HEAT AND MASS TRANSFER
IN LAYERED SEEDBED

A Thesis Submitted to the College of
Graduate Studies and Research
in Partial Fulfillment of the Requirements
for the Degree of Doctor of Philosophy
in the Department of Agricultural and Bioresource Engineering
University of Saskatchewan
Saskatoon

By:
Alireza Keyhani
February 1997

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UNIVERSITY OF SASKATCHEWAN

College of Graduate Studies and Research

SUMMARY OF DISSERTATION

Submitted in partial fulfillment
of the requirements for the

DEGREE OF DOCTOR OF PHILOSOPHY

BY

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The Potential of Dietary Lipases to Improve Fat Utilization in Young Birds

Young chickens and turkeys have a reduced ability to use dietary fat. The reason for the poor fat utilization has not been defined but has been speculated to be due to a deficiency of bile salts and/or pancreatic lipase. Lipase activity is low in the digestive tract of young birds but little research has been completed to examine the role of this enzyme in low fat utilization. Therefore the objective of this study was to investigate the role of dietary lipase in fat malabsorption in young birds. In a series of in vitro studies, mammalian, fungal and bacterial lipase sources were tested under conditions which approximate the proventriculus and small intestine of young birds. It was concluded that Pseudomonas sp. lipase had potential as a supplement in poultry diets.

Two in vivo experiments were completed to test the use of Pseudomonas sp. lipase in diets of young broiler chickens and turkeys. The first experiment studied the impact of five levels of enzyme addition (0, 50, 100, 200 and 400 units per gram of diet) in a corn-soybean meal based diet containing 8% tallow and fed to broiler chickens from 0 to 35 days of age. Lipase addition had a negative impact on body weight gain, feed efficiency and fat digestibility. Analysis of feeds containing 0 and 400 units lipase per gram of diet revealed that triglycerides had been nearly totally hydrolyzed to free fatty acids and glycerol during feed mixing and/or storage in the enzyme supplemented treatment. It was suggested that the presence of free fatty acids would reduce the utilization of fat in the diet and may also have had a negative feed back on the pancreatic output of digestive enzymes. The second experiment utilized the same enzyme source at four lower levels (0, 20, 40 and 60 units per gram of diet) in diets for turkey poult under study from 0 to 21 days of age. The production results of this trial were similar but less severe than those seen for chickens. The apparent digestibility of C18:0 in both experiments was improved by the addition of lipase while that of C18:1 was decreased. The former may indicate insufficient endogenous lipase in young
birds, and the latter that the non-specific nature of the \textit{Pseudomonas sp.} lipase hydrolyzes the fatty acids in the 2 position of the glycerol molecule thereby reducing their digestibility. Questions are raised as to whether the form of enzyme application (liquid or dry) has an impact on lipid hydrolysis and what impact enzyme dosage has on the success of lipase supplementation. Further research is needed to answer to these questions.

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ABSTRACT

Agricultural cultivation and seeding practices often leave a "layered" seedbed structure. Layering is assumed to reduce evaporative losses from the soil surface.

In this study, the effect of layering on temperature and water content variations in a clay soil was investigated. Soil columns 150 mm in height and 200 mm diameter were prepared with four different layering configurations, and three different initial water contents, and allowed to dry for a week in a controlled environment. Settings in the growth chamber were 15 °C and 44% relative humidity for 16 hours and 5 °C and 85% relative humidity for 8 hours. Temperature and water content in different layers of the soil column were monitored continuously.

Statistical analysis of the data revealed that layering had a significant effect on moisture retention in soil columns with low initial water contents, while no effect or even increased moisture losses were found in soils with high initial water contents. Layering had no effect on temperature variations in the soil columns.

A pressure-based coupled heat and mass transfer model was developed to simulate temperature and soil water pressure (suction) in a layered soil profile. A finite difference formulation of the model was solved using a FORTRAN 77 computer code.

Model predictions were compared with experimental data. The model predicted the water content (MRPD values ranged from 2.1% to 7.7%) and temperature (MRPD values ranged from 0.60% to 0.77%) with reasonably low deviations from the measured values.
The model showed very high sensitivity to the proposed hydraulic conductivity function, while lower sensitivity was found for the proposed thermal conductivity function.

For practical purposes in the clay soil tested, layering may be desirable for low initial water content conditions, while in higher water contents, stratification may have an adverse effect on moisture retention.

Verification of the model for field conditions is left for future studies.
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The author wishes to express his sincere appreciation to his supervisor, Dr. Dvoralai Wulfssohn, for her continuous assistance, guidance, patience and encouragement during all stages of this study.

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I acknowledge the full financial support from Ministry of Culture and Higher Education of I. R. of Iran, and partial financial support from the College of Graduate Studies and Research.

I am also thankful to W. Morley and L. Roth, both from the Agricultural and Bioresource Engineering Department who assisted me in preparing the materials and setting up the experiments.

Also, there are some people whose contributions are reflected in this study indirectly, but with great effect. Special recognition is given to Professor E. M. Barber, Head of the Agricultural and Bioresource Engineering Department, for his commitments and contributions to providing a friendly atmosphere in the Department. And last but not least, I would like to thank K. Tischler, the International Student Advisor for the University of Saskatchewan, whose friendly welcome started even before my arrival in Canada.
DEDICATION

This work is dedicated to my wife Fereshteh whose love and support have always been with me. Without her patience and forbearance, I could have never finished this work. In return, this was the least that I could do.
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LIST OF SYMBOLS

\( a \)  
fitting parameter in hydraulic conductivity function

\( a_{11} \ldots a_{22} \)  
matrix components

\( A \)  
lumped coefficient of pressure in numerical model

\( B \)  
lumped coefficient of temperature in numerical model

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

\( C_a \)  
volumetric heat capacity of air \((J \cdot m^3 \cdot K^{-1})\)

\( C_{si} \)  
volumetric heat capacity of \( i \) solid constituent of the soil \((J \cdot m^3 \cdot K^{-1})\)

\( C_{TT} \)  
lumped coefficient of temperature in heat equation

\( C_{Tv} \)  
lumped coefficient of pressure in heat equation

\( C_{vl} \)  
lumped coefficient of pressure in mass equation

\( C_{v2} \)  
lumped coefficient of temperature in mass equation

\( C_w \)  
volumetric heat capacity of water \((J \cdot m^3 \cdot K^{-1})\)

\( C_\theta \)  
pecific water capacity, defined as \( \frac{\partial \theta}{\partial \psi} \) \((m^{-1})\)

\( C_{\psi T} = C_{v2} \)

\( C_{\psi\psi} = C_\theta + C_{v2} \)

\( D_* \)  
diffusion of water in atmosphere at standard temperature \((m^2/s)\)

\( D_T \)  
thermal moisture diffusivity \((m^2/s)\)

\( D_{vap} \)  
diffusion coefficient \((m^2/s)\)

\( D_\theta \)  
isothermal moisture diffusivity \((m^2/s)\)
\( D_{\text{vap}} \) isothermal vapor diffusivity (m\(^2\)/s)

\( E \) internal mass rate of change of liquid to vapor (Mg/Mg s)

\( F \) lumped coefficient of pressure in numerical model

\( G \) lumped coefficient of temperature in numerical model

\( g \) gravitational acceleration (m/s\(^2\))

\( h \) relative humidity

\( j = \sqrt{-1} \)

\( J \) volumetric flux density (m\(^3\) • m\(^{-2}\) • s\(^{-1}\))

\( k \) soil thermal conductivity (W • m\(^{-1}\) • K\(^{-1}\))

\( k_{\text{dry}} \) soil thermal conductivity at dry state (W • m\(^{-1}\) • K\(^{-1}\))

\( k_m \) thermal conductivity of soil minerals (W • m\(^{-1}\) • K\(^{-1}\))

\( k_q \) thermal conductivity of quartz (W • m\(^{-1}\) • K\(^{-1}\))

\( k_{\text{sat}} \) soil thermal conductivity at saturated state (W • m\(^{-1}\) • K\(^{-1}\))

\( k_w \) thermal conductivity of water (W • m\(^{-1}\) • K\(^{-1}\))

\( K \) hydraulic conductivity (m/s)

\( K_e \) Kersten normalized thermal conductivity

\( K_r \) relative hydraulic conductivity (dimensionless)

\( K_{\text{ref}} \) hydraulic conductivity at reference temperature (m/s)

\( K_s \) saturated hydraulic conductivity (m/s)

\( K_{\text{avg}} \) averaged saturated hydraulic conductivity (m/s)

\( K_{\text{si}} \) Saturated hydraulic conductivity of layer \( i \) (m/s)

\( K_{TT} \) lumped coefficient of temperature in heat equation
$K_{Tv}$  lumped coefficient of temperature in mass equation
$K_{v1}$  lumped coefficient of pressure in mass equation
$K_{v2}$  lumped coefficient of temperature in mass equation
$K_{VT} = K_{v2}$
$K_{VV} = K + K_{v1}$
$L$  latent heat of vaporization of water (J/Mg)
$L_o$  fitting parameter in Mualem's hydraulic conductivity model
$L_{di}$  thickness of layer $i$
$m$  fitting parameter in soil-water characteristic function
$n$  fitting parameter in soil-water characteristic function
$N$  number of observations
$P$  pressure (m)
$q_h$  heat flux (W/m$^2$)
$q_i$  mass liquid flux (Mg·m$^{-2}$·s$^{-1}$)
$q_v$  mass vapor flux (Mg·m$^{-2}$·s$^{-1}$)
$Q_h$  heat per unit volume (J/m$^3$)
$R$  universal gas constant (J·kg$^{-1}$·K$^{-1}$)
$S$  degree of saturation
$t$  time (s)
$T$  temperature (K)
$T_s$  initial soil temperature (K)
$T_i$  soil surface temperature (K)
\( T_a \)  
environment temperature (K)

\( T_r \)  
reference temperature (K)

\( u \)  
fitting parameter in vapor diffusivity function

\( v \)  
fitting parameter in vapor diffusivity function

\( v_l \)  
soil liquid velocity (m/s)

\( v_v \)  
soil vapor velocity (m/s)

\( y \)  
measured value of a variable

\( y' \)  
estimated value of a variable

\( z \)  
vertical dimension (m)

\( \alpha \)  
fitting parameter in soil-water characteristic function

\( \beta \)  
a positive constant in sensitivity analysis

\( \delta \)  
thermal gradient coefficient (deg\(^{-1}\))

\( \varepsilon \)  
phase conversion coefficient (dimensionless)

\( \phi \)  
soil total potential (m)

\( \eta \)  
total porosity of soil (m\(^3\)/m\(^3\))

\( \eta_a \)  
air porosity of soil (m\(^3\)/m\(^3\))

\( \eta_m \)  
volume fraction of soil minerals (m\(^3\)/m\(^3\))

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

\( \eta_q \)  
volume fraction of quartz (m\(^3\)/m\(^3\))

\( \eta_{si} \)  
volume fraction of different solid constituents of soil (m\(^3\)/m\(^3\))

\( \eta_w \)  
volume fraction of water (m\(^3\)/m\(^3\))

\( \lambda \)  
ratio of time step to square of grid spacing (s/m\(^2\))
\( \mu \) dynamic viscosity (N \cdot s \cdot m^{-2})

\( \theta \) total volumetric water content (m\(^3\)/m\(^3\))

\( \theta_l \) volumetric water content at liquid phase (m\(^3\)/m\(^3\))

\( \theta_r \) residual volumetric water content (m\(^3\)/m\(^3\))

\( \theta_s \) saturated volumetric water content (m\(^3\)/m\(^3\))

\( \theta_v \) volumetric water content at vapor phase (m\(^3\)/m\(^3\))

\( \rho_s \) saturated vapor density (Mg/m\(^3\))

\( \rho_b \) soil dry bulk density (Mg/m\(^3\))

\( \rho_l \) liquid density (Mg/m\(^3\))

\( \rho_v \) vapor density (Mg/m\(^3\))

\( \sigma \) surface tension (J/m\(^2\))

\( \tau (t) \) a function to represent variable \( T \)

\( \tau' \) function \( \tau (t) \) advanced one temporal increment

\( \xi (t) \) a function to represent variable \( \psi \)

\( \xi' \) function \( \xi (t) \) advanced one temporal increment

\( \psi \) soil pressure or matric suction (m)

\( \psi_i \) initial soil pressure or suction (m)

\( \psi_l \) soil surface pressure or suction (m)

\( \psi_a \) environment pressure (m)

\( \psi_{ref} \) soil suction at reference temperature (m)
Superscripts

\(n\)  temporal increment

Subscripts

\(i\)  spatial increment

T  constant temperature condition

P  constant pressure condition
## LIST OF ABBREVIATIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>B</td>
<td>bottom layer of soil (1.15 Mg/m³ bulk density), also, uniform soil layering configuration (control)</td>
</tr>
<tr>
<td>D</td>
<td>dense layer of soil (1.35 Mg/m³ bulk density)</td>
</tr>
<tr>
<td>DB</td>
<td>layering configuration: dense over bottom layer</td>
</tr>
<tr>
<td>DF</td>
<td>degree of freedom</td>
</tr>
<tr>
<td>EU</td>
<td>experimental unit</td>
</tr>
<tr>
<td>IWC</td>
<td>‘initial water content’</td>
</tr>
<tr>
<td>L</td>
<td>loose layer of soil (0.95 Mg/m³ bulk density)</td>
</tr>
<tr>
<td>LB</td>
<td>layering configuration: loose over bottom layer</td>
</tr>
<tr>
<td>LDB</td>
<td>layering configuration: loose over dense over: bottom layer</td>
</tr>
<tr>
<td>LSD</td>
<td>least significant difference</td>
</tr>
<tr>
<td>LYR</td>
<td>‘layering configuration’</td>
</tr>
<tr>
<td>MRPD</td>
<td>mean relative percentage deviation</td>
</tr>
<tr>
<td>MSE</td>
<td>error mean square</td>
</tr>
<tr>
<td>wc</td>
<td>water content</td>
</tr>
</tbody>
</table>
CHAPTER ONE

INTRODUCTION

1.1 Motivation

The term "seedbed" refers to a cultivated layer of topsoil suitable for the early stages of plant growth, i.e., seed germination and seedling emergence. Although its importance in crop development may last for only a couple of weeks, the seedbed plays a major role in crop establishment. The seedbed's ability to retain moisture and to conduct heat is necessary to provide a proper environment for the newly planted seed.

In dryland farming, especially in arid and semi-arid regions where a delay of one week after seeding to the first precipitation is not unusual, soil undergoes a drying process, hence, the capacity of the top soil to retain more moisture and to reduce evaporative losses is especially important.

Factors contributing to evaporative losses from the soil surface include: external or meteorological factors such as ambient temperature, relative humidity and wind speed; and, internal or soil factors such as texture and structure. To control the moisture loss, a broad knowledge of the way in which each factor affects evaporation and its interactions with other factors is required.

Many methods have been developed to retain soil moisture and to control evaporative losses from the soil surface. Each method, in one way or another, controls the
effect of one of the above mentioned external or internal factors; for example, tillage
operations to control weeds and reduce wind erosion, summer fallow to catch and hold as
much of one seasonal rain as possible, and the use of different types of mulches to cover
the soil to check evaporation and weeds (Brady 1990). These methods are generally
intended for long term effects or for special or valuable crops. In many arid and semi-arid
regions, however, crop residues may not be available. Therefore, a simple and practical
method to reduce short term moisture losses from the top soil is needed.

In this thesis, the terms stratification and layering are used to refer to a
combination of loose and dense layers of soil one upon another with the same texture but
different structures. Many types of agricultural seeding and cultivation equipment produce
a stratified seedbed. For example, tillage using a chisel followed by a roller and a spike
tooth harrow will leave the topsoil layered. In another example, the passage of a
presswheel may leave an indentation which may be filled with a loose layer of soil due to
natural collapse of the slopes of the rut. The dragging of a chain or harrow behind an
implement will also leave a loosened top layer. Depending on the relative position of a
furrow opener (coulter) and presswheel, different types of layering configurations may be
accomplished. Layering may also result as a consequence of soil compaction (heavy
machinery) or soil packing (land packer) due to application of a surface load.

There is evidence that a stratified seedbed is more capable of retaining moisture
than a uniform soil structure, since soil capillary pores are disrupted and no rapid upward
movement of water is allowed (Lemon 1956). This may become more relevant for small
seeds which must be planted near the surface for the purposes of timely emergence, and as
a result are positioned where the most variable conditions of temperature and moisture occur (Waddington and Shoop 1994).

A few studies have been conducted to analyze the effect of layering on the evaporative loss rate from the soil surface (Lemon 1956; Gordiyenko and Kostogryz 1991). Creation of a layered seedbed has long been promoted, but the proposed benefits for moisture conservation have not been investigated directly from a layered seedbed point of view (Nasr et al. 1994; Hakansson and von Polgar 1984). If proven to be efficient, layering the soil can easily be implemented, alone or along with other methods, to reduce soil moisture loss. In this regard, several issues should be addressed: How and to what extent is evaporation from the soil surface affected by soil stratification? What are the roles of initial water content and layering configuration in reducing the moisture loss?

Experimenting with soils of different textures, structures and physical properties in a limited time is not feasible. An alternative is to predict moisture and temperature profile throughout the layered top soil theoretically. The soil undergoes a drying process due to moisture loss from the surface. The study of mass transfer in porous media under isothermal conditions is well established, but its use is limited to very special cases. Mass transfer is coupled with temperature effects, because the presence of temperature gradients is responsible for some of the mass transfer and in turn, heat is transferred due to moisture movement. Available models are generally formulated to predict moisture and temperature in a uniform profile; however, different results are expected in a stratified profile which will have somewhat different soil properties in each layer. Limited experimental data could be used to evaluate the theoretical approach, before extending predictions to a wider range of conditions.
1.2 Objectives

The objectives of this study are:

1. To study the effect of various soil layering configurations on the moisture and temperature distribution in the top 150 mm layer of soil.
2. To develop a model for heat and mass transfer through a layered top soil.
3. To corroborate the model by comparing experimental and predicted results.

To achieve the stated objectives, different stratified topsoil profiles (i.e., combinations of dense and loose layers) will be simulated and the effect of layering configuration on heat and mass transfer will be investigated under controlled conditions.

Results of this study will be applicable to agricultural machinery design, soil tillage practices, and agricultural water management, especially for dryland farming.
CHAPTER TWO

LITERATURE REVIEW

In this chapter, a review of related literature is presented. Evaporation from the soil surface, moisture conservation methods, analysis of heat and mass transfer in agricultural soils and hysteresis are topics covered.

2.1 Evaporation from the Soil Surface

It is not unusual to have a delay of one week or more after seeding before the first precipitation, during which time the soil undergoes drying. This period is one of the most delicate times for the newly planted seed. Inadequate water supply is one of the factors that may doom the entire plant from the very first stages of its growth. When there is no vegetation, in the presence of radiation and wind effects, evaporation occurs entirely from the soil. In many cases the soil surface may remain bare throughout the periods of tillage, germination and early seedling establishment in which preservation of the seedbed moisture is of prime importance to crop growth (Hillel 1982; Brady 1990). Three conditions have to be present for evaporation to occur, namely, a supply of heat to meet the latent heat requirement, removal of vapor by diffusion and/or convection, and a supply of water from the soil to the surface (Hillel 1982).
Often, the top layer of soil will initially be quite wet. Evaporation from the surface induces a large pressure gradient, decreasing from the surface downward, which in turn causes an upward movement of water. Different scenarios of evaporation process may occur; however, evaporation in the absence of a water table (drying) only is considered in this review because of its relevance to the objectives of this study. Other cases are addressed in Hillel (1982).

Under constant atmospheric evaporative demand the drying process of soil follows three distinctive stages (Fig. 2.1) (Fisher 1923; Hillel 1982):

I. Constant rate stage in which the amount of water in the soil is sufficient to supply water to the site of evaporation to meet the demand. This stage is mostly controlled by external factors (e.g., radiation, wind, relative humidity) rather than soil properties. In a dry climate the duration of this stage is short, lasting from a few hours to a few days.

II. Falling rate stage where the drying rate falls behind the evaporative demand. This stage is mostly controlled by soil properties and is sometimes called the soil profile-controlled stage. Its duration usually lasts much longer than the first stage.

III. Slow rate stage during which the evaporation rate may persist at a nearly steady rate for many days, weeks or even months. Liquid water flow is retarded and the extremely slow moisture movement is dominated by adsorptive forces over molecular distances at the solid-liquid interfaces in the soil. This stage is often called the vapor diffusion stage, and can be important
for soils in the form of a loose assemblage of clods which become quickly dried.

![Evaporation rate graph](image)

Fig. 2.1 Change of evaporation rate with time over the drying process.
I. Constant rate stage; II. Falling rate stage; III. Slow rate stage (adapted from Hillel 1982).

Hide (1954) gave another perspective corresponding to similar stages of the evaporation process stated above:

I. The short period while the soil water content is above field capacity and capillary flow to the surface occurs under a low suction gradient.

II. The period after the soil surface has dried to field capacity but before capillary conductivity becomes so slow that it no longer keeps the surface moist.

III. The period when vaporization occurs principally below the surface and diffusion of vapor must go through a static layer of air within the pore space of
dry soil.

Hide (1954) suggests three approaches to suppress the rate of evaporation from the soil surface: (1) decreasing the amount of water that can be transported to the soil surface before surface drying occurs; (2) cooling the upper moist soil layer to lower the driving force for evaporation; and, (3) increasing the thickness of the static layer of air to reduce the vapor pressure gradient.

Considering the brief description of the three stages given above, the effect of seedbed stratification on reducing drying rate in upper layers of the soil will be most influential in the first stage and the early portion of the second stage of the drying process.

2.2 Moisture Conservation Methods

One of the reasons for stratifying the top soil is to conserve more moisture in the vicinity of the seedbed so as to keep the germinated seeds vital for a short period of time until the next watering (precipitation or irrigation) occurs. Many methods have been introduced to control evaporative losses from the soil surface and conserve more water in the soil. In most of the methods, one way or another, the soil structure is changed and the pore size distribution modified. Depending on the method, the resulting structure may be uniform throughout the top soil, such as incorporation of crop residues with the top soil, or abrupt, as in applying a layer of mulch on top. Methods intended for one stage of evaporation may not necessarily be effective for another.
2.2.1 Tillage and fallow methods

Practicing zero tillage in dry semi-arid regions (Jones et al. 1994) and in the Canadian Prairies (Grevers et al. 1986) has resulted in improved water conservation. This is mostly due to reduced manipulation of the soil and also to crop residues left on the soil surface. Chemical fallowing is another method from which more soil water conservation has been shown to result when compared to stubble mulch plots during a 14-month fallow period in a dry year (Tanaka and Aase 1987). Chemical treatments usually act as retarding agents to reduce the vapor pressure of water. A proper crop rotation and tillage system combined has been shown to achieve successful soil conservation for winter wheat production in semi-arid southern Alberta (Larney and Lindwall 1995).

Fall subsoiling plus snow management has been reported to be beneficial in improving the moisture regime in drought years in southwestern Saskatchewan (McConkey et al. 1990). Subsoiling disrupts the continuity of capillary pathways, reducing the conduction of liquid water. Talsma (1963) (as cited in Hillel 1982) related a reduction in evaporation to the formation of stratified soil induced by tillage operations.

2.2.2 Mulching

Mulches are used for various reasons, but water conservation and erosion control are undoubtedly the most important for agriculture in dry regions. A mulch is any material at the soil surface that was grown and maintained in place, any material grown but modified before placement, and any material processed or manufactured and transported before placement (Unger 1975). Numerous studies have been conducted to investigate the effect of mulches on soil water storage and evaporation.
The use of plastic mulches (included are polyethylene, polyvinyl chloride and similar films) usually resulted in higher water contents than bare soils in studies conducted by Army and Hudspeth (1960) and Liptay and Tiessen (1970). Petroleum and asphalt sprays and resins have also been used for water loss control from the soil surface (Kowsar et al. 1969).

Most research with mulches has been concerned with crop residues. The surface soil moisture under the mulch cover produced by reduced tillage is often greater than that of a conventional tillage (Smica and Unger 1986). Application of pine needle mulch has been shown to be effective in reducing the rate of drying of the seedbed (Acharya and Sharma 1994). In a comparison of nine tillage treatments on a sandy loam soil, Kronen (1994) found that soil water content was greater under minimum tillage and under minimum tillage combined with mulching than on sites that were moldboard and disk ploughed.

Gravel mulch is a method in which a layer of gravel with larger pores is applied to the soil surface. Gravel mulch has been shown to be a promising method for increasing infiltration and also for retaining moisture within the topsoil in fallow practices (Corey and Kemper 1968). Hide (1954) reported that partial control of surface evaporation has been achieved through the use of pebble mulches in some of the arid regions of China.

**2.2.3 Stratified soil profile**

Many kinds of stratification can be found in different types of soils. In fact, there are few field soils which have a uniform texture and structure throughout the profile. A change in
texture or structure in the soil profile will be accompanied by a change in water movement. Most studies in this regard have dealt with different textures in the profile.

Miller and Bunger (1963) reported that the moisture retained by soil underlain by sand or gravel was much greater than that in similar depths of a uniform soil. After experimenting with different pairs of soils with different textures in a soil column, Eagleman and Jamison (1962) concluded that water movement from a system of small pores to one of larger pores is very slow in unsaturated media. Clothier et al. (1977) pointed out that coarse-layered soils are free draining in the saturated state but impede water transmission in the unsaturated state. Miller and Gardner (1962) performed a series of experiments to study the effect of stratification on infiltration of water through layers of soil with different textures and different structures. They concluded that the effects of strata in the soil media were related to the pore characteristic differences in the layered soil profile, and that the upward movement of water was more influenced than the downward movement.

According to Willis (1960) for many practical purposes the stratification in the soil profile may be of little consequence when the water table is within a 2.8 m depth; however, in the absence of a water table, stratification might significantly affect evaporation from recently moistened soils. A number of Japanese papers dealing with the flow of water in stratified media, mostly with different soil textures, are cited in Iwata et al. (1995). In these papers, all presented heat and mass transfer models were uncoupled and use of an average hydraulic conductivity was recommended in a stratified medium.

Many tillage and planting operations produce a layered seedbed. A sequence of different tillage operations such as chisel-roller or chisel-roller-spike tooth harrow leave
the entire area layered. On the other hand, seeding machines act as strip stratifiers. Use of presswheels in seed drills enhances the stratification effect and depending on the orientation of a furrow opener (coulter) and presswheel, different configurations of layering may be accomplished.

There is evidence that a stratified seedbed is capable of retaining more moisture than a uniform soil structure since capillary tubes are disrupted and no rapid upward movement of water is allowed. Pore sizes have significant effect on water movement through soils (Nelson and Baver 1940). Larger pores on top (as in gravel mulching) allow water to enter the soil from above the soil surface very easily, but if water moves toward the surface from below due to desaturation of larger pores, hydraulic conductivity will be reduced substantially (Corey and Kemper 1968).

Stratification is one consequence of soil 'compaction' (resulting from large scale surface loads induced by heavy machinery trafficking) and soil 'packing' (resulting from small scale surface loads caused by presswheels and agricultural land packers). Soil compaction is usually considered as a limiting phenomenon in agricultural activities (Soan 1983; Soan and van Ouwerkerk 1995), and is highly unlikely be adopted as a method to control evaporative losses from the soil surface. On the other hand, soil packing by agricultural land packers has proven to be useful in crop production (Djokoto et al. 1971; Hultgreen et al. 1990; Foster 1991) and is one method to stratify the seedbed.

The effect of presswheels (or land packers) in creating a packed layer of soil may reduce the rate of drying by reducing porosity, or it may instead increase the drying rate by increasing unsaturated hydraulic conductivity due to better continuity of pores (Ferraris 1992). To resolve this conflict, Nasr et al. (1994) suggested the use of a stratified seedbed
in which a sudden change in pore size (and thus a disruption of pore continuity) is introduced to prevent the rapid upward movement of water. Some other requirements of a proper seedbed and their conflicting nature were addressed by Braunack and Dexter (1989).

As stated earlier, most studies related to layered seedbed have dealt with the effect on crop development, but have not investigated directly the effect of stratification on moisture conservation (Stout et al. 1961; Johnson and Henry 1964; Hakansson and von Polgar 1984).

Literature that deals with same texture but different structures of soil layers and also focuses on the drying process and evaporative losses from the soil surfaces is almost non-existent. An experiment was conducted by Kolasew (1941) as cited in Lemon (1956) on stratified and unstratified soils under uniform wind tunnel conditions to compare the respective moisture losses from the soil profiles. The results, shown in Fig.2.2, clearly indicated that the rate of moisture loss was reduced under the stratified treatment.

Recently, Gordiyenko and Kostogryz (1991) conducted studies to determine the effect of different bulk densities in the top 50 mm layer on evaporation from the surface of a soil column of 300 mm depth. In the first three days, water loss in the whole soil column was less with lower bulk densities in the top 50 mm layer as compared to compacted layers. They recommended the loosening of the upper soil layer when the initial water content is high, to impose a sudden change in pore sizes and retard the liquid water movement. They also found that evaporation may increase with degree of compaction under strong drying regimes, remain the same under mid-drying conditions, or even
decrease under the mildest drying regimes. It seems that the mobility of capillary water in unsaturated soils does not always show an increasing trend with degree of compaction, but is somehow related to the gradient of the driving force (the moisture or potential gradient).

![Graph showing drying rates of stratified and unstratified chernozem soil](image)

**Fig. 2.2** Drying rates of stratified and unstratified chernozem soil under uniform wind tunnel conditions (after Kolasew 1941, as cited in Lemon 1956).

### 2.3 Analysis of Heat and Mass Transfer in Agricultural Soils

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 has many
applications. The mathematical analysis of the response of soil to atmospheric conditions tend to be complicated since the temperature and moisture dependence of parameters involved in transport equations make these relationships highly nonlinear.

2.3.1 Water movement

There are many factors involved in water transport in the soil. Unlike systems that may be categorized precisely as having solid, liquid or gaseous phases, a soil-water system is no simple combination of these. It has both animal and vegetable parts, it is composed of both inorganic and organic compounds, and its reactions involve chemical as well as physical processes that are influenced by its biological character and by time (Boersma et al. 1972).

Flow of water through soil when both water and air are present in the pores is called *unsaturated flow*. Darcy's law is assumed to be applicable where water exists in small pores while air occupies the large pores. Darcy's law was first formulated by Darcy in 1856 in studying water filtration through a saturated sand column. Later, Wyckoff and Botset (1936) showed a relation between hydraulic conductivity (an important parameter in Darcy's equation) and the degree of water saturation and extended the law to unsaturated flow. Prior to that, Richards (1931) introduced a new concept invoking the mass balance in the form based on Buckingham flux law:

\[
\nabla J = -\left( \frac{\partial \theta}{\partial \psi} \right)_{T,P} \frac{\partial \psi}{\partial t} \tag{2.1}
\]
where \( J \) is the volumetric mass flux \( (\text{m}^3 \cdot \text{m}^{-2} \cdot \text{s}^{-1}) \), \( \theta \) is the volumetric water content \( (\text{m}^3/\text{m}^3) \), \( \psi \) is the matric suction \( (\text{m}) \) and \( t \) is time \( (\text{s}) \). The subscripts \( T \) and \( P \) refer to constant temperature and pressure conditions, respectively. Richards’ paper was based on what Gardner (1972) has since called the best known Ph.D. dissertation in all of soil physics. Richards (1931) developed the following partial differential equation, known as Richards’ equation, which is widely used in modeling liquid water transport in the soil:

\[
\left( \frac{\partial \theta}{\partial \psi} \right)_{T,P} \frac{\partial \psi}{\partial t} = \nabla (K \nabla \psi) - \frac{\partial K}{\partial z}
\]  

(2.2)

where \( K \) is the hydraulic conductivity \( (\text{m/s}) \) and \( z \) is the vertical dimension \( (\text{m}) \). Equation 2.2 is a fundamental equation governing the isothermal-isobaric transport of water through unsaturated soil. Richards’ equation is basically an energy equation, and Sposito (1986) derived the Richards equation directly using the energy balance and Buckingham flux law, by-passing the mass balance equation. A more familiar form of Richards’ equation is written as:

\[
\frac{\partial \theta}{\partial t} = \nabla [K \nabla (\psi + z)]
\]  

(2.3)

The driving force in an unsaturated soil is the water pressure gradient subjected to a sub-atmospheric pressure. The total potential head of soil water is consisted of both gravitational and pressure potential heads, when added is called “hydraulic head” (Hillel
1982). To avoid a negative sign which characterizes the soil pressure, the term “suction” is used for pressure head. Suction is made up of two components: matric and osmotic. Matric suction is solely dependent on physical attraction of water to the surfaces of the soil particles and capillary pores (Hillel 1982). In this study, the terms pressure head or simply pressure and soil suction are used interchangeably and the corresponding value is referred to in a positive number for convenience.

The validity of Darcy’s law at low soil water contents can be questioned because capillary models cannot be reasonably assumed and water is under adsorptive force fields (Iwata et al. 1995). In this regard, Gray and Hassanizadeh (1991a, 1991b) introduced an unsaturated flow theory derived from the well established continuity and thermodynamic equations which took into account the interaction of air-water interfaces. Fredlund and Morgenstern (1977) called this air-water interface the “contractile skin”. This interface is one of the distinctive characteristics of an unsaturated soil and the concept is usually used for stress analyses. The theory proposed by Gray and Hassanizadeh (1991a, 1991b) has not yet been verified by application to practical cases.

Water can move in both liquid and vapor form in unsaturated porous bodies. Vapor movement through most of the soil profile occurs by diffusion and the driving force for the vapor movement is the vapor pressure gradient (Brady 1990). This gradient may be caused by differences in water potential or by temperature differences in the soil. At constant temperature the vapor pressure changes in non-saline soils are very small and can be considered constant (Hillel 1982). The change in vapor density is larger for a temperature difference of 1 °C than for a pressure difference of -153 m (-1500 kPa). Thus
temperature differences are the primary factors that influence vapor flow (Hanks 1992). Examples for vapor movement under two different pressure difference and temperature difference scenarios are shown in Fig. 2.3 (Brady 1990). Vapor tends to move from moist to dry horizons of the soil while it tends to move from warm to cool horizons. In some cases the effects are additive and in other they may cancel each other (Brady 1990). It is almost impossible to separate liquid from vapor movement. Overall flow consists of evaporation, condensation, reevaporation, etc. (Philip and de Vries 1957; Luikov 1961). In an isothermal process, it is usually assumed that liquid flow dominates in moist soils (Miller and Klute 1967).

![Diagram of vapor movement in soil horizons](image)

**(a)**

**(b)**

**Fig. 2.3 Vapor movement in soil horizons.** (a) Temperature and moisture effects are even; (b) effects are added (adapted from Brady 1990).

### 2.3.2 Heat transfer

Analysis of heat transfer in soils is of great importance for the prediction of the temperature for plant-environment interactions (Voorhees et al. 1981; Rendig and Taylor 1989). The transfer of heat through the soil surface may occur by radiation, conduction
and convective modes. When freezing and thawing occurs, a fourth mode called “latent heat transfer” will be present.

Of all modes of heat transfer, the molecular conduction is of prime importance (Hillel 1982). Heat conduction is governed by the well known Fourier equation. Measuring the heat flux at the soil surface is extremely difficult because of abrupt changes in thermal conductivity and temperature differences (Voorhees et al. 1981). The rate of conduction of heat throughout the solid phase of the soil depends on the mineralogical and organic composition (Fuchs 1986). Variation in time and space of the water content leads to dramatic changes in the thermal properties of all soils (de Vries 1963).

### 2.3.3 Coupled heat and mass transfer in unsaturated soils

Early theoretical studies assumed that water was transferred either by capillary action (Haines 1927) or by diffusion (Sherwood 1931). The study of mass transfer in porous media under isothermal conditions is a well developed subject (Philip 1957b; Swartzendruber 1969), but this condition is almost non-existent under natural field conditions. Thermally induced moisture flow may significantly affect the net transfer of the soil water and nutrients by altering the moisture gradients and hydraulic conductivity in addition to the direct effects of mass transfer (Cary 1966).

Matthes and Bowen (1963) pointed out the possibility of controlling water-vapor movement as a practical tool for increasing germination under adverse moisture conditions where daily reversal of the temperature gradients exists. Because of the exponential relation between temperature and the vapor pressure of water, thermal gradients will
produce significant fluxes of water vapor in a moist soil profile subjected to a diurnal
temperature regime. Hence, the isothermal soil moisture diffusion theory cannot be
expected to fully describe the drying of soil (Cary 1967).

Gurr et al. (1952), and Taylor and Cavazza (1954) reported that in a closed soil
column the net movement of water due to temperature gradients occurs in both liquid and
vapor phases in opposite directions: vapor in the direction of decreasing temperature and
that of liquid in the direction of increasing temperature. Condensation at the cold end
results in liquid water flow back to the warm regions due to the developed moisture
gradient. Also, using closed soil columns, Cassel et al. (1969) and Joshua and de Jong
(1973) reported that the effect of temperature gradient on the water movement was
greatest for the intermediate initial water contents.

Cary (1965) indicated that temperature gradients are important under moist
conditions while Philip (1957a) reported their significance under dry conditions. Milly
(1984) calculated the total water flux and its thermal liquid component at the surface and
at depths of 20 mm and 150 mm and found that in most cases the thermal liquid flux was
of the order of or less than 1% of the total flux at each depth (with an exception in a very
wet soil). In a series of experiment and employing the modified model of Philip and de
Vries (1957), Bach (1992) found that the effect of temperature on water transport in soil
is small for very high and very low initial water contents. Bach (1992) indicated that the
temperature gradients of 1 °C per 10 mm depth and higher has much greater effect on
thermally induced water flow than lower temperature gradients. Bach (1992) concluded
that the use of isothermal predictive equations could introduce significant errors in the estimation of overall soil-water movement.

Thermally induced vapor and liquid flow invalidates the Darcy-Buckingham flux law embedded in Eq. 2.3. In addition to that, temperature-dependent soil properties have been overlooked in formulating the Darcy-based equations. Because of the dependence of the transport equations on temperature, an internal energy balance equation should be considered in models of non-isothermal flow in porous media. The result is coupled heat and mass transfer equations. Pioneers in modeling coupled heat and mass transfer in porous media are Philip and de Vries (1957), de Vries (1958), Luikov (1964) and Cary and Taylor (1962a and 1962b). The work of Philip and de Vries (1957) is based on a mechanistic approach, while Luikov (1964), Taylor and Cary (1964) and Cary (1965) incorporated the thermodynamics of irreversible processes in deriving their models. Although Cary and Taylor’s model is considerably more general, Milly (1988) reports no significant difference between their model and that of Philip and de Vries. More recent formulations largely involve modifications of either Philip and de Vries’ or Luikov’s approaches.

Philip and de Vries (1957) extended the isothermal theory of liquid water flow by incorporating vapor flow and temperature gradients into their governing equations. Their governing differential equations for moisture (Eq. 2.4) and heat transfer (Eq. 2.5) for one-dimensional flow read as follows:

\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( D_r \frac{\partial T}{\partial z} \right) + \frac{\partial}{\partial z} \left( D_\theta \frac{\partial \theta}{\partial z} \right) + \frac{\partial K}{\partial z} \quad (2.4)
\]
\[
C \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) - L \frac{\partial}{\partial z} \left( D_{\text{vap}} \frac{\partial \theta}{\partial z} \right)
\]  \hspace{1cm} (2.5)

where \( D_T \) is the thermal moisture diffusivity (m\(^2\)/s), \( D_\theta \) is the isothermal moisture diffusivity (m\(^2\)/s), \( T \) is the temperature (K), \( C \) is the volumetric heat capacity (J \cdot m\(^{-3}\) \cdot K\(^{-1}\)), \( k \) is the thermal conductivity (W \cdot m\(^{-1}\) \cdot K\(^{-1}\)), \( L \) is the latent heat of vaporization of water (J/Mg) and \( D_{\text{vap}} \) is the isothermal vapor diffusivity (m\(^2\)/s).

Equation 2.4 indicates that the rate of change of volumetric water content depends on driving potentials \( \partial T/\partial z \) and \( \partial \theta/\partial z \), with corresponding diffusivity coefficients, plus gravity effects represented by the gradient of hydraulic conductivity \( \partial K/\partial z \). Thermal and moisture diffusivity coefficients are composed of corresponding coefficients in liquid and vapor modes. Equation 2.5 states that the rate of change of temperature depends on the amount of heat transfer by conduction minus the distillation effect induced by the moisture gradient.

Shortly thereafter, de Vries (1958) presented a more general system of heat and mass transfer equations in which heat of wetting and transfer of sensible heat were taken into account. The resulting formulation consisted of a set of three complex simultaneous differential equations with too many parameters that were difficult to determine. Besides, the interactable nature of the new equations limited the usefulness of the model (Thomas 1985). After careful calculations and sensitivity analysis of parameters included in the de Vries (1958) mass equation, Rose (1968) found that many terms in the equation had little effect and could be neglected.
Luikov's (1964) mass transfer equation is very similar to that of Philip and de Vries (1957), but the heat transfer equation is somewhat different. For one-dimensional flow, and after some manipulation Luikov's (1964) heat and mass transfer equations can be written as (Tzimopoulos and Sidiropoulos 1981):

\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( \delta D_\theta \frac{\partial T}{\partial z} \right) + \frac{\partial}{\partial z} \left( D_\theta \frac{\partial \theta}{\partial z} \right) + \frac{\partial K}{\partial z}
\]  

(2.6)

\[
C \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) - L \varepsilon \frac{\partial \theta}{\partial t}
\]

(2.7)

where \( \delta \) is the thermal gradient coefficient (deg\(^{-1}\)), \( \varepsilon \) is the phase conversion coefficient (dimensionless). Although the parameter \( \delta \) has the dimension of (deg\(^{-1}\)), its dependence on temperature is negligible; however, it has strong relationship with water content (Luikov 1964). The value of \( \varepsilon \) ranges from 0 (liquid movement only) to 1 (vapor movement only). After carrying out a sensitivity analysis Sidiropoulos and Tzimopoulos (1983) found that the solution of Luikov's equations shows very small sensitivity to changes in \( \varepsilon \), providing some justification for the omission of this term. This is of a practical advantage since determining \( \varepsilon \) involves a lot of difficulty (Sidiropoulos and Tzimopoulos 1983); however, eliminating \( \varepsilon \) leads to decoupling of Luikov's heat and mass transfer equations. Couvillion and Hartley (1984) question the validity of \( \varepsilon \) in Luikov's equation arguing that the assumption of an instant change in water content from a high liquid fraction to a high vapor fraction cannot be justified physically since the process is continuous. It appears that
one can derive Luikov's model, under some assumptions, from that of Philip and de Vries (Tzimopoulos and Sidiropoulos 1981; Thomas 1985).

Many researchers in the soil area have followed Philip and de Vries model in its original form or in some modified form. Sophocleous (1979) adapted the Philip and de Vries model to the more general pressure (or matric suction) based approach and proposed a new model for thermal liquid diffusivity. Thomas (1987) incorporated the phase conversion coefficient from Luikov's model to Philip and de Vries governing equations and came up with a heat equation similar to that of Luikov's. Benjamin et al. (1990) extended the Philip and de Vries' (1957) model to a two-dimensional pressure-based model. Nassar et al. (1992) applied the original Philip and de Vries equations to a closed soil column and found reasonable results when the mean soil temperature was lower than 27 °C. Kharab and Guenther (1994), in a pressure-based model, presented a mass transfer equation in which thermal liquid diffusivity was eliminated. Milly (1982, 1984) followed de Vries' (1958) approach and modified the formulation to derive a pressure-based model. Thomas and King (1992), starting from Darcy's law and the continuity equations, derived a pressure-based solution suitable for geotechnical engineering practice for coupled heat and mass transfer. Following Philip and de Vries' (1957) approach, Thomas and King (1994) extended their 1992 model to two-dimensional applications.

Luikov's model has been primarily used for porous media other than soil. Mikhailov and Shishedjeev (1975) applied Luikov's model to the drying process of a porous sheet of paper. Irudayaraj et al. (1990) applied Luikov's governing equations for a

Whitaker (1977) introduced another set of equations for simultaneous heat and mass transfer in porous media which was based on a volume averaging technique along with continuity and heat equations. Whitaker (1977) incorporated the internal mass rate of vaporization in the mass transfer equation. The final derived governing equations were somewhat similar to Philip and de Vries and Luikov's models. Whitaker (1977), in this paper erroneously questions Luikov's governing equation for mass transfer for not including the term for mass rate of vaporization (which was considered in Luikov's model but was cancelled out in deriving the final equations). In a later paper Whitaker and Chou (1983) criticized Luikov's equations for not including the gravity effect but didn't mention anything regarding the mass rate of vaporization.

2.3.4 Analysis of stratified soil profile

Water moves according to its energy state represented by a potential gradient. In a homogeneous profile in a porous body, water transfers under isothermal conditions from higher water content to the lower one. However, when two dissimilar porous bodies come in contact, the opposite may occur. For example, if a layer of moist peat (gravimetric water content = 300%) comes in contact with a layer of moist sand (gravimetric water content = 10%), then the transfer of water occurs from sand to peat (Luikov 1964). The affinity of water molecules to peat particles is much higher than that of the sand particles.
This produces a large pressure gradient between the two dissimilar media forcing the water to move towards the higher suction, in this case from sand to peat.

In a stratified soil profile, a jump in water content exists at adjacent layers (Fig. 2.4) which becomes more profound as the soil dries. This discontinuity makes the solution of the mass transfer equation difficult if solved in the mass-based form, due to different inter-layer boundary conditions. It seems that developed models in pressure-based form are more capable of handling the transport phenomena in stratified media since the pressure head or matric suction can be considered as a continuous variable at the intermediate interfacial contacts between different layers. For this reason, Luikov (1966)

---

**Matric Potential**

![Matric Potential Diagram]

**Water Content**

![Water Content Diagram]

**Fig. 2.4** Flow of water through two different layers of soil with different properties. (A): The matric potential curve is continuous across the boundary (B): the water content curve shows a discontinuity at the boundary (Hanks 1992).
and Scanlon (1992) recommended the use of pressure-based equations when dealing with layered profiles, and the use of mass-based equations for homogeneous media.

Most theoretical approaches in solving the flow equation in stratified soil profiles appear to be under isothermal and steady state conditions (Tagaki 1960; Zaslavsky 1964; Srinilta et al. 1969). In these studies, two layered systems with different textures were considered and discussions revolved around the pressure head development as a function of flow rate and whether a lower permeability layer overlies a less permeable region or vice versa.

Warrick and Yeh (1990) analyzed the steady isothermal flow through multi-layered soil profiles for any number of layers. The outcome of their theoretical analysis for two and four-layered profiles is shown in Fig. 2.5. Sudden changes where two layers meet can readily be distinguished in Fig. 2.5. This is due to changes in parameters in different layers.

Fig. 2.5 Profile of pressure head vs depth for evaporation at the soil surface in stratified profiles. L: loam; S: Sand. In profiles A and B, layers L and S are 800 mm in depth; in C and D, L and S are 400 mm in depth (Warrick and Yeh 1990).
For unsteady cases but still under isothermal conditions, one can refer to Sisson (1987) and Sirvastava and Yeh (1991). Gardner and Fireman (1958) developed a solution for flow upward from a shallow water table in a uniform soil profile which was extended to a two layer system by Willis (1960). Milly (1988) subdivided the problem of flow through heterogeneous media into deterministic and stochastic approaches. By deterministic, it is meant that the spatial distribution of soil properties and their magnitudes are defined, whereas in a stochastic problem the soil properties are represented by random variables. For the deterministic approach one can refer to Willis (1960), Philip (1967), Broadbridge (1987), and Warrick and Yeh (1990). In stochastic problems, one can refer to Yeh et al. (1985a, b, c) and Eaton and McCord (1995). Adjacent homogeneous layers is the simplest mode of a deterministic nature. In this case, the effective saturated hydraulic conductivity, $K_{\text{avg}}$, when the direction of flow is normal to the layers is given as (Iwata et al. 1995):

$$K_{\text{avg}} = \frac{\sum L_{di}}{\sum (L_{di} / K_i)} \quad (2.8)$$

where $L_{di}$ is the thickness of layer $i$ (m) and $K_i$ is the saturated hydraulic conductivity of stratum $i$ (m/s).

### 2.4 Hysteresis Effects

The relationship between water pressure and soil water content, the soil-water characteristic curve, is not unique but is dependent upon the previous moisture history of
the soil. This characteristic is called hysteresis. Usually, the water content at a given pressure for a wetting soil is less than that for a draining soil (Haines 1930). This means that at the end of a complete drying and wetting cycle in the soil-water characteristic curve, the initial starting point will not be met again and a lower value for the water content is expected. This water content is called natural saturation or satiated water content (Klute 1986). The intermediate curves between the main wetting and drying curves are called scanning curves (Hillel 1982).

Although hysteresis occurs when cyclic drying and wetting is present, depending on boundary conditions and temperature gradients, one can expect hysteresis effects even in a monotonic drying or wetting process, which in turn may introduce a source of error in predicting the moisture variation in the soil profile.

There are three generally accepted theories for hysteresis, namely, the bottle neck, the contact angle, and the delayed formation of the meniscus. All of these theories are based upon the Kelvin equation which relates the free energy of the liquid to the radius of the pore. For more description of these theories one can refer to Taylor and Ashcroft (1972).

Parker and Lenhard (1987) and Lenhard and Parker (1987) proposed a theoretical model for hysteresis in rigid porous media subjected to complex saturation history. The model considers hysteresis due to non-wetting fluid entrapment in addition to hysteresis caused by irregular pore geometry and contact angle.

Hassanizadeh and Gray (1993) proposed a new explanation for hysteresis and related the macroscopic capillary pressure to fluid densities, temperature, medium
porosity, specific interfacial areas, interfacial mass densities and degree of saturation. They argued that hysteresis is due to many effects which are usually lumped in a pressure-saturation relationship. They concluded that hysteresis in microscopic capillary pressure and contact angle are related to the elastic forces developed within the solid-fluid interfaces. These forces act upon the contact line and resist its movement within the tube. Along similar lines, Fredlund and Rahardjo (1993) pointed out that the effect of adsorptive forces between clay particles could produce highly negative pore water pressures, something which is not predictable by ordinary capillary law.

In a stratified profile where different bulk densities are present in adjacent layers, abrupt changes in total specific interfacial area of the solid-liquid interfaces per unit volume are expected. As a result, a retardation of liquid movement is expected.

In most transport equations, the hysteresis effect is ignored. The reason is not the lack of knowledge of the researcher, but rather the lack of sufficient data to adequately calibrate a hysteresis model (Kool and Parker 1987). Another reason for disregarding hysteresis which was pointed out by Royer and Parker (1975), is that spatial variability of hydraulic properties may overwhelm local hysteretic effects. Also, there are some who believe that hysteretic effects in the field are small (Pickens and Gillham 1980). Hillel (1982) noted that the relation of hydraulic conductivity to matric suction appears to be more affected by hysteresis than does the relation of hydraulic conductivity to water content. Hopmans and Dane (1986) found that the effect of both temperature and hysteresis were mostly dependent on the type of boundary conditions applied. Hopmans
hysteresis were mostly dependent on the type of boundary conditions applied. Hopmans and Dane (1986) noted that hysteresis tended to dominate the temperature effects during the simulation of water movement.

There have been many attempts to formulate the hysteresis phenomenon and the effort still continues (Poulolvasilis 1962; Topp 1971; Mualem 1974; Kool and Parker 1987; Philip 1991). Milly (1982) and Yu et al. (1993) incorporated hysteresis effects in their models. There are still some problems encountered in models dealing with hysteresis. First, to determine the transport properties in which hysteresis effects are included and second, to judge the flow condition and determine the finite time step in numerical solutions of the transport equations (Yu et al. 1993).

In Summary

The literature search found only a few studies conducted on stratified soil profiles, especially in soil columns having similar textures but different structures. The number of studies narrowed down further when it came to the investigation of moisture and temperature variations since most experiments were related to crop response. Shortage of related studies extends to theoretical approach as well, since uniform soil profiles are usually dealt with. This justifies further experimental and theoretical studies on the heat and mass transfer in stratified profiles.
CHAPTER THREE

EXPERIMENTAL STUDY

In this chapter, the experimental treatments are described, materials needed to carry out
the experiment are outlined, and the procedure for designing and conducting an
experiment according to the objectives is presented. Also, experimental results are
presented and discussed.

3.1 Treatments

There can be many layering configurations in a seedbed resulting from different
tillage methods or seeding operations. To study the effect of layering on evaporative
losses from the soil surface and on moisture and temperature variations through the soil
profile, four layering configurations commonly occurring in the seedbed were used as
treatments (Fig. 3.1). Treatment B, or no-layering, is considered as the control. Layers L
and D are 30 mm deep loose and dense layers of soil, respectively. In this study, the focus
was only on the top portion of agricultural soils, hence, soil columns were restricted to
150 mm in height. Since initial water content (IWC) may have an important influence on
the final result, three IWC levels: low, intermediate and high, were considered as another
Fig. 3.1. Layering configurations. L, B and D refer to loose, bottom layer and dense layers with 0.95, 1.15 and 1.35 Mg/m$^3$ bulk densities, respectively. (a): B configuration, (b): LB configuration, (c): DB configuration, (d): LDB configuration.

set of treatments, bringing the total number of treatments to twelve.

Soil columns were prepared and kept for one week without watering in a growth chamber under controlled temperature and relative humidity. Water content and temperature of different layers were monitored.

The detailed procedure of the experimental procedure and design along with the results are given in the following sections.
3.2 Soil Classification

The soil used in this study was obtained from the Kernen research farm, north east of Saskatoon, Saskatchewan (52° 08’ N and 106° 38’ W). The soil is classified as an Orthic Dark Brown chernozem (Souster 1979). Procedures for determining some properties of the soil sample used along with corresponding values are given in Table 3.1. Values were determined either by the author or by personnel of the Soil Science Department of the University of Saskatchewan.

<table>
<thead>
<tr>
<th>Property</th>
<th>Method</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle size fractions</td>
<td>Hydrometer</td>
<td>57% clay, 34% silt, 9% sand</td>
</tr>
<tr>
<td>Particle density</td>
<td>Pycnometer</td>
<td>2.72 Mg/m³</td>
</tr>
<tr>
<td>Organic matter content</td>
<td>Dry combustion</td>
<td>4.83%</td>
</tr>
<tr>
<td>Quartz content</td>
<td>X-ray diffraction</td>
<td>40%</td>
</tr>
</tbody>
</table>

The result indicated that the soil texture is a clay according to the USDA soil classification triangle (Brady 1990). The relatively high organic matter content made the preparation of soil samples easier for higher initial water contents, otherwise, the high percentage of clay particles could have resulted in unfavorable structural characteristics. Particle density was found to be higher than average (but still a typical value) which could be due to the type of clay minerals and also to the high percentage of quartz in the soil.
Bulk densities (dry) of 0.95, 1.15 and 1.35 Mg/m$^3$ were chosen for the “loose”, “bottom” and “dense” soil layers, respectively, when preparing the soil columns. The magnitudes were chosen similar to the range of bulk densities reported for the same location from which the soil was obtained (Moazed 1996). Due to the fine texture of the soil, water content at field capacity was determined at 5.1 m (50 kPa) suction rather than 3.64 m (33 kPa) as recommended by Cassel and Nielsen (1986). Water content at 153 m (1500 kPa) pressure (suction), representing the wilting point, was determined as well. Both field capacity and wilting point, limits for determining the available water, are controversial subjects (Hillel 1982). In particular, the lower limit varies with the plant species and corresponds to different soil suctions (Cassel and Nielsen 1986). In this study, these limits were considered as arbitrary points and not as intrinsic physical properties of the soil. For 1.15 Mg/m$^3$ bulk density, a water content of 40% corresponded to 5.1 m pressure and 24% to 153 m pressure. Accordingly, low, intermediate and high initial water contents of 27.2%, 32% and 36.8%, respectively, were selected to correspond to 20%, 50% and 80% of field capacity.

3.3 Preparation of Experimental Units

Three containers to be used for experimental units (EUs) were constructed out of clear acrylic tube. Cylindrical containers of 200 mm diameter, 160 mm height, 6.35 mm thick with a 6.35 mm thick solid base were made. A solid base was used so as to restrict moisture losses to evaporation from the top surface.
The soil was air dried, ground and sieved (<4.5 mm) to make a more uniform soil structure and to remove foreign objects. Soil was brought to the selected initial water content by carefully adding the necessary amount of distilled water to the air dried soil. To compensate for the amount of water evaporating during the preparation of EUs given the very dry environment, 5% more water was added to the soil. The prepared soil was sealed in a plastic bag and stored in a sealed plastic container for one week before final preparation of EUs to reach equilibrium state. Mini-gypsum blocks were embedded in the soil 24 hours prior to preparing the EUs to reach to equilibrium with the soil. Since during the preparation of EUs the relative humidity was not constant (18% to 25%), a small variation in the initial water content for each replication was expected. After preparing the soil samples the actual initial gravimetric water contents (IWC) obtained were: 27.4% ± 0.32, 31.8% ± 0.37 and 36.6% ± 0.38.

When preparing each soil layer for the specified bulk density, 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 predetermined amount of wetted soil using a manually driven hydraulic press.

To monitor the soil moisture in 30 mm thick layers, mini-gypsum blocks (dimensions 17 mm x 15 mm x 10 mm) were constructed and calibrated for both moisture and temperature effects (Appendix A). Thermocouples (copper-constantan type) were constructed, selected (Appendix A) and used for temperature measurements. Water content and temperature were measured at 15, 45, 75, and 135 mm depths and temperature was also measured at the surface. The experimental units were insulated using
25.4 mm thick fiberglass insulation around the wall, and 25.4 mm thick Styrofoam at the base (Fig. 3.2).

![Diagram of cross section of an experimental unit]

3.4 Experimental Design and Setup

To test the interaction of layering with initial water contents as well as the effect of stratification on moisture loss, an experimental design consisting of 12 treatments (4 layering configurations and 3 different IWCs) in 4 incomplete blocks of 3 EU’s with 3 replications was established. Blocks were incomplete because not all treatments were present in each block.

Wires from moisture and temperature sensors, coming out of the chamber through a hole, were hooked up to Campbell 21X data-logger (Campbell Scientific, Inc., Logan,
UT) via an AM416 multiplexer from the same company (Fig. 3.3). Data were collected hourly and stored in a computer for analysis.

![Diagram](image)

**Fig. 3.3 The schematic diagram of the experimental setup.** T and RH represent temperature and relative humidity, respectively.

The plan for randomized treatments (Table 3.2) was taken from a template available in Cochran and Cox (1957). In this plan, the first replication (Rep. I) consists of blocks X1-X4, the second replication (Rep. II) consists of blocks Y1-Y4 and the third replication (Rep. III) consists of blocks Z1-Z4. Each category (X, Y and Z) contains all 12 randomized treatments (i.e., four layering configurations x three initial water contents).
Table 3.2 Plan of experimental design (Cochran and Cox 1954)

<table>
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</tr>
</thead>
<tbody>
<tr>
<td>X1</td>
<td>1 2 3</td>
<td>Y1</td>
<td>4 7 10</td>
<td>Z1</td>
<td>6 8 12</td>
</tr>
<tr>
<td>X2</td>
<td>4 5 6</td>
<td>Y2</td>
<td>1 8 11</td>
<td>Z2</td>
<td>2 9 10</td>
</tr>
<tr>
<td>X3</td>
<td>7 8 9</td>
<td>Y3</td>
<td>2 5 12</td>
<td>Z3</td>
<td>3 4 11</td>
</tr>
<tr>
<td>X4</td>
<td>10 11 12</td>
<td>Y4</td>
<td>3 6 9</td>
<td>Z4</td>
<td>1 5 7</td>
</tr>
</tbody>
</table>

Each block consisted of 3 experimental units. The sole reason for blocking the treatments was to compensate for the possible variability of the temperature and relative humidity in different places of the growth chamber.

3.5 Ambient Conditions

In all EUs, the initial temperature throughout the soil column depth was found to be approximately 18 ±1°C at the beginning of the experiments. A 1.4 m² growth chamber located in the Phytotron facility of the University of Saskatchewan was used to provide a controlled environment (Fig.3.4). The chamber settings were periodically checked using a humidity and temperature meter (model HM 34, Vaisala Company, Finland).

Each block of EUs were placed in the controlled chamber in which temperature and relative humidity, respectively, were set to 15 °C and 44% for 16 hours and to 5 °C and 85% for 8 hours. These approximate settings were chosen according to the local
Fig. 3.4 Controlled environment chamber in the Phytotron facility, University of Saskatchewan.
meteorological data representing the time of seeding which is usually in early May for a
typical grain crop in Saskatoon (Wittrock and Wheaton 1991; Environment Canada

In the growth chamber, air was flowing upward from the floor. Using an air
velocity transducer (model 8470-5AM-V, TSI Inc., St. Paul, Min) no air movement was
sensed (in the range of the sensitivity of the instrument) at the surface of the EUs.

3.6 Experimental Results and Discussion

3.6.1 Moisture variations in different layers

Figures 3.5-3.8 show the variation of water content with time in samples with IWC of
0.27 Mg/Mg (average of 3 replicates). Similar drying trends were found in samples with
other IWCs from which Figs. 3.9-3.10 are presented for IWC of 0.32 (Mg/Mg) and Fig.
3.11 is shown for 0.37 (Mg/Mg) IWC (the rest are shown in Appendix B).

For a B configuration and IWC of 0.32 (Mg/Mg), measured water contents after
elapsed time of 24 hours for 3 different replications ranged from 0.27-0.29 (Mg/Mg) at 15
mm to 0.31-0.32 at 135 mm. At the end of the experiment, measured water contents
ranged from 0.31-0.32 (Mg/Mg) at 135 mm and ranged from 0.16-0.20 (Mg/Mg) at 15
mm. The variability in the range of 0.01 to 0.04 (Mg/Mg) was also observed in other
IWCs as well.

Although the mini-gypsum blocks were brought to equilibrium with the soil to be
used in each experiment, due to their small size (high specific area) and to the very dry
Fig. 3.5 Variation of water content with time at 15 mm depth and 0.27 (Mg/Mg) IWC. Each point is the average of 3 replications.
Fig. 3.6 Variation of water content with time at 45 mm depth and 0.27 (Mg/Mg) IWC. Each point is the average of 3 replications.
Fig. 3.7 Variation of water content with time at 75 mm depth and 0.27 (Mg/Mg) IWC. Each point is the average of 3 replications.
Fig. 3.8 Variation of water content with time at 135 mm depth and 0.27 (Mg/Mg) IWC. Each point is the average of 3 replications.
Fig. 3.9 Variation of water content with time at 15 mm depth and 0.32 (Mg/Mg) IWC. Each point is the average of 3 replications.
Fig. 3.10 Variation of water content with time at 135 mm depth and 0.32 (Mg/Mg) IWC. Each point is the average of 3 replications.
Fig. 3.11 Variation of water content with time at 135 mm depth and 0.37 (Mg/Mg) IWC. Each point is the average of 3 replications.
state of compactness and the IWC of the soil, a period of 10 to 24 hours was required for equilibrium as seen by the initial rising portion of the graphs.

Readings from mini-gypsum blocks showed high instability when the soil became very dry. The calibration formulas for mini-gypsum blocks (Eqs. A1 and A.4 in Appendix A) cover the range of water contents from approximately 0.15 to 0.38 Mg/Mg where calibrating the mini-gypsum blocks, soil water contents less than 0.15 Mg/Mg produced high fluctuations in soil resistance, exceeding the resolution of the data acquisition system and thus giving unreliable readings. Corresponding soil resistances for water contents lower than 0.15 Mg/Mg are reflected in a flattened curve as can be seen in Fig. 3.5. Over this range, confidence in the reliability of the data is greatly reduced.

Occurrence of small bumps at the beginning of the cool cycle, especially at 15 mm depths (Figs. 3.5 and 3.9), can be due to three mechanisms. First, absorption of moisture from the environment due to the higher relative humidity in the cool cycle. This reason holds only for the upper layers near the soil surface and reflects itself in the larger amplitude of the bumps for these drier layers. Second, diffusion and transfer of water vapor from moist and warm areas to dry and cool horizons. This happens due to the temperature and vapor pressure gradients imposed at the soil surface. Third, the influence of temperature changes on the mini-gypsum blocks' readings. At deeper soil horizons, the amplitude of the bumps is very small (Figs. 3.8, 3.10 and 3.11). When calibrating the mini-gypsum blocks, temperature effects were satisfactorily accounted for (Appendix A), but a very small portion of this change can still be caused by the effect of temperature on gypsum blocks. The most likely reason for this phenomenon (bumps), lies in the diffusion
and transfer of water vapor caused by step changes in the boundary conditions in the upper horizons and on temperature effects on mini-gypsum blocks in the lower horizons.

3.6.2 Moisture conservation

From the figures it is clear that the influence of layering on moisture retention didn’t extend to depths lower than about 45 mm. In samples with lower IWC, the effect of layering on moisture retention is more evident (Figs. 3.6 and 3.7). As water evaporates from the soil surface, more air is introduced into the soil medium, which in turn blocks the water movement and reduces the hydraulic conductivity, thus retaining moisture in deeper horizons (Fig 3.8). In samples with higher IWC, more water is lost due to the imposed boundary conditions (compare Figs. 3.8, 3.10 and 3.11). This is probably due to more continuous capillary pathways supplying the water commensurate to the evaporative demand.

The low overall moisture variations in each treatment, especially in deeper horizons, is due to the fine texture of the soil used, with its high percentage of clay particles and thus low hydraulic conductivity. The high percentage of organic matter and the short drying period for each experiment are other reasons for overall low moisture loss from the soil columns.

Since a major objective of this study is to investigate the effect of stratification on moisture conservation in soil samples, a thorough statistical analysis was conducted to evaluate the experimental data. Since the top 30 mm layer, especially in the dry loose state, gave unreliable readings for water content in mini-gypsum blocks, corresponding
data for this layer was excluded in calculating the final volume of water retained in the soil
samples. Besides, water available for a seedling would likely come from soil layers below
the seed, typically from the 25-40 mm depth.

To obtain a meaningful index to compare the amount of water retained in the
samples at the end of each experiment, a normalized volume of water (the ratio of final to
the initial volume of water, excluding the top 30 mm layer) was used in the statistical
analysis. For calculating the retained volume of water in 30 mm thick zones, the final
measured gravimetric water content at the mid-point of the range was used as the average
(i.e., 15 mm above and 15 mm below) and converted to volumetric basis using the known
bulk density for each layer. Since there was no sensor embedded at 105 mm depth,
average readings for 75 mm and 135 mm depths were used for the corresponding layer. A
constant volume was assumed for the soil layers throughout the experiment. This could be
one source of error, especially in the top layers where some shrinkage was experienced.
Occurrence of random cracks especially on denser top layers was another source of error
since moisture could have escaped at different rates from different replicates. Data used in
the statistical analysis are given in Appendix D.

Table 3.3 shows the result of the analysis of variance for the experimental design.
Due to the exclusion of the top 30 mm layer and due to the fine texture of the samples,
total evaporation was small. This resulted in near unity values for the normalized volume
of water and less variation among samples. Nevertheless, the results show that layering
had a significant effect on final normalized volume of water (p < 0.05).
### Table 3.3 Analysis of variance for four layering configurations (B, LB, DB and LDB) with 3 different initial water contents (0.27, 0.32 and 0.37 (Mg/Mg)) and 3 replications

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<th>MS</th>
<th>F value</th>
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<tr>
<td>Total</td>
<td>35</td>
<td>0.024712</td>
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</table>

\[ R^2 = 0.9095 \quad CV = 1.42\% \quad \text{Root MSE} = 0.01312 \quad \text{Norm Vol} = 0.92433 \]

<table>
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<tr>
<th>Source</th>
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<td>0.000141</td>
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<td>0.6093</td>
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<td>Lyr</td>
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<td>0.000591</td>
<td>3.44</td>
<td>0.0490</td>
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<td>0.005427</td>
<td>31.5</td>
<td>0.0001</td>
</tr>
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Control as

<table>
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<th>Lyr x IWC</th>
<th>DF</th>
<th>Type III SS</th>
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<td></td>
</tr>
</tbody>
</table>

Among

<table>
<thead>
<tr>
<th>Lyr x IWC</th>
<th>DF</th>
<th>Type III SS</th>
<th>MS</th>
<th>F value</th>
<th>Pr &gt; F</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0.000770</td>
<td>0.000193</td>
<td>1.12</td>
<td>0.3890</td>
<td></td>
</tr>
</tbody>
</table>

**LYR** = Layering configurations; **IWC** = Initial water content; **DF** = Degrees of freedom; **CV** = Coefficient of variation; **NormVol** = Normalized volume

The interaction of layering configurations with the initial water contents (Lyr x IWC) was found to be non-significant. This result was in contrast to the T grouping based on a Least Significant Difference (LSD) analysis (Table 3.4) in which all layering configurations with low IWC, and the DB configuration with high IWC, show significant differences.
Table 3.4 Grouping of final normalized means of volume of water according to LSD analysis

<table>
<thead>
<tr>
<th>Normalized means</th>
<th>No. of replications</th>
<th>Treatment</th>
<th>T grouping</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.963</td>
<td>3</td>
<td>LB27</td>
<td>a</td>
</tr>
<tr>
<td>0.953</td>
<td>3</td>
<td>LDB27</td>
<td>a</td>
</tr>
<tr>
<td>0.950</td>
<td>3</td>
<td>DB27</td>
<td>ab</td>
</tr>
<tr>
<td>0.940</td>
<td>3</td>
<td>LB32</td>
<td>abc</td>
</tr>
<tr>
<td>0.928</td>
<td>3</td>
<td>LDB32</td>
<td>bcd</td>
</tr>
<tr>
<td>0.926</td>
<td>3</td>
<td>DB32</td>
<td>cd</td>
</tr>
<tr>
<td>0.924</td>
<td>3</td>
<td>B27*</td>
<td>cd</td>
</tr>
<tr>
<td>0.922</td>
<td>3</td>
<td>B32*</td>
<td>cde</td>
</tr>
<tr>
<td>0.907</td>
<td>3</td>
<td>B37*</td>
<td>de</td>
</tr>
<tr>
<td>0.901</td>
<td>3</td>
<td>LB37</td>
<td>ef</td>
</tr>
<tr>
<td>0.899</td>
<td>3</td>
<td>LDB37</td>
<td>ef</td>
</tr>
<tr>
<td>0.878</td>
<td>3</td>
<td>DB37</td>
<td>f</td>
</tr>
</tbody>
</table>

α = 0.05    DF = 13    MSE = 0.000172    $T_{cr} = 2.16$    LSD = 0.0231

* Controls

compared to no-layering or control treatments. Therefore, the sum of squares of the interaction effect was separated into its two components: (1) that of Control as LYR x IWC, (i.e., the control samples with no-layering only, namely B27, B32 and B37); and (2) among LYR x IWC (i.e., among all layered configurations, excluding the control samples). The ANOVA (Table 3.3) indicated that there was no interaction between different layering configurations and initial water content except for those configurations with uniform bulk densities (controls). This is now consistent with the results of T grouping based on LSD analysis shown in Table 3.4. The LSD results indicate that stratification
conserved more water in low IWC treatments, whereas in high IWC treatments more water was lost in the DB configuration. No significant difference among means of normalized volume of water was observed in the intermediate IWC treatments.

In the above analysis, the total volume of water retained in the samples at the end of the experiments was analyzed. Another approach is to consider the retained water in specific layers. From this respect, more water was present in LDB configuration at 45 mm depth compared to B (control) treatment for the low IWC of 0.27 (Mg/Mg). This difference corresponds to an almost 7% change (corresponding data is shown in Fig. 3.6). This may be due to the large difference between the pore sizes in the dense and loose layers overlaying one another, impeding the flow of liquid water. This is a hysteresis phenomenon referred to as the bottle-neck effect (Hillel 1982). Such a layering configuration (LDB) could correspond to seeds being planted into a packed layer which is covered with a loose layer of soil. Water loss in the DB configuration with high IWC of 0.37 (Mg/Mg) could be due to more continuity of pathways in the packed layer.

One of the implications of the results of this study applies to seeding operations in similar soil textures. In clay soils with low initial water content, a layered seedbed, preferably a loose over a dense layer is recommended. This configuration can easily be implemented by using presswheels near to the furrow openers in a seed drill (to prepare the packed or dense layer) followed by a small harrow or drag chain (to create a loose overlying layer) attached to the seed drill. In soils with higher initial water content, where layering the seedbed may have small or even adverse effect on moisture conservation, avoiding layering the seedbed would be recommended (e.g., removing presswheels from
the seed drills or reducing the weight of the presswheels). Furthermore, packing a moist clay soil may result in a densely compacted layer which in turn impedes the emergence of newly planted seeds. This is more critical for smaller seeds, such as canola, which have limited energy to emerge to the surface in a short period of time.

3.6.3 Temperature variation in different layers

Figure 3.12 shows the temperature variation with time at 75 mm depth with IWC of 0.27 (Mg/Mg). Similar trends were found at the other depths and IWC's. The results showed that temperature was not significantly affected by layering treatments at any depth and IWC.

The temperature at the surface (not shown) rapidly became very close to that of the ambient temperature. Luikov (1964) suggested the use of wet bulb temperature as a boundary condition at the surface of a porous body undergoing a drying process. This cannot be assumed, at least for the type of soil being used in this study. At a relative humidity of 44%, a wet bulb temperature of around 9 °C is obtained from a psychrometric chart, significantly different from that measured (13.5 °C to 15 °C). The measured surface temperatures were almost the same as the ambient temperature.
Fig. 3.12 Temperature variation with time at 75 mm depth and 0.27 (Mg/Mg) IWC. Each point is the average of 3 replications.
CHAPTER FOUR
MODEL DEVELOPMENT

In this chapter the governing coupled heat and mass transfer equations are derived. The numerical solutions to the governing equations and conditions for stability are developed and the computer program to solve the numerical equations is outlined.

4.1 Mass Transfer Governing Equation

In developing the model, hysteresis effects are ignored since a process that is monotonic with no cycling of wetting and drying is of interest in this study. It is recognized that this may not be entirely correct since even under no precipitation with respect to hysteresis effects, the boundary conditions (i.e., in terms of temperature and relative humidity) will undergo cyclic changes. In this development, this is assumed to have negligible effect.

Applying Darcy's law for one-dimensional unsaturated flow, the liquid mass flux \( q_l \) for each layer can be written as:

\[
q_l = -p_l K \frac{\partial \phi}{\partial z}
\]  

(4.1)
where:

\[ q_t = \text{liquid mass flux (Mg} \cdot \text{m}^2 \cdot \text{s}^{-1}) \],

\[ \rho_t = \text{liquid density (Mg/m}^3 \),

\[ K = \text{hydraulic conductivity (m/s)}, \]

\[ \phi = \text{total pressure (m)}, \]

\[ z = \text{depth (m)}. \]

Total pressure or hydraulic head in the absence of osmotic pressure is equal to the sum of gravitational head corresponding to depth \( z \) (m) and the soil pressure head \( \psi \) (m) which is sometimes called the "capillary potential" or "soil matric potential".

Since the pressure corresponding to the depth under study (0.15 m) is small compared to the vapor pressure imposed at the surface, it is neglected and the total potential is assumed to be equal to the matric potential. Therefore, rewriting Eq. 4.1 in terms of velocity, the liquid velocity \( v_t \) can be written as:

\[ v_t = -K \frac{\partial \psi}{\partial z} \]  \hspace{1cm} (4.2)

Based on the conservation of mass:

\[ \frac{\partial \theta_t}{\partial t} = -\frac{\partial v_t}{\partial z} - E \]  \hspace{1cm} (4.3)
where \( \theta_i \) is the volumetric water content in liquid phase \( (m^3/m^3) \) and \( E \) is the internal mass rate of change of liquid to vapor \( (m^3/m^3 \text{ s} \) or \( \text{Mg/Mg s} \)).

In a stratified soil profile in which there may be sudden changes in water content at the interfaces of adjacent layers, a potential-based equation is preferred. To transform Eq. 4.3 into a pressure-based equation, the chain rule is applied:

\[
\frac{\partial \theta_i}{\partial t} = \frac{\partial \theta_i}{\partial \psi} \left( \frac{\partial \psi}{\partial t} \right) + \frac{\partial \theta_i}{\partial T} \left( \frac{\partial T}{\partial t} \right) \quad (4.4)
\]

Application of the chain rule requires that the variable \( \theta_i \) be continuous, but writing the transport equation in pressure-based form gives the benefit of smooth transition of pressure at interlayer boundaries.

In Eq. 4.4 the ratio \( \partial \theta_i/\partial \psi \) is called the "specific water capacity", \( C_\theta \) and is equal to the slope of the soil-water characteristic curve (Hillel 1982). The contribution of the ratio \( \partial \psi/\partial T \) is somewhat controversial. Ten Berge and Bolt (1988) stated that in accordance with thermodynamics of irreversible process (TIP), the primary temperature-moisture coupling effect arises with \( \nabla \psi \) as the driving force and not \( \nabla \theta \). Kay and Groenvelt (1974) and Groenvelt and Kay (1974) showed that at a constant pressure, a temperature gradient induces a driving force on the water vapor in the direction of the lower temperature (i.e., the same direction as found under a temperature gradient at a constant water content in the mechanistic approach of Philip and de Vries 1957). On the
other hand, for the liquid phase, such a temperature gradient at constant pressure induces a driving force on the liquid in the direction from cold to warm (i.e., opposite to that of the mechanistic approach). To understand the net thermally induced flux, Ten Berge and Bolt (1988) added the effect of thermo-osmosis induced flux towards the higher temperature and the surface tension induced flux towards the lower temperature in a hydrophilic media. Thermo-osmosis is a term for the $\nabla T$-induced mass transport under the condition of $\nabla \psi = 0$. Also, Ten Berge and Bolt (1988) showed that the magnitude of these opposite $\nabla T$-driven liquid fluxes are likely to be of the same order. Therefore, in a potential-based equation, the effect of $\nabla T$-driven liquid fluxes can safely be neglected. Even in the water content-based equations the overall effect of thermally induced liquid flux was shown to be less than 1% of the total flux (Milly 1984). Figure 4.1 illustrates the idealized capillary model for $\nabla T$-induced liquid transport based on the TIP described above.

Assuming then that thermally driven liquid fluxes are negligible, the ratio $\partial \theta / \partial T$ can be eliminated. Substituting for $v_l$ from Eq. 4.2 into Eq. 4.3 and using Eq. 4.4, the following relationship is derived:

$$C_a \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left[ K \frac{\partial \psi}{\partial z} \right] - E$$

where $C_a = \partial \theta / \partial \psi$ (m⁻¹). Equation 4.5 is the transport equation for the liquid phase.
Fig. 4.1 Idealized capillary model for thermally induced liquid transport in a hydrophilic media (where heat of adsorption is positive). Surface tension-governed flow to the right, thermo-osmosis-governed flow to the left. The flow is associated with a sensible heat flux from left to right due to adsorption (right) and desorption (left) (adapted from Ten Berge and Bolt 1988).
Water pressure, temperature and relative humidity in the absence of solutes are related by the following thermodynamic relationship (Edlefsen and Anderson 1943):

$$\psi = \frac{RT}{g} \ln(h) \quad (4.6)$$

where:

- $R$ = universal gas constant (J·kg$^{-1}$·K$^{-1}$),
- $T$ = temperature (K),
- $h$ = relative humidity.

In Eq. 4.6, the water pressure $\psi$ is in thermodynamic equilibrium with the water in the medium with atmospheric pressure as datum, provided that chemical reactions have negligible effect.

Noting that:

$$\rho_v(\psi, T) = \rho_o(T) h(\psi, T) \quad (4.7)$$

where $\rho_v = \text{vapor density (Mg/m}^3\text{)}$ and $\rho_o = \text{saturated vapor density (Mg/m}^3\text{)}$, the vapor density gradient $\nabla \rho_v$ in one-dimensional form can be expressed as:

$$\frac{\partial \rho_v}{\partial z} = \rho_o \frac{\partial h}{\partial T} \frac{\partial T}{\partial z} + \rho_o h \frac{\partial \rho_v}{\partial T} \frac{\partial T}{\partial z} \quad (4.8)$$
One should keep in mind that $\rho_v$, $\rho_o$ and $h$ are related according to Eq. 4.6 so that $h$ is not an independent variable. Relative humidity $h$ is retained in the expression at this point solely to simplify mathematical manipulations.

The ratios $\partial h/\partial T$ and $\partial h/\partial \psi$ can be found from Eq. 4.6. From Eq. 4.7 the relative humidity is given by:

$$h = \exp \left( \frac{\psi g}{R T} \right), \quad (4.9)$$

so that

$$\frac{\partial h}{\partial \psi} = \frac{g}{R T} h, \quad (4.10)$$

and

$$\frac{\partial h}{\partial T} = -\frac{\psi g}{R T^2} h. \quad (4.11)$$

Since the temperature is expressed in K, it would appear that the dependence of relative humidity on temperature is very small. Sophocles (1979) made the assumption of negligible effect of temperature on relative humidity in the development of a pressure-
based equation. Herkelrath (1981) and Milly (1982) criticized Sophocles’ method and pointed out some erroneous outcomes resulted from this assumption. Equation 4.11 includes a pressure variable in the numerator implying that in a very dry state, the ratio \( \partial h/\partial T \) may be significant. In this study, this may occur in the top few centimeters of the soil profile where the top layer dries rapidly. In this situation the ratio \( \partial h/\partial T \) may no longer be negligible compared to the \( \partial h/\partial \psi \) term.

Mass vapor flux \( q_v \) (Mg \cdot m^{-2} \cdot s^{-1}) is written as:

\[
q_v = -D_{vap} \frac{\partial \rho_v}{\partial z}
\]  

(4.12)

where \( D_{vap} \) is the vapor diffusivity (m\(^2\)/s).

Vapor velocity \( v_v \) (m/s) is written as:

\[
v_v = \frac{q_v}{\rho_l}
\]  

(4.13)

Substituting Eqs 4.8, and 4.10–4.12 into Eq. 4.13 yields:

\[
v_v = \frac{D_{vap}}{\rho_l} \left( \rho^* \frac{gh}{RT} \frac{\partial \psi}{\partial z} + \frac{\partial \rho^*}{\partial T} \frac{\partial T}{\partial z} - \rho^* h \frac{\psi}{RT^2} \frac{\partial T}{\partial z} \right)
\]  

(4.14)
Applying the principle of conservation of mass to Eq. 4.13 produces the following relationship:

\[
\frac{\partial \theta_v}{\partial t} = -\frac{\partial v_v}{\partial z} + E
\]  
(4.15)

where \( \theta_v \) (m\(^3\)/m\(^3\)) is the volumetric vapor content of perceptible water, defined as (Thomas and King 1992):

\[
\theta_v = \frac{(\eta - \theta_i) \rho_v}{\rho_i}
\]  
(4.16)

where \( \eta \) is the total porosity (m\(^3\)/m\(^3\)). Again, applying the chain rule to \( \partial \theta_v / \partial t \) the following relationship is found:

\[
\frac{\partial \theta_v}{\partial t} = \frac{\partial \theta_v}{\partial \psi} \left| \frac{\partial \psi}{\partial t} \right| + \frac{\partial \theta_v}{\partial T} \left| \frac{\partial T}{\partial t} \right|
\]  
(4.17)

Differentiating Eq. 4.16 with respect to pressure and temperature, respectively, leads to the following equations:

\[
\frac{\partial \theta_v}{\partial \psi} = \frac{\rho_v h}{\rho_i} \left[ \frac{\theta_v}{RT} - C_0 \right]
\]  
(4.18)
\[
\frac{\partial \theta}{\partial T} = \frac{h(\eta - \theta)}{\rho_i} \left( \frac{\partial \rho}{\partial T} - \frac{\rho \psi g}{RT^2} \right)
\]  
(4.19)

where the relationships given by Eqs. 4.9-4.11 have been used. Differentiating Eq. 4.16 once more with respect to time, applying the chain rule and substituting into Eqs. 4.18-4.19, results in the following relationship:

\[
\frac{\partial \theta}{\partial t} = C_{v1} \frac{\partial \psi}{\partial t} + C_{v2} \frac{\partial T}{\partial t}
\]  
(4.20)

where:

\[
C_{v1} = \frac{\rho_i h}{\rho_i} \left[ \frac{g(\eta - \theta)}{RT} - C_g \right],
\]

\[
C_{v2} = \frac{h}{\rho_i} (\eta - \theta) \left( \frac{\partial \rho}{\partial T} - \frac{\rho \psi g}{RT^2} \right).
\]

Substituting Eq. 4.14 into Eq. 4.15 and using Eq. 4.20 leads to the following governing equation for vapor flow:

\[
C_{v1} \frac{\partial \psi}{\partial t} + C_{v2} \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( K_{v1} \frac{\partial \psi}{\partial z} \right) + \frac{\partial}{\partial z} \left( K_{v2} \frac{\partial T}{\partial z} \right) + E
\]  
(4.21)
where:

\[ K_{vl} = \frac{D_{vl} g \rho \cdot h}{\rho_l RT} \]

\[ K_{v2} = \frac{D_{v2} h}{\rho_l} \left( \frac{\partial \rho}{\partial T} - \frac{g \psi \rho}{RT^2} \right) \]

The overall mass transfer governing equation is found by adding the liquid and vapor mass transfer equations 4.5 and 4.21, in which the internal evaporation rate \( E \) is eliminated:

\[ C_{vv} \frac{\partial \psi}{\partial t} + C_{vT} \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( K_{vv} \frac{\partial \psi}{\partial z} \right) + \frac{\partial}{\partial z} \left( K_{vT} \frac{\partial T}{\partial z} \right) \]

(4.22)

where:

\[ C_{vv} = C_v + C_{vl} \]

\[ C_{vT} = C_{v2} \]

\[ K_{vv} = K + K_{vl} \]

\[ K_{vT} = K_{v2} \]

4.2 Heat Transfer Governing Equation

Assuming that the heat transfer occurs only by conduction and latent heat, total flux of the sensible and latent heat of vaporization per unit area can be written as:
\[ q_h = -k \frac{\partial T}{\partial z} + L \theta_v \]  

(4.23)

where:

\[ q_h \] = heat flux (W/m^2),
\[ k \] = thermal conductivity (W/m\( \cdot \)K^{-1}),
\[ L \] = latent heat of vaporization (J/Mg).

Heat per unit volume \( Q_h \) (J/m^3) is written as:

\[ Q_h = C(T - T_r) + L \rho \theta_v \]  

(4.24)

where \( T_r \) is a reference temperature. Differentiating Eq. 4.24 with respect to time and applying the principle of conservation of energy leads to:

\[ C \frac{\partial T}{\partial t} + L \rho_i \frac{\partial \theta_v}{\partial t} = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) - L \frac{\partial \theta_v}{\partial z} \]  

(4.25)

Rearranging produces:

\[ \frac{C}{\rho_i} \frac{\partial T}{\partial t} + L \rho_i E = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) \]  

(4.26)
where \( E \) can be determined from Eq. 4.5 or Eq. 4.21. After some manipulation, the final form of the governing heat transfer equation can be written as:

\[
C_T \frac{\partial T}{\partial t} + C_{T_w} \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left( K_T \frac{\partial T}{\partial z} \right) + \frac{\partial}{\partial z} \left( K_{T_w} \frac{\partial \psi}{\partial z} \right)
\]

where:

\[
C_T = \frac{C}{\rho_l} + L C_{v_2},
\]

\[
C_{T_w} = L C_{v_1},
\]

\[
K_T = \frac{k}{\rho_l} + L K_{v_2},
\]

\[
K_{T_w} = L K_{v_1}.
\]

4.3 Model Application to Stratified Soil Profile

The final developed coupled model, governing mass and heat transfer for a uniform soil profile, are presented in Eqs. 4.22 and 4.27. For a stratified soil profile, it is assumed that all soil parameters are well defined within each layer. Therefore, the overall mass and heat transfer equations are applied within each layer while matching the common points in adjacent layers.

In solving the governing equations 4.22 and 4.27 the following initial conditions are assumed:
\[ \psi = \psi_o \]  \hspace{2cm} (4.28)

\[ T = T_o \]  \hspace{2cm} (4.29)

where \( \psi_o \) and \( T_o \) are initial pressure head (suction) and temperature, respectively. It is assumed that initial pressure head and temperature are the same for all layers.

The following boundary conditions are imposed at the surface to correspond to the experimental conditions described in chapter 3:

\[ T_1 = T_o = 15 \, ^\circ C, \psi_1 = \psi_o = -11130 \, m \, (h = 0.44), \text{ for 16 hours}, \]

\[ T_1 = T_o = 5 \, ^\circ C, \psi_1 = \psi_o = -2127 \, m \, (h = 0.85), \text{ for 8 hours}. \]

where \( T_o \) and \( \psi_o \) are ambient temperature and pressure head, respectively. The values -11130 m and -2127 m were obtained from Eq. 4.6 with corresponding values for temperature (in K) and relative humidity. It was assumed that surface pressure \( \psi_1 \) and temperature \( T_1 \) are equal to the environment pressure \( \psi_o \) and temperature \( T_o \). Since the model is pressure-based, smooth transitions of pressure and temperature are assumed and no additional boundary conditions are required.

At the bottom end and also around the wall, it is assumed that no mass and heat transfer occurs. The boundary conditions are:
\[
\frac{\partial \psi_s}{\partial t} = 0
\]  
\[
\frac{\partial T_n}{\partial t} = 0
\]  

A schematic diagram of the layered soil column is shown in Fig. 4.2.

![Diagram](image)

**Fig. 4.2 Schematic diagram of boundary conditions of the layered soil column.** Environment temperature and pressure are represented by \( T_o \) and \( \psi_o \), and soil surface temperature and suction are represented by \( T_f \) and \( \psi_f \), respectively.
4.4 Numerical Solution

Due to the coupled nature and nonlinear parameters involved in the developed equations of heat and mass transfer, a numerical solution approach is unavoidable. Various numerical methods, from simple finite difference to advanced finite elements, can be implemented. Since finding an efficient numerical solution or comparing different numerical methods is not an objective of this study, a simple explicit Forward Time Central Space (FTCS) method is employed. The advantage of using this method is its simplicity and its straight-forward implication (no matrix needed to be solved). The disadvantage is its conditional stability reflected in the size of the time steps which makes it impractical for long simulation periods.

The following equations are approximate FTCS solutions for partial differential equations of pressure and temperature (Press et al. 1992):

\[
\frac{\partial \psi}{\partial t} = \frac{\psi_{i+1}^n - \psi_i^n}{\Delta t} \quad (4.32)
\]

\[
\frac{\partial^2 \psi}{\partial z^2} = \frac{\psi_{i+1}^n - 2\psi_i^n + \psi_{i-1}^n}{(\Delta z)^2} \quad (4.33)
\]

\[
\frac{\partial T}{\partial t} = \frac{T_{i+1}^n - T_i^n}{\Delta t} \quad (4.34)
\]
\[
\frac{\partial^2 T}{\partial z^2} = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta z)^2}
\]  

(4.35)

where \(n\) and \(i\) refer to temporal and spatial increments, respectively, and \(\Delta t\) is the time step.

It is assumed that all parameters remain constant over a small increment of time.

Therefore, substituting Eqs 4.32-4.35 into Eqs. 4.22 and 4.27 leads to:

\[
C_{\psi \psi} \frac{T_{i+1}^n - T_i^n}{\Delta t} + C_{\psi \psi} \frac{T_{i+1}^n - T_i^n}{\Delta t} = K_{\psi \psi} \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta z)^2} + K_{\psi \psi} \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta z)^2}
\]

(4.36)

\[
C_{\tau \psi} \frac{T_{i+1}^n - T_i^n}{\Delta t} + C_{\tau \tau} \frac{T_{i+1}^n - T_i^n}{\Delta t} = K_{\tau \psi} \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta z)^2} + K_{\tau \tau} \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta z)^2}
\]

(4.37)

In each time step, all parameters are evaluated at the 'current' state. Solving for \(\psi_i^{n+1}\) and \(T_i^{n+1}\) as the new pressure and temperature, results in the following equations:

\[
\psi_i^{n+1} = \lambda A \psi_i^n + [1 - 2\lambda A] \psi_i^n + \lambda A \psi_i^n + \lambda B T_i^{n+1} - 2\lambda B T_i^n + \lambda B T_i^n
\]

(4.38)

\[
T_i^{n+1} = \lambda F \psi_i^n - 2\lambda F \psi_i^n + \lambda F \psi_i^n + \lambda G T_i^{n+1} + [1 - 2\lambda G] T_i^n + \lambda G T_i^n
\]

(4.39)
where:

\[ \lambda = \frac{\Delta t}{(\Delta z)^2}, \]

\[ A = \left( \frac{C_{VT}K_{TV} - K_{VV}C_{TT}}{C_{VT}C_{TV} - C_{VV}C_{TT}} \right), \]

\[ B = \left( \frac{C_{VT}K_{TT} - K_{VT}C_{TT}}{C_{VT}C_{TV} - C_{VV}C_{TT}} \right), \]

\[ F = \left( \frac{K_{VV}C_{TV} - C_{VV}K_{TV}}{C_{VT}C_{TV} - C_{VV}C_{TT}} \right), \]

\[ G = \left( \frac{K_{VT}C_{TV} - K_{VV}K_{TT}}{C_{VT}C_{TV} - C_{VV}C_{TT}} \right). \]

4.5 Stability Analysis

Referring to a numerical solution technique, the term stability addresses a property of the particular finite difference equation(s) used, as the time step is made extremely small (Carnahan et al. 1969). This implies that there is an upper limit for the time step to maintain a stable solution. The following procedure (O’Brien et al. 1951; Carnahan et al. 1969) is applied to find the largest time step in an explicit finite difference method.
It is assumed that at any stage (at a time arbitrarily called \( t = 0 \)) Fourier expansions can be found for functions \( \psi \) and \( T \). Further, it is assumed that a separation of time and space is made and at time \( t \) the pressure and temperature can be expressed in the form:

\[
\psi = \xi (t) e^{\beta z} \tag{4.40}
\]

\[
T = \tau (t) e^{\beta z} \tag{4.41}
\]

where \( j = \sqrt{-1} \) and \( \beta \) is a positive constant. Substituting Eqs. 4.40 and 4.41 into Eqs. 4.36 and 4.37 leads to:

\[
C_{\psi\psi} \frac{\xi^{'}}{\Delta t} e^{\beta z} + C_{\psi T} \frac{\tau^{'}}{\Delta t} e^{\beta z} = K_{\psi\psi} \frac{\xi}{\Delta z^2} \left[ e^{\beta (z-\Delta z)} - 2e^{\beta z} + e^{\beta (z+\Delta z)} \right] + K_{\psi T} \frac{\tau}{\Delta z^2} \left[ e^{\beta (z-\Delta z)} - 2e^{\beta z} + e^{\beta (z+\Delta z)} \right] \tag{4.42}
\]

\[
C_{T\psi} \frac{\xi^{'}}{\Delta t} e^{\beta z} + C_{T T} \frac{\tau^{'}}{\Delta t} e^{\beta z} = K_{T\psi} \frac{\xi}{\Delta z^2} \left[ e^{\beta (z-\Delta z)} - 2e^{\beta z} + e^{\beta (z+\Delta z)} \right] + K_{T T} \frac{\tau}{\Delta z^2} \left[ e^{\beta (z-\Delta z)} - 2e^{\beta z} + e^{\beta (z+\Delta z)} \right] \tag{4.43}
\]
where $\xi'$ and $\tau'$ (updated functions of $\xi$ and $\tau$ which were introduced in Eqs. 4.40 and 4.41) are substituted for $\xi_{i+1}^*$ and $\tau_{i+1}^*$, respectively. The following relationship is used to simplify Eqs. 4.42 and 4.43:

$$\cos(\beta \Delta z) = \frac{e^{\beta \Delta z} + e^{-\beta \Delta z}}{2}$$  \tag{4.44}$$

Therefore, Eqs. 4.42 and 4.43 reduce to:

$$C_{vv} \frac{\xi' - \xi}{\Delta t} + C_{vr} \frac{\tau' - \tau}{\Delta t} = K_{vv} \frac{2\xi [\cos(\beta \Delta z) - 1]}{\Delta z^2}$$
$$+ K_{vr} \frac{2\tau [\cos(\beta \Delta z) - 1]}{\Delta z^2}$$  \tag{4.45}$$

$$C_{rv} \frac{\xi' - \xi}{\Delta t} + C_{rr} \frac{\tau' - \tau}{\Delta t} = K_{rv} \frac{2\xi [\cos(\beta \Delta z) - 1]}{\Delta z^2}$$
$$+ K_{rr} \frac{2\tau [\cos(\beta \Delta z) - 1]}{\Delta z^2}$$  \tag{4.46}$$

Solving for $\xi'$ and $\tau'$ leads to:

$$\xi' = \left\{ \frac{C_{vr} C_{rv} - C_{vv} C_{rr} + 2\lambda (C_{vr} K_{rv} - C_{rr} K_{vv}) [\cos(\beta \Delta z) - 1]}{C_{vr} C_{rv} - C_{vv} C_{rr}} \right\} \xi$$
$$+ \left\{ \frac{2\lambda (C_{vr} K_{rr} - K_{rr} C_{vv}) [\cos(\beta \Delta z) - 1]}{C_{vr} C_{rv} - C_{vv} C_{rr}} \right\} \tau$$  \tag{4.47}$$
\[
\tau = \left( \frac{2\lambda (K_{vv} C_{Tv} - C_{vv} K_{Tv})[\cos(\beta \Delta Z) - 1]}{C_{vr} C_{Tv} - C_{vv} C_{rr}} \right) \xi \\
+ \left( \frac{C_{vr} C_{Tv} - C_{vv} C_{rr} + 2\lambda (K_{vr} C_{Tv} - C_{vv} K_{rr})[\cos(\beta \Delta Z) - 1]}{C_{vr} C_{Tv} - C_{vv} C_{rr}} \right) \tau
\]  

(4.48)

Equations 4.47 and 4.48 can be written in matrix form:

\[
\begin{bmatrix}
\xi \\
\tau
\end{bmatrix} = 
\begin{bmatrix}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{bmatrix}
\begin{bmatrix}
\xi \\
\tau
\end{bmatrix}
\]  

(4.49)

where \(a_{11}, a_{12}, a_{21}, \text{ and } a_{22}\) are corresponding coefficients of \(\xi\) and \(\tau\) from Eqs. 4.47 and 4.48. For stability, the eigen-values \(a_{11}\) and \(a_{22}\) must not exceed unity. Hence, the stability conditions are:

\[|a_{11}| \leq 1 \quad \text{and} \quad |a_{22}| \leq 1\]

Substituting the corresponding coefficients for \(a_{11}\) and \(a_{22}\) from Eqs. 4.47 and 4.48 results in the following inequalities:

\[
\left| 1 + \frac{2\lambda (C_{vr} K_{Tv} - C_{rr} K_{vv})[\cos(\beta \Delta Z) - 1]}{C_{vr} C_{Tv} - C_{vv} C_{rr}} \right| \leq 1
\]  

(4.50)
\[
1 + \left\{ \frac{2\lambda (K_{vt} C_{tv} - C_{vv} K_{TT}) [\cos(\beta \Delta z) - 1]}{C_{vt} C_{tv} - C_{vv} C_{TT}} \right\} \leq 1
\] (4.51)

In inequalities 4.50 and 4.51 the worst possible case occurs when \(\cos(\beta \Delta z) = -1\) leading to the following inequalities:

\[
1 - \frac{4\lambda (C_{vt} K_{tv} - C_{TT} K_{vv})}{C_{vt} C_{tv} - C_{vv} C_{TT}} \leq 1
\] (4.52)

\[
1 - \frac{4\lambda (K_{vt} C_{tv} - C_{vv} K_{TT})}{C_{vt} C_{tv} - C_{vv} C_{TT}} \leq 1
\] (4.53)

The most negative allowable value for the inequalities is -1, thus, the stability conditions for the governing numerical equations of coupled heat and mass transfer developed in Eqs. 4.36 and 4.37 are:

\[
\lambda \leq \frac{C_{vt} C_{tv} - C_{vv} C_{TT}}{2(C_{vt} K_{tv} - C_{TT} K_{vv})}
\] (4.54)

\[
\lambda \leq \frac{C_{vt} C_{tv} - C_{vv} C_{TT}}{2(K_{vt} C_{tv} - C_{vv} K_{TT})}
\] (4.55)
Substituting for \( \lambda = \frac{\Delta t}{\Delta z^2} \) into inequalities 4.54 and 4.55, the following inequalities for the maximum permissible time step must both be satisfied:

\[
\Delta t \leq \frac{\Delta z^2 \left( C_{\nu T} C_{\nu T} - C_{\nu \nu} C_{\nu \nu} \right)}{2 \left( C_{\nu T} K_{\nu T} - C_{\nu \nu} K_{\nu \nu} \right)}
\]  
(4.56)

and,

\[
\Delta t \leq \frac{\Delta z^2 \left( C_{\nu \nu} C_{\nu \nu} - C_{\nu \nu} C_{\nu \nu} \right)}{2 \left( K_{\nu T} C_{\nu T} - C_{\nu \nu} K_{\nu \nu} \right)}
\]  
(4.57)

Inequalities 4.56 and 4.57 imply that the maximum permissible time step is itself variable. However, with the help of inequalities 4.56 and 4.57, the permissible time step can always be checked during the computation if necessary.

### 4.6 Computer Programming

The volume of computational operations involved in solving Eqs. 4.36 and 4.37 with corresponding boundary conditions, makes the use of computer programming unavoidable.

For this study, a program was written in FORTRAN 77 language (Appendix C). The code is not intended for a general application of the derived governing equations, but
rather for the specific conditions applied. Since soil parameters in each layer differ from those of the adjacent layers, generalization of the code to include all these changes is left for future studies.

For this study, a 7 mm distance between nodes was used. This spacing ensures at least 4 nodes in each 30 mm thick layer and that none of the nodes lies on the inter-layer boundaries (Fig. 4.3). Continuity of pressure and temperature throughout the soil column assures the smooth transition of these two variables from one layer to another.

![Diagram showing grid spacing between layers.](image)

**Fig. 4.3 Schematic diagram of the grid spacing.**
CHAPTER FIVE
PARAMETER ESTIMATION

Equations 4.22 and 4.27 contain several parameters related to soil hydraulic and thermal properties. These parameters have to be determined to make the solution of the coupled heat and mass transfer equations possible. There are two approaches to determine these parameters: parameter estimation using a statistical non-linear regression analysis or sum of square method, and experimental or semi-empirical values preferably in the form of closed-form functions (Whitaker and Chou 1983). Both statistical and semi-empirical methods were used.

5.1 Estimation of Soil Hydraulic Properties

For mathematical simulation of soil drying, knowledge of hydraulic properties of the medium is essential. The natural spatial variability of these properties requires intensive sampling within the soil volume of interest. In this regard, laboratory experiments along with functions for the soil-water characteristic curve, saturated and unsaturated hydraulic conductivities and vapor diffusivity are of prime importance. Closed-form expressions for
hydraulic functions of soil, in particular, can be useful in modeling and predicting the mass transport in the soil media.

5.1.1 Soil-water characteristic curves

Experimental and theoretical studies have indicated that the soil-water characteristic or moisture retention curve can be used to describe hydraulic properties of an unsaturated soil (Fredlund and Xing 1994). The shape of the curve depends on the parent materials, pore size distribution and soil texture. The relationship also exhibits hysteresis in drying and wetting cycles.

Three different pressure plates were used for obtaining data for the soil-water characteristic curve: (1) for pressures up to 30.6 m (300 kPa), an acrylic pressure cell made by Engineering Shops at the University of Saskatchewan was used (Fig. 5.1); (2) for pressures of 40.8 m (400 kPa) and 60 m (500 kPa) a null pressure plate, University of Saskatchewan design (Fig. 5.2), and, (3) a Pressure Membrane Extractor (Soil Moisture Equipment, Santa Barbara, CA) for 102 m (1000 kPa) and 153 m (1500 kPa) pressures (Fig. 5.3). Ceramic porous plates were used in the first two pressure cells, and cellulose membrane disks were used in the Pressure Extractor Membrane.

In a layered soil profile, one would expect different soil-water characteristic relations for different layers, due to the different bulk densities. There can be two approaches to describing the volumetric water content-pressure (θ-ψ) of a stratified profiles. One is to consider each stratum as a homogeneous layer to which is assigned a specific soil-water characteristic curve (Willis 1960). Alternatively, a weighting procedure can be used to computationally homogenize the properties in each layer.
Fig. 5.1 Acrylic pressure cell, University of Saskatchewan design.
Fig. 5.2 Metal null pressure plate, University of Saskatchewan design.
Fig. 5.3 Pressure Membrane Extractor (Soil Moisture Equipment, Santa Barbara, CA).
(Constantz 1995). Since the layers were prepared so as to achieve a uniform bulk density within each layer, the first approach was followed.

Bulk density affects the available water capacity of a soil (Archer and Smith 1972; Reeve et al. 1973). The effect of bulk density is usually more influential in the lower suction range and tends to attenuate at higher suctions (Warkentin 1971). Therefore, water contents at 102 m and 153 m pressures were determined using sieved (<2 mm), loose samples of soil, while for other pressures, soil samples were compacted to the specified bulk densities.

One of the frequently used equations for the soil-water characteristic curve is that of van Genuchten (1980) whose work is based on pore size distribution theory of Mualem (1976). Van Genuchten's (1980) model can be written as:

\[
\theta = \theta_r + \frac{\theta_s - \theta_r}{1 + |\alpha\psi|^{n}}^{m} \quad (\theta_r \leq \theta \leq \theta_s)
\]  

(5.1)

where:

\(\theta_r\) = residual volumetric water content (m\(^3\)/m\(^3\)),

\(\theta_s\) = saturated volumetric water content (m\(^3\)/m\(^3\)),

\(\psi\) = pressure or suction (m),

\(m = 1 - 1/n\),

\(\alpha\) and \(n\) = fitting parameters.
Campbell et al. (1993) presented a one-parameter equation for the soil-water characteristic curve. Lack of flexibility of the equation, due to only one parameter being involved, limits its use to a narrow range of soils. Fredlund and Xing (1994) derived very similar equations to that of van Genuchten (1980) and illustrated the effect of varying the three parameters on the shape of the soil-water characteristic curve. Since the suction for the oven-dry soil is around 102,000 m (10^6 kPa) (Ross et al. 1991) and is essentially the same for different types of soils, Fredlund and Xing (1994) introduced a correction function to force the soil-water characteristic curve to zero at a suction of 102,000 m. For the purpose of this study, there is no need to go beyond the residual water content, hence, Eq. 5.1 was considered satisfactory for representing the soil-water characteristic curve.

The parameters \( m \), \( n \) and \( \alpha \) in van Genuchten's (1980) equation were estimated using SAS non-linear estimation program (SAS Institute, Cary, NC) for data obtained from the pressure-water content measurements corresponding to the bulk densities for each layer.

Although \( \theta_r \) and \( \theta_s \) can also be estimated from Eq. 5.1, it is better to minimize the number of parameters determined in this way to maximize available degrees of freedom. Mualem (1976) proposed a method to extrapolate \( \theta_s \), but the method doesn't always give reliable values (the author of this study even determined negative values for residual water content using Mualem's method). Residual water content \( \theta_r \) can be determined as the water content at the air-dried state of the soil (van Genuchten 1980) which has more physical meaning than just a fitting parameter. The natural saturated water content \( \theta_s \) can be readily determined using standard methods (Klute 1986). In this study, prepared
samples in specified bulk densities were soaked in distilled water to saturate overnight and tested the next day. The results are shown in Table 5.1.

<table>
<thead>
<tr>
<th>Bulk density (Mg/m³)</th>
<th>θ_r (m³/m³)</th>
<th>θ_s (m³/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.95</td>
<td>0.038</td>
<td>0.686</td>
</tr>
<tr>
<td>1.15</td>
<td>0.046*</td>
<td>0.608</td>
</tr>
<tr>
<td>1.35</td>
<td>0.054*</td>
<td>0.567</td>
</tr>
</tbody>
</table>

* Calculated based on the residual water content for 0.95 Mg/m³ bulk density

Figure 5.4 shows the soil-water characteristic curves for different bulk densities according to the experimental data. Fitted curves up to the last experimental datum using Eq. 5.1 with corresponding values for parameters α, m and n are also shown on the same figure. As the soil dries, the soil water pressure is likely to exceed the range of pressures found for the soil-water characteristic curve by experiment, hence, extrapolation will be necessary.

In this study, there can be two main sources of error in determining the soil-water characteristic curves for different soil bulk densities. Soil samples were all prepared (except for 102 m and 153 m pressures) at different bulk densities at 28% water content (corresponding to the optimum dry bulk density) and then allowed to saturate. Therefore, desorption curves may not follow the same trend as the sorption curves (hysteresis phenomenon) in other IWC's. Also, using different equipment for different pressure
Fig. 5.4 Soil-water characteristic curves. $L = 0.95 \text{ Mg/m}^3$; $B = 1.15 \text{ Mg/m}^3$; $D = 1.35 \text{ Mg/m}^3$.

(markers are measured data and lines are fitted curves using Eq. 5.1).
ranges and combining the results could introduce considerable amount of error. Figure 5.4 clearly shows resulting shifts in data at the corresponding ranges of pressure for different equipment. Besides, natural variability of structure of remolded soil samples will also introduce variation in results.

The parameters in Eq. 5.1, span pressure (suction) well beyond the experimental data. Tables 5.2 to 5.4 show the results of the non-linear parameter estimation using soil-water characteristic data for corresponding bulk densities.

While running the SAS program, the solution was found to be very sensitive to the initial assigned values for the parameters. This could be due to the low number of data points obtained from soil-water characteristic data compared to the number of parameters. The solution was even sensitive to the non-linear method itself. The Steepest Descent method gave better results in terms of convergence and lower sum of squares than Marquardt or Gauss methods.

The results for the loose soil (0.95 Mg/m³) show the highest mean square which means the variability of data around the fitted curve is larger. This was expected since soil aggregates in loose state have more space to arrange themselves during soil preparation in switching from one pressure plate apparatus to another. The best result was obtained for the dense soil (1.35 Mg/m³) which showed very small change in the trend of its soil-water characteristic curve (Fig. 5.4). As opposed to soil in the loose state, soil particles in the dense state have less space to move around, giving a more uniform structure each time the soil samples are prepared.
Table 5.2 Summary statistics for non-linear parameter estimation for soil-water characteristic curve parameters $m$, $n$ and $\alpha$ for “loose” soil (0.95 Mg/m$^3$)

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>SS</th>
<th>MS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
<td>3</td>
<td>1.78</td>
<td>0.594</td>
</tr>
<tr>
<td>Residual</td>
<td>9</td>
<td>0.007</td>
<td>0.001</td>
</tr>
<tr>
<td>Uncorrected total</td>
<td>12</td>
<td>1.79</td>
<td></td>
</tr>
<tr>
<td>Corrected total</td>
<td>11</td>
<td>0.180</td>
<td></td>
</tr>
</tbody>
</table>

DF = degrees of freedom  SS = sum of squares  MS = mean square

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Estimate</th>
<th>SE</th>
<th>Lower limit*</th>
<th>Upper limit*</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>11.0</td>
<td>36.0</td>
<td>-70.5</td>
<td>92.4</td>
</tr>
<tr>
<td>$n$</td>
<td>1.15</td>
<td>0.02</td>
<td>1.11</td>
<td>1.20</td>
</tr>
<tr>
<td>$m$</td>
<td>0.133</td>
<td>0.015</td>
<td>0.098</td>
<td>0.167</td>
</tr>
</tbody>
</table>

* at 95% confidence interval  SE = standard error

Table 5.3 Summary statistics for non-linear parameter estimation for soil-water characteristic curve parameters $m$, $n$ and $\alpha$ for “uniform” soil (1.15 Mg/m$^3$)

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>SS</th>
<th>MS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
<td>3</td>
<td>2.05</td>
<td>0.685</td>
</tr>
<tr>
<td>Residual</td>
<td>9</td>
<td>0.004</td>
<td>0.000</td>
</tr>
<tr>
<td>Uncorrected total</td>
<td>12</td>
<td>2.06</td>
<td></td>
</tr>
<tr>
<td>Corrected total</td>
<td>11</td>
<td>0.103</td>
<td></td>
</tr>
</tbody>
</table>

DF = degrees of freedom  SS = sum of squares  MS = mean square

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Estimate</th>
<th>SE</th>
<th>Lower limit*</th>
<th>Upper limit*</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>2.94</td>
<td>4.31</td>
<td>-6.81</td>
<td>12.7</td>
</tr>
<tr>
<td>$n$</td>
<td>1.13</td>
<td>0.038</td>
<td>1.047</td>
<td>1.22</td>
</tr>
<tr>
<td>$m$</td>
<td>0.117</td>
<td>0.024</td>
<td>0.064</td>
<td>0.171</td>
</tr>
</tbody>
</table>

* at 95% confidence interval  SE = standard error

91
Table 5.4 Summary statistics for non-linear parameter estimation for parameters \( m \), \( n \) and \( \alpha \) for "dense" soil (1.35 Mg/m\(^3\))

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>SS</th>
<th>MS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
<td>3</td>
<td>2.44</td>
<td>0.813</td>
</tr>
<tr>
<td>Residual</td>
<td>9</td>
<td>0.001</td>
<td>0.000</td>
</tr>
<tr>
<td>Uncorrected total</td>
<td>12</td>
<td>2.44</td>
<td></td>
</tr>
<tr>
<td>Corrected total</td>
<td>11</td>
<td>0.063</td>
<td></td>
</tr>
</tbody>
</table>

DF = degrees of freedom  SS = sum of squares  MS = mean square

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Estimate</th>
<th>SE</th>
<th>Lower limit*</th>
<th>Upper limit*</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha )</td>
<td>0.264</td>
<td>0.107</td>
<td>0.021</td>
<td>0.507</td>
</tr>
<tr>
<td>( n )</td>
<td>1.17</td>
<td>0.023</td>
<td>1.12</td>
<td>1.23</td>
</tr>
<tr>
<td>( m )</td>
<td>0.147</td>
<td>0.017</td>
<td>0.109</td>
<td>0.186</td>
</tr>
</tbody>
</table>

* at 95% confidence interval  SE = standard error

In Eq. 5.1, \( \theta_r \) and \( \theta_s \) can also be considered as independent parameters and estimated using the non-linear estimation procedure. Due to the high number of parameters and limited number of data points, empirically determined residual and saturated water contents (presented in Table 5.1) were treated as known parameters.

Variability of parameters \( m \) and \( n \) was found to be small compared to changes in \( \alpha \) for different bulk densities (Tables 5.2-5.4). Figure 5.5 is the graphical representation of the extrapolated soil-water characteristic curves for the different bulk densities. Since water pressure ranges from 0.01 to 10000 m, curves were plotted against a logarithmic scale. Figure 5.5 shows a common point around 0.2 m pressure at which all soil water-pressure functions give the same volumetric water content. At high suctions, three curves
tend to move closer to each other implying that the influence of soil structure on soil-water characteristic curve decreases as the soil dries out.

5.1.2 Saturated hydraulic conductivity

Saturated hydraulic conductivity is an index which describes the “ease” or “ability” of a saturated porous medium to transmit water (Reynolds 1993). Its determination is essential since it is usually an integral part of an unsaturated hydraulic conductivity function.

There are two common methods for determining saturated hydraulic conductivity (Klute and Dirksen 1986; Reynolds 1993); namely, falling head and constant head methods. The saturated hydraulic conductivities for 1.15 and 1.35 Mg/m³ bulk densities were determined using the falling head method (Fig. 5.6). Due to very fast falling of the head, the constant head method was used in the soil columns with 0.95 Mg/m³ bulk density. The experimental setup for constant head method is the same as that shown in Fig. 4.8 except that input and output water flows were regulated using adjustable valves to give a constant head.

Saturated hydraulic conductivities for different bulk densities were determined as:

\[ K_s = 2.66 \times 10^{-6} \, \text{m/s} \] for 0.95 Mg/m³ bulk density

\[ K_s = 1.00 \times 10^{-7} \, \text{m/s} \] for 1.15 Mg/m³ bulk density

\[ K_s = 6.23 \times 10^{-9} \, \text{m/s} \] for 1.35 Mg/m³ bulk density
Fig. 5.5 Closed form functions for volumetric water content vs water pressure.

L, B and D represent 0.95, 1.15 and 1.35 Mg/m³ bulk densities, respectively.
Fig. 5.6 Schematic diagram of the falling head method for measuring saturated hydraulic conductivity (Klute and Dirksen 1986).
5.1.3 Unsaturated hydraulic conductivity

Without doubt, hydraulic conductivity is the most influential parameter in any coupled heat and mass transfer governing equations. During a wetting or drying process, soil undergoes physical changes in its structure which are not reflected in any available closed form hydraulic conductivity function. It is clear that water plays an important role in binding layers of the soil column. This was more evident when the initial water content was low. At the end of each experiment, while emptying the containers, separation of top layers of dissimilar bulk densities in samples with lower IWC was evident. This discontinuity of conductive pores can dramatically change the hydraulic conductivity of a soil column.

The saturated hydraulic conductivity for a particular soil is fairly constant with time; however, in unsaturated state, hydraulic conductivity changes dramatically and can vary by several orders of magnitude. Both soil and fluid characteristics contribute to a change in hydraulic conductivity. The characteristics of soil which affect hydraulic conductivity are the porosity, pore size distribution and tortuosity, and that of fluid are density and viscosity (Hillel 1982).

For simulation models, a closed form relationship for unsaturated hydraulic conductivity is preferred. One of the most frequently used models in this regard is that of Mualem-van Genuchten (Mualem 1976; van Genuchten 1980). In this model, the unsaturated hydraulic conductivity function estimated from the soil-water characteristic and the saturated hydraulic conductivity. De Jong (1993) describes Mualem-van Genuchten’s model as a standard procedure for determining the unsaturated hydraulic
conductivity function. When the van Genuchten (1980) equation for the soil-water characteristic is used, the unsaturated hydraulic conductivity as a function of pressure (suction) can be written as:

\[ K = K_s \left( \frac{(1+|\alpha \psi|^n)^m - |\alpha \psi|^{n-1}}{[1+|\alpha \psi|^{m(L_o+2)}]} \right) \]  \hspace{1cm} (5.2)

where \( K_s \) is the saturated hydraulic conductivity (m/s) and \( \alpha, m \) and \( n \) are the same parameters as in Eq. 5.1. The only new parameter is the coefficient \( L_o \) (dimensionless) for which Mualem (1976) conducted an analysis of over 45 soil hydraulic data sets and reported an average value of about 0.5.

Despite the popularity of Eq. 5.2, its validity may not hold for all circumstances (Khaleel and Relyea 1995). Using Eq. 5.2, the author of this thesis found some strange results (increasing hydraulic conductivity with suction in a certain range), which had no physical meaning.

Brutsaert (1967) presents a very simple and attractive model which was first attributed to Blake (1922) (cited in Brutsaert 1967). The equation is of form:

\[ K_r = S_e^a \]  \hspace{1cm} (5.3)

where \( S_e \) is called the “effective saturation”, defined as:
\[ S_e = \frac{\theta - \theta_s}{\theta - \theta_r} \] (5.4)

and \( K_r \) is termed the "relative hydraulic conductivity", defined as:

\[ K_r = \frac{K}{K_r} \] (5.5)

Zhang and van Genuchten (1994), after proposing new models for unsaturated hydraulic conductivity, still recommended the use of Eq. 5.3 along with some other options. For this study, Eq. 5.1 and Eqs. 5.3-5.5 were combined to fully describe the unsaturated hydraulic conductivity function. The final form for the hydraulic conductivity function for each distinctive layer reads as:

\[ K = K_r \left[ \frac{1}{(1 + |\alpha \psi|^a)^n} \right]^a \] (5.6)

In general, \( a \) takes values from 3 to 3.5 for sands, 3.5 to 5 for loams and 5 to 8 for clays, but values more than 24 are also reported in the literature (Mualem 1986). Since the soil type in this study was clay, the value for \( a \) was expected to be in the high range. The recommended range of 5-8 (Mualem 1986) for \( a \) was found to produce unreasonable results regarding the equilibrium pressure of the soil water to the imposed boundary
conditions. For instance, by substituting a value of 8 for $a$ in Eq. 5.6, the heat and mass
transfer equations predicted an equilibrium state for the entire soil column to the boundary
conditions (i.e., pressures in all layers equilibrated with the pressure imposed at the
boundary) after 12 hours. This was opposed to that of experimental data shown in Figs.
3.5-3.11.

Parameter $a$ was estimated by using the sum of square of residuals method. Results
are shown in Tables 5.5 and 5.6. Parameter $a$ was found to be considerably higher for the
top 30 mm layer than for the deeper horizons. Therefore, parameter $a$ was determined for
1.15 Mg/m$^3$ bulk density at different IWCs excluding the first 30 mm. The first 24-hour
data were excluded to avoid the data related to the equilibrium time of the mini-gypsum
blocks. For loose and dense layers, the results for LB and DB configurations were used.

Plots of the final predicted hydraulic conductivity functions for the three soil
structures are shown in Fig. 5.7. The figure shows that at pressures (suctions) near 1 m, all
functions predict almost the same hydraulic conductivity, while at very high pressures
loose and dense states of soil tend to the same hydraulic conductivity. Figure 5.7 also
shows that the influence of saturated hydraulic conductivities is mostly at the beginning of
the drying process and as the drying front advances through the soil column, the overall
function becomes dominant rather than only the saturated hydraulic conductivity. This is
evident by comparing the corresponding functions of loose and dense states of the soil.
Table 5.5 Sum of square of residuals for determining optimum values of hydraulic conductivity function parameter $a$ at different depths and IWCs for 1.15 Mg/m$^3$ bulk density

<table>
<thead>
<tr>
<th>IWC (%)</th>
<th>Depth (mm)</th>
<th>Sum of square of residuals</th>
<th>$a = 15$</th>
<th>$a = 16$</th>
<th>$a = 17$</th>
<th>$a = 18$</th>
<th>$a = 19$</th>
<th>$a = 20$</th>
</tr>
</thead>
<tbody>
<tr>
<td>27.4</td>
<td>45</td>
<td></td>
<td>0.107</td>
<td>0.010</td>
<td>0.014</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>75</td>
<td></td>
<td>0.036</td>
<td>0.003</td>
<td>0.015</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>135</td>
<td></td>
<td>0.002</td>
<td>0.005</td>
<td>0.005</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td>0.145</td>
<td>0.018</td>
<td>0.034</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>31.8</td>
<td>45</td>
<td></td>
<td>0.052</td>
<td>0.001</td>
<td>0.031</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>75</td>
<td></td>
<td>0.011</td>
<td>0.009</td>
<td>0.030</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>135</td>
<td></td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td>0.063</td>
<td>0.010</td>
<td>0.061</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>36.6</td>
<td>45</td>
<td></td>
<td>0.051</td>
<td>0.001</td>
<td>0.022</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>75</td>
<td></td>
<td>0.072</td>
<td>0.012</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>135</td>
<td></td>
<td>0.000</td>
<td>0.003</td>
<td>0.007</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td>0.123</td>
<td>0.016</td>
<td>0.029</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Shaded area is used to highlight the minimum sum of square of residuals.
Table 5.6 Sum of square of residuals for determining optimum values of hydraulic conductivity function parameter $a$ at 15 mm depth and different IWCs for 0.95 Mg/m$^3$ and 1.35 Mg/m$^3$ bulk densities

<table>
<thead>
<tr>
<th>IWC (%)</th>
<th>Bulk density (Mg/m$^3$)</th>
<th>$a = 15$</th>
<th>$a = 16$</th>
<th>$a = 17$</th>
<th>$a = 18$</th>
</tr>
</thead>
<tbody>
<tr>
<td>27.4</td>
<td>0.95</td>
<td>0.097</td>
<td>0.088</td>
<td>0.093</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>1.35</td>
<td>*</td>
<td>0.037</td>
<td>0.016</td>
<td>0.023</td>
</tr>
<tr>
<td></td>
<td>$a = 17$</td>
<td>$a = 18$</td>
<td>$a = 19$</td>
<td>$a = 20$</td>
<td></td>
</tr>
<tr>
<td>31.8</td>
<td>0.95</td>
<td>0.046</td>
<td>0.017</td>
<td>0.021</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>1.35</td>
<td>*</td>
<td>0.052</td>
<td>0.0226</td>
<td>0.0227</td>
</tr>
<tr>
<td></td>
<td>$a = 18$</td>
<td>$a = 19$</td>
<td>$a = 20$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$a = 22$</td>
<td>$a = 23$</td>
<td>$a = 24$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>36.6</td>
<td>0.95</td>
<td>0.051</td>
<td>0.021</td>
<td>0.032</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>1.35</td>
<td>*</td>
<td>0.022</td>
<td>0.012</td>
<td>0.021</td>
</tr>
</tbody>
</table>

Shaded area is used to highlight the minimum sum of square of residuals.

5.1.4 Vapor diffusivity

Gases flow in porous media due to two major transport mechanisms: mass flow and diffusion. Gaseous diffusion is considered the most important process causing gaseous interchange between the soil and the atmosphere. Diffusion occurs in the air-filled pore space due to the presence of a pressure gradient such as evaporative conditions or temperature differences (Rolston 1986).
Fig. 5.7 Closed form functions for unsaturated hydraulic conductivity vs water pressure.

L, B and D represent 0.95, 1.15 and 1.35 Mg/m$^3$ bulk densities, respectively.
Experimental studies cited in the literature show that gas transport in the soil is directly proportional to a diffusion coefficient $D_{vp}$ and to the gas concentration gradient (Kirkham and Powers 1972). Therefore, determination of diffusivity coefficient is essential in predicting the vapor flux. Because of the difficulty involved in measurement of the diffusion coefficient of a soil, many studies have been undertaken to develop functions relating the diffusion coefficient to some easily measured soil properties. One of these properties is air porosity. Xu et al. (1992) concluded that the relationship between diffusion coefficient and air porosity is nearly the same regardless of soil type and soil water content. Many relationships for diffusion coefficient were reviewed by Glinski and Stepniewski (1985). Two different forms of equations are usually used to relate the diffusion coefficient to air porosity: linear and power functions. Troeh et al. (1982) combined the two types of equations to come up with the following model:

$$D_{vp} = D_e \left( \frac{\eta_a - u}{1 - u} \right)^v$$  \hspace{1cm} (5.7)

where:

$D_{vp} =$ diffusion coefficient (m$^2$/s),

$D_e =$ diffusion in a standard medium, $21.6 \times 10^{-6}$ (m$^2$/s),

$\eta_a =$ air porosity (m$^3$/m$^3$),

$u$ and $v =$ fitting parameters.
Troeh et al. (1982) applied the model to different sets of data available in the literature and found reasonable results. Xu et al. (1992) found that the model of Troeh et al. (1982) satisfactorily represented the diffusion coefficient for the types of soil in their study.

Troeh et al. (1982) used data reported by Ayres et al. (1972) for a wide range of Saskatchewan soils and found values of $u$ and $v$ in Eq. 5.7 of 0.03 and 1.5, respectively. The relationship for diffusion coefficient then becomes:

$$D_{\text{vap}} = D_* \left( \frac{n_a - 0.03}{1 - 0.03} \right)^{1.5}$$ \hspace{1cm} (5.8)

Parameter $u$ (= 0.03) in Eq. 5.7 represents isolated pore spaces that remain in the medium when diffusion ceases. This means that $u \leq n_a \leq 1$ and $0 \leq u \leq 1$ to have meaningful values for diffusion. Values of $n_a \leq u$ corresponds to $D_{\text{vap}} = 0$. Parameter $v$ (= 1.5) in Eq. 5.7 controls the curvature of the relationship and no value greater than 2 was found for this parameter in the literature (Troeh et al. 1982). Graphical representation of Eq. 5.8 is shown in Fig. 5.8. Non-linearity of vapor diffusivity and intersection of the graph with the x-axis rather than through the origin is clearly shown in the figure.

5.1.5 Saturated vapor density

The partial derivative $\partial \rho / \partial T$, which appears in both heat and mass transfer equations can be evaluated by differentiating the following closed-form equation for saturated vapor density with respect to temperature (Thomas and King 1992):

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Fig. 5.8 Vapor diffusivity vs air porosity

\[ \rho_e = 5.14 \times 10^{-3} \exp \left[ 0.064 (T - 273) - 0.163 \times 10^{-3} (T - 273)^2 \right] \]  \hspace{1cm} (5.9)

where \( T \) is in K.

5.2 Estimation of Soil Thermal Properties

In modeling heat and mass transfer in soils, a knowledge of thermal properties of the medium is also necessary. Thermal conductivity and volumetric heat capacity have strong
influences on soil thermal behavior. Both can be formulated on the basis of soil physical composition.

5.2.1 Soil volumetric heat capacity

The volumetric heat capacity \( C \, (J \cdot m^3 \cdot K^{-1}) \) is defined as the change in heat content of a unit bulk volume of soil per unit change in temperature (Hillel 1982). The definition implies that the composition of the soil and the volume fraction of its constituents come into account. Table 5.7 shows the density and volumetric heat capacities of different constituents of soils.

<table>
<thead>
<tr>
<th>Constituents</th>
<th>Density (Mg/m³)</th>
<th>Heat capacity (J \cdot m^{-3} \cdot K^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>2.66</td>
<td>( 2.13 \times 10^6 )</td>
</tr>
<tr>
<td>Other minerals (average)</td>
<td>2.65</td>
<td>( 2.39 \times 10^6 )</td>
</tr>
<tr>
<td>Organic matter</td>
<td>1.3</td>
<td>( 2.50 \times 10^6 )</td>
</tr>
<tr>
<td>Water (liquid)</td>
<td>1.0</td>
<td>( 4.18 \times 10^6 )</td>
</tr>
<tr>
<td>Ice</td>
<td>0.92</td>
<td>( 1.90 \times 10^6 )</td>
</tr>
<tr>
<td>Air</td>
<td>0.00125</td>
<td>( 1.26 \times 10^3 )</td>
</tr>
</tbody>
</table>

There are standard methods available to measure the heat capacity of a soil (Taylor and Jackson 1986), but since the volumetric heat capacity in an unsaturated medium
undergoing drying or wetting continuously changes, it is preferred to have a closed-form function to estimate its value as a function of varying water content. De Vries (1963) proposed a relationship for volumetric heat capacity of soils based on the constituents. This approach has become popular ever since. According to de Vries (1963) volumetric heat capacity can be expressed as:

\[ C = \sum \eta_i C_i + \eta_w C_w + \eta_a C_a \] (5.10)

where:

\( \eta_i \) = volume fraction of solid constituent \( i \) of the soil \( (m^3/m^3) \),

\( C_i \) = volumetric heat capacity of solid constituent \( i \) of the soil \( (J \cdot m^3 \cdot K^{-1}) \),

\( \eta_w \) = volume fraction of water or volumetric water content \( \theta \) \( (m^3/m^3) \),

\( C_w \) = volumetric heat capacity of water soil \( (J \cdot m^3 \cdot K^{-1}) \),

\( \eta_a \) = volume fraction of air \( (m^3/m^3) \),

\( C_a \) = volumetric heat capacity of air soil \( (J \cdot m^3 \cdot K^{-1}) \).

Table 5.7 shows that the contribution of water content determines the heat capacity to a large extent, whereas that of air is very small. For this reason the air component of heat capacity is usually neglected (Hillel 1982). The particle density for the soil used in this study was determined to be 2.72 Mg/m³ (Table 3.1) and the corresponding volumetric heat capacity becomes 2.45x10⁶ soil J/m³ K. Therefore, the equation for the volumetric heat capacity is:
\[ C = 2.45 \times 10^6 \eta_m + 2.5 \times 10^6 \eta_o + 4.18 \times 10^6 \eta_w \quad (5.11) \]

where \( \eta_m \) (m\(^3\)/m\(^3\)), \( \eta_o \) (m\(^3\)/m\(^3\)) and \( \eta_w \) (m\(^3\)/m\(^3\)) stand for volume fractions of minerals, organic matter and water, respectively.

In 100 g of dry soil sample, the volume of organic matter is 3.72 cm\(^3\) (= 4.83/1.3) and its volume ratio to that of solid matter becomes 0.096 m\(^3\)/m\(^3\). Hence, the volume fraction of the soil minerals in 100 g of dry soil becomes 1-0.096 = 0.904 m\(^3\)/m\(^3\). Equation 5.11 can therefore be written as:

\[ C = 2.45 \times 10^6 (1-\eta) \times 0.904 + 2.5 \times 10^6 (1-\eta) \times 0.096 + 4.18 \times 10^6 \eta_w \quad (5.12) \]

In Eq. 5.12, \( \eta_w \) is the same as volumetric water content \( \theta \) and is the only parameter that varies. Plots of Eq. 5.12 for different bulk densities are shown in Fig. 5.9. The steep slope of the curves shows the high influence of water. Also, denser soil show higher heat capacity since more soil minerals are present per unit volume of soil (or more air is expelled).

### 5.2.2 Soil thermal conductivity

Thermal conductivity \( k \) (W \( \cdot \) m\(^{-1}\) \( \cdot \) K\(^{-1}\)) is defined as the amount of heat transferred through a unit area in a unit time under a unit temperature gradient (Hillel 1982). Just as with heat
capacity, soil constituents play important role in determining the thermal conductivity.

Table 5.8 shows values of thermal conductivities for different soil constituents.

![Graph showing heat capacity vs water content](image)

**Fig. 5.9** Heat capacity vs water content. L, B and D stand for 0.95, 1.15 and 1.35 Mg/m³ bulk densities, respectively.

| Table 5.8 Thermal conductivities of soil constituents (Hillel 1982) |
|-----------------|------------------|
| Constituent     | W·m⁻¹·K⁻¹        |
| Quartz          | 8.8              |
| Other minerals (average) | 2.9             |
| Organic matter  | 0.25             |
| Water           | 0.57             |
| Ice             | 2.2              |
| Air             | 0.025            |

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Measuring methods are also available for thermal conductivity of soils (Jackson and Taylor 1986), but thermal conductivity varies with water content and closed-form equations are preferred for mathematical modeling.

Farouki (1986) presented an excellent review of the studies conducted on thermal conductivity of soils. After comparing many methods, Farouki (1986) recommended Johansen’s method (1975) (cited in Farouki 1986) which in turn was based on Kersten’s (1949) approach. Johansen’s method has been verified for unfrozen and frozen soils over a wide range of soil types, and degrees of saturation above 0.1; however, de Vries’ (1963) method was recommended for coarse soils and degrees of saturation between 0.1 and 0.2.

For the purpose of this study, Johansen’s (1975) model was used for the closed-form function representing the thermal conductivity of soils. In this model, the thermal conductivity of an unsaturated soil, \( k \), is expressed as a function of its thermal conductivity in a completely dry soil \( k_{\text{dry}} \), and in its saturated state \( k_{\text{sat}} \), at the same dry density. This is expressed by the Kersten normalized thermal conductivity \( K_e \):

\[
K_e = \frac{k - k_{\text{dry}}}{k_{\text{sat}} - k_{\text{dry}}} \tag{5.13}
\]

The thermal conductivity is thus an interpolation between the dry and saturated states. Rearranging Eq. 5.13 for thermal conductivity:

\[
k = (k_{\text{sat}} - k_{\text{dry}})K_e + k_{\text{dry}} \tag{5.14}
\]
For $k_{\text{dry}}$, Johansen (1975) derived a semi-empirical equation for natural soils. Substituting the corresponding value for particle density of the soil sample used in this study from Table 3.1, the relationship becomes:

$$k_{\text{dry}} = \frac{0.135 \rho_b - 64.7}{2720 - 0.947 \rho_b}, \quad (\text{W/m K}) \quad (5.15)$$

where the dry bulk density, $\rho_b$, is in kg/m$^3$. For $k_{\text{sat}}$, Johansen (1975) (cited in Farouki 1986) proposed the following function, which is the geometric mean of the thermal conductivities of the most important constituents of the soil:

$$k_{\text{sat}} = k_w^{\eta_w} k_q^{\eta_q} k_m^{\eta_m} \quad (5.16)$$

where $k_w$, $k_q$ and $k_m$ are the thermal conductivities, and $\eta_w$, $\eta_q$ and $\eta_m$ are volume fractions of water, quartz and other minerals, respectively.

Finally, the Kersten number for fine textured soils is defined as (Farouki 1986):

$$K_e = \log_{10} S + 10, \quad S > 0.1 \quad (5.17)$$

where $S$ is the degree of saturation. Equations 5.14-5.17 fully describe the thermal conductivity of an unsaturated fine-textured soil.
Using Eq. 5.15, thermal conductivities for dry soil were determined as 0.106, 0.135 and 0.171 W/m K for 0.95, 1.15 and 1.35 Mg/m$^3$ bulk densities, respectively. Using Eq. 5.16 thermal conductivities for saturated soil were found as 1.1, 1.3 and 1.42 W/m K for 0.95, 1.15 and 1.35 Mg/m$^3$ bulk densities, respectively. Using the percentage of quartz in the soil (Table 3.1), in 100 g of soil the volume of quartz and minerals are found to be as 16.2 cm$^3$ and 21.5 cm$^3$. The corresponding volume fraction of quartz and minerals are found as $(1-\eta) \times 0.43$ and $(1-\eta) \times 0.57$, respectively.

Using values of thermal conductivities for dry and saturated states and substituting in Eq. 5.14, the final closed form functions can be stated as:

$$k = 1.1 + 0.994 \times \log \left( \frac{\theta}{0.651} \right), \text{ for } 0.95 \text{ Mg/m}^3 \text{ bulk density} \quad (5.18)$$

$$k = 1.3 + 1.16 \times \log \left( \frac{\theta}{0.577} \right), \text{ for } 1.15 \text{ Mg/m}^3 \text{ bulk density} \quad (5.19)$$

$$k = 1.42 + 1.25 \times \log \left( \frac{\theta}{0.504} \right), \text{ for } 1.35 \text{ Mg/m}^3 \text{ bulk density} \quad (5.20)$$

The only parameter changing in Eqs. 5.18-5.20 is the volumetric water content. Thermal conductivities for different soil bulk densities are shown in Fig. 5.10. At a given water content, due to the low thermal conductivity of air, a more packed soil shows higher thermal conductivity than that of a loose soil.
Fig. 5.10 Thermal conductivity vs water content. L, B and D stand for 0.95, 1.15 and 1.35 Mg/m$^3$ bulk densities, respectively.

5.3 Temperature Dependence of Soil Hydraulic and Thermal Properties

Soil properties are influenced by temperature. The range of the temperature itself plays a major role in deciding whether or not the parameter should be modified. In Eqs. 4.22 and 4.27 many parameters are temperature dependent. Prior to solving these equations, proper adjustments should be applied.

The behavior of hydraulic properties is linked to the change of properties of water. These properties are believed to be the kinematic viscosity $\mu$ and the surface tension $\sigma$ (Hopmans and Dane 1985). The surface tension of the soil water decreases with increasing
temperature; as a result, a reduction of water content at a given pressure occurs (Klute 1986). Also, the increase in hydraulic conductivity at a given water content with increasing temperature is almost entirely related to the decrease in viscosity of water (Haridasan and Jensen 1972).

Thomas and King (1992) proposed the following relationships between the pressure and hydraulic conductivity:

\[
\psi(\theta, T) = \frac{\sigma(T)}{\sigma(T_r)} \psi_{\text{ref}}(\theta)
\]  

(5.21)

where:

\( \sigma(T) = \) surface tension at temperature \( T \) (J/m\(^2\)),

\( \sigma(T_r) = \) surface tension at reference temperature (J/m\(^2\)),

\( \psi_{\text{ref}}(\theta) = \) pressure at a reference temperature (m).

and,

\[
K(\theta, T) = \frac{\mu(T_r)}{\mu(T)} K_{\text{ref}}(\theta)
\]  

(5.22)

where:

\( \mu(T) = \) dynamic viscosity at temperature \( T \) (Ns/m\(^2\)),

\( \mu(T_r) = \) dynamic viscosity at reference temperature (Ns/m\(^2\)),

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\( K_{\text{ref}}(\theta) \) = hydraulic conductivity at reference temperature (m/s).

Equations for surface tension and dynamic viscosity are given as (Thomas and King 1992):

\[
\sigma (T) = 0.117 - 0.00015T
\]

(5.23)

\[
\mu (T) = 0.661 \times (T - 229)^{-1.56}
\]

(5.24)

where \( T \) is in K.

Ten Berge (1990) ignored the effect of temperature on both pressure and hydraulic conductivity, reasoning that the effects cancel out since \( \nabla \psi \) is multiplied by \( K \) in calculating the flux. This reasoning is not correct, since the change of surface tension with change in temperature is much less than the change in dynamic viscosity with the same temperature gradient. According to Eq. 5.23, a change from 278 K to 288 K leads to almost 2% change in surface tension, while the same temperature gradient contributes to almost 34% change in viscosity from Eq. 5.24. For this study, both pressure and hydraulic conductivity were adjusted for temperature according to Eqs. 5.21-5.22.

Vapor diffusivity is also affected by temperature. The following equation was provided by Pakowski et al. (1991) for diffusivity of water vapor in air for atmospheric pressure:
\[ D_s = 2.16 \times 10^{-6} \left( \frac{T}{273} \right)^{1.8} \] 

(5.25)

where \( T \) is in K. In this study, Eq. 5.25 was used in conjunction with Eq. 5.8 to adjust vapor diffusivity for temperature.

Thermal conductivity is also affected by changes in temperature (Sepaskhah and Boersma 1979). Kersten (1949) reported an average 4% change in thermal conductivity of 19 different soils with a temperature change from 278 K to 294 K. Since the dependence of thermal conductivity on temperature is relatively small, no adjustment was made for it in this study.
CHAPTER SIX

CORROBORATION OF COUPLED HEAT AND MASS TRANSFER MODEL

In this chapter, the comparison method is described. The simulation results are presented and measured and predicted values for temperature and water content are compared. Sensitivity of the model to hydraulic and thermal conductivities are tested. Also, the nature of the coupled heat and mass transfer governing equations is discussed.

6.1 Procedure for Comparing Numerical and Experimental Results

To compare theoretical and experimental results, a mean relative percentage deviation (MRPD) procedure was adopted (Yang and Cenkowski 1995). In this method, the sum of normalized absolute values of residuals are 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:

\[
MRPD = \frac{100}{N} \sum \frac{|y - y'|}{y}
\]  

(6.1)
where \( MRPD = \) mean relative percentage deviation,

\[ y = \text{measured value}, \]

\[ y' = \text{estimated value}, \]

\[ N = \text{number of observations}. \]

For evaluation of models by comparing estimated and measured values, this method quantifies the prediction error using a percentage value which is more familiar and easier to interpret than, say, sum-of-squares error number.

### 6.2 Numerical Results

Corresponding parameters estimated in chapter 5 were substituted in Eqs. 4.36 and 4.37. Time steps of up to 20 s in the computer program were used to produce stable solutions. Each run simulating a total time of 168 h with a time step of 20 s, took approximately 75-80 seconds of CPU time using a Pentium 90 MHz personal computer.

### 6.2.1 Predicted water content in different layers

Figures 6.1-6.4 show the predicted water content with time in simulations with IWC of 0.27 (Mg/Mg), corresponding to Figs. 3.5-3.8. Similar trends were found in simulations with other IWCs from which Figs. 6.5-6.6 are presented for IWC of 0.32 (Mg/Mg) corresponding to Figs. 3.9-3.10 and Fig. 6.7 is shown for 0.37 (Mg/Mg) IWC corresponding to Fig. 3.11. The rest are shown in Appendix B. The trends predicted by the model agree with the experimental
Fig. 6.1 Predicted variation of water content with time at 15 mm depth and IWC of 0.27 (Mg/Mg).

(note that LB and LDB are the same line).
Fig. 6.3 Predicted variation of water content with time at 75 mm depth and IWC of 0.27 (Mg/Mg).
Fig. 6.4 Predicted variation of water content with time at 135 mm depth and IWC of 0.27 (Mg/Mg).
Fig. 6.5 Predicted variation of water content with time at 15 mm depth and IWC of 0.37 (Mg/Mg),

(note that LB and LDB are the same line).
Fig. 6.6 Predicted variations of water content with time at 135 mm depth and IWC of 0.37 (Mg/Mg).
Fig. 6.7 Predicted variation of water content with time at 135 mm depth and IWC of 0.37 (Mg/Mg).
findings. Predicted variations of water content in the top (i.e., "loose") layer of LB and LDB configurations are coincident (Figs. 6.1 and 6.5). Occurrence of small bumps (see Figs. 6.1 and 6.5) were also predicted reflecting the effect of cyclic changes in the boundary conditions. Comparison of Figs. 6.4, 6.6 and 6.7 reveals that the model predicts negligible loss of moisture in the deeper horizons, with somewhat greater loss for the high IWC (Fig. 6.7)

Due to some shrinkage during drying, especially for the loose layer on top, separation of layers of dissimilar bulk densities could introduce a thin layer of air between adjacent layers (which is not included in the model). This could significantly influence the mass transfer rate.

6.2.2 Predicted temperature variations in different layers

To show how the model predicted the temperature throughout the soil column, the result for B configuration at IWC of 0.37 (Mg/Mg) is shown as an example in Fig 6.8. Since a constant temperature is assumed, the surface temperature (not shown) is represented only by a straight line during each period with a step change at corresponding cycles.

No difference in predicted temperatures was observed between different layering configurations at any depth and IWC. Figure 6.9 shows the result of simulated temperature variation at 75 mm depth and IWC of 0.27 (Mg/Mg). Similar graphs were obtained for other IWCs.
Fig. 6.9 Predicted temperature variation with time at 75 mm depth and IWC of 0.27 (Mg/Mg).
6.3 Comparison of Water Content Predictions

To compare the experimental (average of 3 replicates) and numerical results, the mean relative percentage deviation method described above was used. The results are shown in Table 6.1. Over the entire time, data for the first 24 hours were excluded to avoid the rising measured water contents.

Deviation of measured and predicted values is reflected in the MRPDs presented in Table 6.1. There are a number of reasons for this deviation. For example, estimated parameters, the occurrence of random cracks in the surface layer during drying, separation of the top layer after drying, hysteresis effect in mini-gypsum blocks and the assumed boundary conditions are among the most possible reasons for this deviation. In solving the heat and mass transfer equations, Dirichlet type boundary conditions were assumed. Luikov (1964) suggested a boundary condition of saturated vapor pressure and wet bulb temperature for the surface of a porous body undergoing a drying process. Since the measured surface temperatures were close to that of the environment, surface temperature was equated to ambient temperature in the calculations. This introduces a source of error since the true surface temperature and thus relative humidity would be different from that of the environment.

Better results may be achieved by measuring the surface relative humidity along with surface temperature and assuming a convection surface (third type) condition (Incropera and Dewitt 1990). Keeping in mind that measuring the surface temperature and relative humidity of soils are extremely difficult, simplifying assumptions are always preferred, hence, one can expect differences in theoretical and experimental results.
Table 6.1 Mean relative percentage deviation for water content prediction for different layering configurations with different IWCs, using averaged experimental data

<table>
<thead>
<tr>
<th>IWC (Mg/Mg)</th>
<th>LYR</th>
<th>MRPD (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>15 (mm)</td>
<td>45 (mm)</td>
</tr>
<tr>
<td>0.27</td>
<td>B</td>
<td>10.7</td>
</tr>
<tr>
<td></td>
<td>LB</td>
<td>15.3</td>
</tr>
<tr>
<td></td>
<td>DB</td>
<td>4.65</td>
</tr>
<tr>
<td></td>
<td>LDB</td>
<td>15.1</td>
</tr>
<tr>
<td>0.32</td>
<td>B</td>
<td>8.07</td>
</tr>
<tr>
<td></td>
<td>LB</td>
<td>4.64</td>
</tr>
<tr>
<td></td>
<td>DB</td>
<td>4.27</td>
</tr>
<tr>
<td></td>
<td>LDB</td>
<td>6.21</td>
</tr>
<tr>
<td>0.37</td>
<td>B</td>
<td>19.9</td>
</tr>
<tr>
<td></td>
<td>LB</td>
<td>4.6</td>
</tr>
<tr>
<td></td>
<td>DB</td>
<td>2.96</td>
</tr>
<tr>
<td></td>
<td>LDB</td>
<td>3.94</td>
</tr>
</tbody>
</table>

\(y_{\text{me}}\) = measured value; \(y'_{\text{me}}\) = predicted value; \(N\) = number of observations; LYR = layering configuration
Another explanation for the disagreement between theoretical and experimental results is the preparation of the soil columns in thin layers. Each 30 mm layer is prepared in two 15 mm layers where each layer is a separate layer. As a result, each layer may have different pore size distribution leading to a different hydraulic behavior. Layers may become more distinctive if IWC is low (insufficient binding agent to stick layers together). Higher deviation in the upper 30 mm depth of B configuration in any IWC (Table 6.1) is due to the fact that in estimating parameter \( a \) in Eq. 5.6, the first layer was excluded to get better results for other depths. However, the overall average of the percentage deviation in all different layering configurations is relatively low which means that the model prediction of the water content is acceptable.

Another source of discrepancy between numerical and experimental results is the assumption of one-dimensional flow in the soil media. Shrinkage of the soil especially at the top layer due to drying, left a gap of about 5 mm between the soil and the wall of the container. Seepage through the gap is another possibility which is not predicted by the derived governing equations. In this study, low overall percentage deviation from the experimental results justified the one-dimensional assumption of the mass flow.

Determination of parameters either experimentally or semi-empirically can also introduce a source of error. Estimated parameters using the regression analysis, become a lumped representative of all of these experimental errors and theoretical assumptions. No matter how accurate and mathematically sound the derived model is, its evaluation depends on the accuracy of the parameters involved.
As long as simplifying assumptions, extrapolations and sources of errors are involved, in a drying process, one can expect sometimes significant differences between experimental and theoretical results. The differences become more evident especially in a heterogeneous shrinkable medium with random occurrence of cracks on the surface.

As examples, Figs. 6.10 and 6.11 are presented to show the comparison between predicted and measured values of water content at 45 mm depth and IWC of 0.27 (Mg/Mg) and 0.37 (Mg/Mg), respectively. As can be seen from figures, considerable amount of moisture was lost from the layer while the mini-gypsum block was equilibrating with the medium. Lower MRPD value for the B configuration at 45 mm depth and IWC of 0.32 (Mg/Mg) (Table 6.1) is reflected in the closer graphs in Fig. 6.11 compared to that of Fig. 6.10.

6.4 Comparison of Moisture Conservation Predictions

The procedure outlined as in section 3.6.2 is followed to find the predicted moisture conservation after the end of the experiment. Table 6.2 presents predicted normalized volume of water as well as the experimental mean normalized values taken from Table 3.4.

All layering configurations give higher values for predicted normalized volume of water for all IWCs with respect to the no-layering or B configuration. The result is somehow different for the measured values especially for 0.32 (Mg/Mg) and 0.37 (Mg/Mg) IWC's. This is mostly due to the soil shrinkage and occurrence of cracks especially in higher initial water contents.
Fig. 6.10 Comparison between measured and predicted water contents in B configuration at 45 mm depth and IWC of 0.27 (Mg/Mg). An MRPD value of 3.29% was obtained.
Fig 6.11 Comparison between measured and predicted water contents in B configuration at 45 mm depth and IWC of 0.32 (Mg/Mg). An MRPD value of 0.88% was obtained.
Table 6.2 Comparison between predicted and measured normalized volume of water remained at the end of the experiment

<table>
<thead>
<tr>
<th>IWC</th>
<th>Configuration</th>
<th>Normalized volume of water (m³/m³)</th>
<th>Measured</th>
<th>Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Mg/Mg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.27</td>
<td>B</td>
<td>0.924</td>
<td>0.924</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LB</td>
<td>0.963</td>
<td>0.954</td>
<td></td>
</tr>
<tr>
<td></td>
<td>DB</td>
<td>0.950</td>
<td>0.969</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LDB</td>
<td>0.953</td>
<td>0.954</td>
<td></td>
</tr>
<tr>
<td>0.32</td>
<td>B</td>
<td>0.922</td>
<td>0.931</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LB</td>
<td>0.940</td>
<td>0.964</td>
<td></td>
</tr>
<tr>
<td></td>
<td>DB</td>
<td>0.926</td>
<td>0.950</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LDB</td>
<td>0.928</td>
<td>0.948</td>
<td></td>
</tr>
<tr>
<td>0.37</td>
<td>B</td>
<td>0.907</td>
<td>0.875</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LB</td>
<td>0.901</td>
<td>0.917</td>
<td></td>
</tr>
<tr>
<td></td>
<td>DB</td>
<td>0.875</td>
<td>0.905</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LDB</td>
<td>0.899</td>
<td>0.907</td>
<td></td>
</tr>
</tbody>
</table>

6.5 Comparison of Temperature Predictions

Table 6.3 is the result of applying Eq. 6.1 to numerical and experimental temperature (average of 3 replicates) values. Data for the first 16 hours were excluded to avoid the variations in initial temperatures. As an example, Fig. 6.12 is presented to show the comparison between predicted and measured values in B configuration at 75 mm depth.
Table 6.3 Mean relative percentage deviation for temperature prediction for different layering configurations with different IWC, using averaged experimental data

| IWC (Mg/Mg) | LYR | \( \frac{\sum |y_T - y'_T|}{N} \times 100 \) | Average MRPD |
|-------------|-----|---------------------------------|--------------|
|             |     | 15 (mm) | 45 (mm) | 75 (mm) | 135 (mm) | (%) |
| 0.27        | B   | 0.978    | 0.797   | 0.461   | 0.346   | 0.646 |
|             | LB  | 0.872    | 0.769   | 0.434   | 0.326   | 0.600 |
|             | DB  | 1.02     | 0.843   | 0.482   | 0.350   | 0.674 |
|             | LDB | 0.925    | 0.758   | 0.441   | 0.330   | 0.619 |
| 0.32        | B   | 1.21     | 0.893   | 0.551   | 0.370   | 0.756 |
|             | LB  | 1.08     | 0.885   | 0.657   | 0.331   | 0.738 |
|             | DB  | 1.24     | 0.884   | 0.546   | 0.394   | 0.767 |
|             | LDB | 1.15     | 0.835   | 0.511   | 0.346   | 0.711 |
| 0.37        | B   | 1.14     | 0.925   | 0.586   | 0.417   | 0.767 |
|             | LB  | 0.996    | 0.833   | 0.530   | 0.416   | 0.694 |
|             | DB  | 1.08     | 0.881   | 0.583   | 0.487   | 0.758 |
|             | LDB | 1.04     | 0.873   | 0.554   | 0.426   | 0.723 |

\( y_T \) = measured value (K); \( y'_T \) = predicted value (K); \( N \) = number of observations; LYR = layering configuration
Fig. 6.12 Comparison between measured and predicted temperatures in B configuration at 75 mm depth and IWC of 0.27 (Mg/Mg). An MRPD value of 12% was obtained.
and IWC of 0.27 (Mg/Mg). Since the governing equations are coupled, all errors involved in the mass transfer are reflected in the heat transfer as well and one can expect differences between the experimental and theoretical results. Deviation of measured and predicted values is reflected in MRPDs calculated in Table 6.3. Low calculated MRPD values are due to the fact that degree Kelvin was used. Mean relative percentage deviation is highest for the first layer, just as that for the predicted water contents. Possible sources of differences are: the simplified assumption of constant temperature at the surface, errors involved in the thermal properties incorporated in the model, coupling with mass transfer and corresponding errors, two-dimensional flow of heat, equilibrium time for the chamber to reach to a constant temperature in each cycle and finally, not perfectly insulated containers.

6.6 Sensitivity Analysis

Two important parameters in the coupled heat and mass transfer governing equations are hydraulic conductivity $K$ (m/s) and thermal conductivity $k$ (W/m K). Both $K$ and $k$ were presented as closed form functions in chapter 5. To study the effect of overall hydraulic and thermal conductivity functions on predicted values of water content and temperature, after decreasing and increasing both functions by 20%, MRPD method was applied. Tables 6.4 and 6.5 show the results of changing hydraulic and thermal conductivities. Presented values for MRPD show the profound influence of the hydraulic conductivity function on predicted water contents (reflected in two or three fold MRPD values in Table 6.4). This emphasizes the importance of proper estimation of hydraulic conductivity to
Table 6.4 Mean relative percentage deviation for temperature prediction for 0.32 (Mg/Mg) IWC and B configuration with different thermal conductivities

| Thermal conductivity (W/m K) | Average $\sum |y_T - y_T' | / y_T N \times 100$ | MRPD (%) |
|-----------------------------|--------------------------------------------|-----------|
| 15 mm                       | 45 mm                                     | 75 mm     | 135 mm |
| 0.8 $k$                     | 1.18                                       | 0.810     | 0.448   | 0.316   | 0.689   |
| 1.0 $k$                     | 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

Table 6.5 Mean relative percentage deviation for water content prediction for 0.32 (Mg/Mg) IWC and B configuration with different hydraulic conductivities

| Hydraulic conductivity (m/s) | Average $\sum |y_{wc} - y_{wc}' | / y_{wc} N \times 100$ | MRPD (%) |
|------------------------------|--------------------------------------------|-----------|
| 15 mm                       | 45 mm                                     | 75 mm     | 135 mm |
| 0.8 $K$                     | 7.47                                       | 5.32      | 10.9    | 0.385   | 6.02    |
| 1.0 $K$                     | 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

minimize the overall deviation. Figure 6.13 shows the variation of measured (all 3 replications) and predicted values of water content with time by taking into account the change in hydraulic conductivity. On the other hand, a 20% change in thermal conductivity (decrease or increase) resulted in almost 10% change in MRPD (Table 6.5). Since the
Fig. 6.13 Variation of measured (all 3 replications) and predicted water contents with time. K: hydraulic conductivity (m/s).
accuracy needed for predicting temperature is not usually high for agricultural purposes, a rough estimation of thermal conductivity may be sufficient.

Full sensitivity analysis of other parameters and percentage of their contribution in predicting water content and temperature remains for future studies.

6.7 Effect of Temperature Change on Mass Transfer

Table 6.6 shows the effect of surface temperature on overall MRPD. Using an average temperature of 10 °C gave an almost 15% improved overall MRPD (Table 5.4). For practical purposes, it is much more convenient to be able to use an average value for the environment temperature as the boundary condition at the soil surface rather than a varying one.

As the temperature rises, the deviation increases; for example, imposing a constant 20 °C at the surface, led to 3.61% change in overall deviation while 30 °C led to more than 107% change in the overall deviation. This shows that the model reflects the coupling effect between heat and mass transfer and the effect may become very large under certain circumstances. More studies are needed to find the proportion of this deviation due to different origins: the effect of temperature on mass transfer and the effect of temperature on pressure head (suction), versus its effect on parameters adjusted for temperature. The proposed model incorporates both coupling effect and adjusted parameters for temperature.
Figure 6.14 shows the effect of different surface temperatures on the change of water content during the drying process at 45 mm depth and IWC of 0.32 (Mg/Mg). As the temperature increases, the rate of change of the water content increases. This could be due to the decrease in the viscosity of water which in turn increases the hydraulic conductivity.

### Table 6.6 Mean relative percentage deviation for water content prediction with 0.32 (Mg/Mg) IWC and different depths with different surface temperatures

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Average MRPD (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(°C)</td>
<td>15 mm</td>
</tr>
<tr>
<td>5, 15 (cyclic)</td>
<td>8.07</td>
</tr>
<tr>
<td>10</td>
<td>5.83</td>
</tr>
<tr>
<td>20°</td>
<td>5.32</td>
</tr>
<tr>
<td>30°</td>
<td>8.84</td>
</tr>
</tbody>
</table>

* compared with the numerical result for constant 10 °C at the surface as the base

\( y_{wc} = \) measured or base value; \( y'_{wc} = \) predicted value; \( N = \) number of observations

6.8 Overall Discussion

The model developed in this study is theoretically sound and can easily be applied in different situations. Even in its one-dimensional form, the model predicted reasonable results, for example, the model may be used to simulate water content and temperature
predictions under draining situation. The problem remains in determining the parameters involved in the model. Using the experimental results to estimate the unknown parameters in a model lumps many phenomena in the estimated parameters. In soil related studies, due to many factors involved (e.g., shrinkage, cracks, Neumann, Dirichlet or third type boundary conditions), this is an unavoidable procedure. Hence, part of the shortcomings is compensated by the parameter estimation.

Low MRPD values presented in Tables 6.1 and 6.3 illustrates the ability of the model to predict water content and temperature in a layered soil profile. Elimination of the ratio \( \partial \theta / \partial T \) and presented vapor diffusivity function (Eq. 5.8) made the developed pressure-based model much easier to apply than earlier models (e.g. Thomas and King 1992). Also, with the help of a simple finite difference solution, the model was applied to a layered seedbed satisfactorily.

The stability analysis revealed that the model is stable under time steps of up to 20 s. Using today’s desktop fast computers, the model can simulate long periods of time in a matter of minutes.
Fig. 6.14 Effect of surface temperature on drying rate at 45 mm depth and IWC of 0.32 (Mg/Mg).
CHAPTER SEVEN

SUMMARY AND CONCLUSIONS

7.1 Summary

The followings were accomplished to fulfill the objectives of this study:

1. An experiment with four layering configurations and three (low, medium and high) initial water contents with three replications was designed and conducted.

2. Mini-gypsum blocks and thermocouples were constructed and calibrated for measuring soil water content and temperature, respectively.

3. Statistical analyses were carried out to determine the significant differences among treatments.

4. Coupled heat and mass transfer governing equations were developed.

5. Closed form functions were found for parameters used in the model.

6. Numerical formulations were derived using fully explicit Forward Time Central Space finite difference method.

7. Conditions for numerical stability of the coupled governing equations were developed.
8. A code was developed in FORTRAN 77 language to solve the finite difference forms of the governing equations.

9. Optimum values for the only unknown parameter in the hydraulic conductivity function were found for different bulk densities using a sum of the square of residuals procedure.

10. Sensitivity of the model to hydraulic and thermal conductivities was tested.

11. Coupling effect of heat and mass transfer was studied by simulating different temperature levels at the soil surface.

12. Numerical (predicted) and experimental (measured) results were compared using the mean relative percentage deviation method.

### 7.2 Conclusions

This section is intended to list some of the conclusions that can be drawn from the present study. These conclusions are considered mainly in the context of the materials, methods and conditions in this study and any generalization should be viewed with caution. The important conclusions corresponding to objectives of this study are outlined as follows:

1. A significant amount of moisture was conserved in layered profiles compared to that of no-layering in samples with low initial water content of 0.27 (Mg/Mg). Also, a significant amount of moisture was lost in a profile of dense layer over uniform bulk density compared to that of no-layering in samples with a high initial water content of 0.37 (Mg/Mg).
Comparing the retained volume of water in different layers, at 45 mm depth more moisture corresponding to 7% change with respect to control or no-layering was conserved in a loose-over-dense-over uniform (LDB) configuration in samples with initial water content of 0.27 (Mg/Mg).

Layering didn’t affect the temperature variations in the soil strata.

2. The developed model is theoretically sound and in its numerical form is capable of predicting water pressure (water content) and temperature in layered soil profile. In solving the numerical form of the developed model, time steps of up to 20 s produced stable solutions.

3. Low overall mean percentage deviation for measured and predicted water contents (ranged from 2.1% to 7.7%) and temperature (ranged from 0.60% to 0.77%) justified the use of the developed model for water content prediction in its one-dimensional form. Predicted retained volume of water was more comparable with the measured ones in lower initial water contents.

   The model is capable of reflecting the coupled effect of heat and mass transfer. Changing the surface temperature from 10 to 20 and 30 °C led to 2.6% and 5.2% average deviation from measured values of water content, respectively. Also, using the average value for the surface temperature instead of a cyclic change, led in better results in terms of average mean relative percent deviation (15% improve) in a uniform soil column with 1.15 Mg/m³ bulk density and initial water content of 0.32 (Mg/Mg).

   The model is very sensitive to hydraulic conductivity. Suggested values for parameter a (6-8) in the closed form function used for the hydraulic
conductivity were inappropriate. Higher values ranged from 17 to 23 were obtained. A 20% change in hydraulic conductivity led to almost 100% to 200% change in average mean relative percent deviation for the predicted water contents in a uniform soil column of 1.15 Mg/m³ bulk density and initial water content of 0.32 (Mg/Mg). On the other hand, a 20% change in thermal conductivity led to only 10% change in average mean percentage deviation for the predicted temperatures in a uniform soil column of 1.15 Mg/m³ bulk density and initial water content of 0.32 (Mg/Mg).

In overall, layering may be desirable for a clay type soil with low initial water content, while in higher initial water contents, stratification may have an adverse effect in terms of moisture conservation. The developed pressure-based heat and mass transfer model proved to be capable of reasonably predicting water content, provided that good estimates of hydraulic and thermal parameters are available. The model is linked to the soil-water characteristic curve which makes it more flexible.

7.3 Suggestions for Future Work

One of the goals of most researchers is the generalization of the results. On the contrary, specific conditions, materials and simplifying assumptions in any research as opposed to many possible scenarios, force the researcher to limit the result. This study is not an exception. For example, had it been a different type of soil could have led to completely different results. However, close involvement in the subject, enables the researcher to shed some light on further studies.
To minimize the deviation between the theoretical and experimental results and to make the model more applicable to more common agricultural soils, the following recommendations are given:

1. Measuring soil surface relative humidity and temperature to incorporate better boundary conditions into the model. This will definitely improve the overall prediction of the model.

2. Verifying model using more common soil types with lower percentage of clay to minimize the shrinkage in drying process, otherwise, volume change should be considered in the model. High percentage of clay particles introduces dramatic structural changes (shrinkage and cracks), especially in the top layer. The model should be applied to the field conditions to compare the predicted and measured values. Laboratory experiments occur under controlled conditions. In real field conditions, natural soil and constantly changing boundary conditions could introduce higher non-linearity into the model which in turn may lead to further modifications.

3. Developing and applying two-dimensional model for both temperature and pressure to encounter the lateral transfer of heat and mass. This may be more useful when dealing with strip stratification (layering due to passage of row stratifiers or seed drills).

4. Performing a detailed sensitivity analysis for all parameters involved when using the model under layered soil condition. Further simplification may result by analyzing the model’s response to changes in different parameters.
5. Investigating the separation of layers with dissimilar bulk densities in a drying process and possible formation of a layer of air between layers.

6. Linking the model to soil mechanics models in which soil strength is related to the soil-water characteristic curve (Wulfsohn et al. 1996).
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Appendix A

Sensor calibration

Since both thermocouples and mini-gypsum blocks were hand made, variation in responses were expected. Therefore, each sensor had to be calibrated. Also, in calibrating mini-gypsum blocks the effect of temperature were taken into account.

A.1 Thermocouples

The procedure for calibrating and selecting copper-constantan thermocouples was as follows: thermocouples were inserted in the mixture of water and ice for a low temperature reading and put into an open end box for a room temperature reading (20.8 °C at the time). The outputs were read using a Campbell CR-21X (Campbell Scientific, Inc., Logan, UT) with a built-in thermistor for reference temperature hooked up to a computer. Fifteen thermocouples that showed the most similar readings, were selected. For the room temperature very low deviation (20.8 °C ± 0.1) and for the water-ice mixture a higher deviation (0.0 °C ± 0.2) of thermocouple outputs were obtained. No further adjustments were applied to the readings of thermocouples in the experiment.

A.2 Mini-gypsum blocks

Mini-gypsum blocks were constructed using a clear acrylic mold (capable of making four blocks at a time) prepared in four layers (57 mm x 160 mm) in Engineering Shops at the
University of Saskatchewan. The base layer (6 mm thick) was solid and the other three layers (3 mm thick) had four openings of dimensions 3 x 15 x 17 mm. For each gypsum block two probes of stainless steel mesh screen No. 14 (0.64 mm) with dimensions of 10 x 10 mm were used. The first layer of the mold was placed on the base layer and secured with four pins at the corners. A mixture of Plaster of Paris with distilled water (10g Plaster of Paris: 7ml of distilled water) was prepared and then poured into the openings. After approximately 2 min (to allow the mixture to partially set), the first probe for each block was placed and positioned in the middle of each opening. Placing the second layer on top of the first one, the openings were again filled with the mixture and allowed to set for 2 min. Then, the last layer was placed and the second probe for each block was positioned in the middle of each opening. The openings were filled with the mixture and allowed to set for 40 min (Fig. A.1). Gypsum blocks were pushed out from the mold and placed in distilled water for 24 hours to gain more strength (complete the setting process). Figure A.2 shows four mini-gypsum blocks after completion of the above procedure.

Mini-gypsum blocks were calibrated for both water content and temperature. Toth and Maulé (1993) presented a method to calibrate a probe-type sensor for measuring soil electrical resistance, in which the temperature effect was also taken into account. A similar procedure was followed in this study.

For calibration, mini-gypsum blocks were embedded into soil samples in small sealed plastic containers (Fig. A.3). Gravimetric water contents used for the soil varied from approximately 0.15 to 0.37 Mg/Mg. The mini-gypsum blocks were allowed to equilibrate with the media for 24 hours, then the containers were placed in a controlled
Fig. A.1 Acrylic clear type mold for preparing mini-gypsum blocks
Fig. A.2 Mini-gypsum blocks at final stage
Fig. A.3 Mini-gypsum block and plastic container used for calibration.
environment. Temperature was changed every 8 hours from 5 °C to 15 °C in increments of 5 °C for a period of 24 hours. Sensors were hooked up to the Campbell CR-21X data-logger and the sensor resistances were stored in a computer for further analysis. The small size of the cylindrical containers (60 mm height x 80 mm diameter) and relatively long period of time for each temperature setting ensured the temperature equilibrium throughout each container within each 8-hour setting.

Due to the perishable nature of the mini-gypsum blocks and possible destruction during calibration and the main experiment (which happened for four of the gypsum blocks) 42 sensors were made and calibrated.

The water content-resistance showed a power (logarithmic) relationship; for example, the following equation was obtained for one of the sensors at 15 °C:

\[
WC = 0.361 R_{15}^{-0.156} \quad (R^2 = 0.998) \tag{A.1}
\]

where  
\[WC = \text{gravimetric water content (Mg/Mg)},\]
\[R_{15} = \text{reference resistance at 15 °C (kΩ/kΩ)}.
\]

Equation A.1 was found to be temperature dependent. Figure A.4 shows the dependency of the soil resistance on temperature for the same sensor. To eliminate the effect of temperature, variable Y is defined as normalized resistance deviation from a reference resistance (15 °C):
Fig. A.4 Temperature effect on soil resistance readings with different water contents.

\[ Y = \frac{R_k - R_{15}}{R_{15}} \]  \hspace{1cm} (A.2)

where \( Y \) = normalized resistance deviation (kΩ/ kΩ),

\( R_k \) = soil resistance (kΩ).

Figure A.4 is now transformed into Fig. A.5 in which the variations of both temperature and water content are reflected in the graphs.
Fig. A.5 Variation of normalized resistance deviation with temperature at different water contents.

Using a multiple linear regression analysis on sensor readings versus normalized resistance deviation and temperature, the following relationship was found:

\[ Y = 0.0009 \, R_x - 0.0487 \, T + 0.6812 \quad (R^2 = 0.956) \]  
(A.3)

Substituting Eq. A.3 into A.2 and solving for \( R_{15} \) and then substituting into Eq. A.1 produced the following final calibration equation for the mini-gypsum block:

\[ WC = 0.361 \left( \frac{R_x}{0.0009R_x - 0.0486T + 1.681} \right)^{-0.156} \]  
(A.4)
Equation A.4 predicts the water content provided that the soil resistance and the temperature are known.

The same procedure was followed for calibrating the other mini-gypsum blocks. Of the 42 sensors made, those with the highest coefficients of determination were used in the experimental program.

During calibration of mini-gypsum blocks, it was found that in low water contents (less than approximately 0.15 Mg/Mg) the readings were unstable and exceeded the resolution of the data acquisition system. Toth and Maulé (1993) reported the same problem in low water contents as well.
Appendix B

Graphs of experimental and predicted water content variations
Fig. B.1 Variation of water content with time at 45 mm depth and IWC of 0.32 Mg/Mg. Each point is the average of 3 replications.
Fig. B.2 Predicted variation of water content with time at 45 mm depth and IWC of 0.32 Mg/Mg.
Fig. B.3 Variation of water content with time at 75 mm depth and IWC of 0.32 Mg/Mg. Each point is the average of 3 replications.
Fig. B.4 Predicted variation of water content with time at 75 mm depth and IWC of 0.32 Mg/Mg.
Fig. B.5 Variation of water content with time at 15 mm depth and IWC of 0.37 Mg/Mg. Each point is the average of 3 replications.
Fig. B.6 Predicted variation of water content with time at 15 mm depth and IWC of 0.37 Mg/Mg,
(note that LB and LDB are the same line).
Fig. B.7 Variation of water content with time at 45 mm depth and IWC of 0.37 Mg/Mg. Each point is the average of 3 replications.
Fig. B.8 Predicted variation of water content with time at 45 mm depth and IWC of 0.37 Mg/Mg.
Fig. B.9 Variation of water content with time at 75 mm depth and IWC of 0.37 Mg/Mg. Each point is the average of 3 replications.
Fig B.10 Predicted variation of water content with time at 75 mm depth and IWC of 0.37 Mg/Mg.
Appendix C

Program code

The following notations have been used in the code written in FORTRAN 77 language:

AB = power for the unsaturated hydraulic conductivity
BLAN5A = the ratio of time step to the square of space step
CE095 = specific water capacity for the loose layer
CE115 = specific water capacity for the bottom layer
CE135 = specific water capacity for the dense layer
CHECK1 = check for being in 16 h period
CHECK2 = check for being in 8 h period
DAY = number of days past
DAYMAX = maximum number of days
DNOTT = vapor diffusion adjusted for temperature
DR001 = partial derivative of vapor density with respect to temperature
DTIME = time step
DVPI095 = vapor diffusivity for the loose layer
DVPI115 = vapor diffusivity for the bottom layer
DVPI315 = vapor diffusivity for the dense layer
DZ = space step
FLOATN = changing integer value of N to real value
HV095 = volumetric heat capacity for the loose layer
HV115 = volumetric heat capacity for the bottom layer
HV135 = volumetric heat capacity for the dense layer
I = an integer used in DO loops
LCFG1 = 1 for bottom layer, 2 for loose layer and 3 for dense layer
LCFG2 = 1 for bottom layer and 2 for dense layer
ICOUNT = an integer for counting loops
IFREQ = frequency of loops prior to printing
N = number of nodes
NODES(I) = an array for number of nodes
NP1 = number of nodes plus one
PA095 = air porosity of the soil in the loose state
PA115 = air porosity of the soil in the bottom layer
PA135 = air porosity of the soil in the dense state
POR095 = total porosity of the soil in the loose state
POR115 = total porosity of the soil in the bottom layer
POR135 = total porosity of the soil in the dense state
RH095 = relative humidity in the loose layer
RH115 = relative humidity in the bottom layer
RH135 = relative humidity in the dense layer
RO = saturated vapor density
S095 = soil suction in the loose layer
S115 = soil suction in the bottom layer
S135 = soil suction in the dense layer
SI(1) = soil surface suction
SI095 = soil suction in the loose layer
SI115 = soil suction in the bottom layer
SI135 = soil suction in the dense layer
SI(\text{T}) = array of current values of soil suctions
SIN\text{EW}(\text{T}) = array of new values of soil suctions
SK095 = saturated hydraulic conductivity for the loose layer
SK115 = saturated hydraulic conductivity for the bottom layer
SK135 = saturated hydraulic conductivity for the dense layer
T = temperature
T(1) = soil surface temperature
T095 = temperature in the loose layer
T115 = temperature in the bottom layer
T135 = temperature in the dense layer
T(\text{T}) = array of current values of temperature
TET095 = volumetric water content in the loose layer
TET115 = volumetric water content in the bottom layer
TET135 = volumetric water content in the dense layer
\text{T\text{HETA}(\text{T})} = array of volumetric water contents
\text{T\text{IME} = time}
TTNI = initial temperature
TK095 = thermal conductivity for the loose layer
TK115 = thermal conductivity for the bottom layer
TK135 = thermal conductivity for the dense layer
T\text{NEW}(\text{T}) = array of new temperatures
U = kinematic viscosity
UK095 = unsaturated hydraulic conductivity for the loose layer
UK115 = unsaturated hydraulic conductivity for the bottom layer
UK135 = unsaturated hydraulic conductivity for the dense layer
WC = gravimetric water content
Z\text{MAX} = depth of the soil column
* This program is written in FORTRAN 77 language to solve the coupled heat and mass
* transfer governing equations formulated in Finite Difference in FTCS mode in this study.
* Soil water pressures are converted back to volumetric water content for comparison
* with experimental results. In the main program initial water content, initial temperature,
* time step should be specified. Also, layering configuration is determined by assigning
* specified values for LCFG1 and LCFG2.

```
PROGRAM LAYERS
REAL T(26), TNEW(26), DAYMAX, ZMAX, BLANDA,
1 FLOATN, DZ, DTIME, DAY, CHECK1, CHECK2,
2 WC, TIME, TINI, THETA(26)
DOUBLE PRECISION SI(26), SINEW(26)
INTEGER I, N, NP1, ICOUNT, IFREQ, LCFG1, LCFG2,
1 NODE(26)
OPEN(UNIT=6, FILE='filename.DAT', STATUS='NEW')
LCFG1=1
LCFG2=1
WC=0.318
TINI=291.16
DAYMAX=7.0
ZMAX=0.147
IFREQ=180
N=21
NP1=N+1
FLOATN=N
DZ=ZMAX/FLOATN
DTIME=20.0
BLANDA=DTIME/DZ**2.0
DO 10 I=1,26
   SI(I)=0.0
   T(I)=0.0
   SINEW(I)=0.0
   TNEW(I)=0.0
   NODE(I)=0
   THETA(I)=0.0
10 CONTINUE
CALL INITIA(NP1, LCFG1, LCFG2, WC, TINI, SI, T,
1    NODE)
ICOUNT=0
TIME=0.0
DAY=1.0
100 IF(DAY.GT.DAYMAX) THEN
   PRINT *, 'NO MORE DAY TO GO!
   GO TO 600
ELSE
```

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CHECK1 = 28800.0*(3.0*DAY-1.0)
CHECK2 = 86400.0*DAY
IF(TIME.LT.CHECK1) THEN
    T(1) = 288.16
    SI(1) = -11130.0
    IF(LCFG1.EQ.1) THEN
        THETA(1) = 0.046+0.562/(1.0+(DABS(2.94*SI(1)))**1.13)**0.117
    ELSEIF(LCFG1.EQ.2) THEN
        THETA(1) = 0.038+0.648/(1.0+(DABS(11.0*SI(1)))**1.15)**0.133
    ELSEIF(LCFG1.EQ.3) THEN
        THETA(1) = 0.054+0.513/(1.0+(DABS(0.264*SI(1)))**1.17)**
    ENDIF
ENDIF
CALL NEWSIT(WC, LCFG1, LCFG2, SI, T, BLANDA, N, NP1,
    1 THETA, SINEW, TNEW)
DO 150 I=2,NP1
    SI(I) = SINEW(I)
    T(I) = TNEW(I)
150 CONTINUE
TIME = TIME + DTIME
ICOUNT = ICOUNT + 1
IF(ICOUNT.NE.IFREQ) THEN
    GO TO 100
ELSE
    ICOUNT = 0
    THETA(23) = THETA(3)+(1.0/7.0)*(THETA(3)-THETA(4))
    THETA(24) = THETA(7)+(3.0/7.0)*(THETA(7)-THETA(8))
    THETA(25) = THETA(11)+(5.0/7.0)*(THETA(11)-THETA(12))
    THETA(26) = THETA(20)+(2.0/7.0)*(THETA(20)-THETA(21))
    T(23) = T(3)+(1.0/7.0)*(T(3)-T(4))
    T(24) = T(7)+(3.0/7.0)*(T(7)-T(8))
    T(25) = T(11)+(5.0/7.0)*(T(11)-T(12))
    T(26) = T(20)+(2.0/7.0)*(T(20)-T(21))
    CALL PRINTS(NP1, LCFG1, LCFG2, WC, THETA,
        1 SI, T, NODE, TIME)
ENDIF
GO TO 100
ELSEIF(TIME.GE.CHECK1.AND.TIME.LT.CHECK2) THEN
    T(1) = 278.16
    SI(1) = -2127.0
    IF(LCFG1.EQ.1) THEN
        THETA(1) = 0.046+0.562/(1.0+(DABS(2.94*SI(1)))**1.13)**0.117
    ELSEIF(LCFG1.EQ.2) THEN
        THETA(1) = 0.038+0.648/(1.0+(DABS(11.0*SI(1)))**1.15)**0.133
    ELSEIF(LCFG1.EQ.3) THEN

THETA(1)=0.054+0.513/(1.0+(DABS(0.264*SI(1)))**1.17)**
1 0.147
ENDIF
CALL NEWSIT(WC, LCFG1, LCFG2, SI, T, BLANDA, N, NP1,
1 THETA, SINEW, TNEW)
DO 155 I=2,NP1
   SI(I)=SINEW(I)
   T(I)=TNEW(I)
155 CONTINUE
TIME=TIME+DTIME
ICOUNT=ICOUNT+1
IF(ICOUNT.NE.IFREQ) THEN
   GO TO 100
ELSE
   ICOUNT=0
   THETA(23)=THETA(3)+(1.0/7.0)*(THETA(3)-THETA(4))
   THETA(24)=THETA(7)+(3.0/7.0)*(THETA(7)-THETA(8))
   THETA(25)=THETA(11)+(5.0/7.0)*(THETA(11)-THETA(12))
   THETA(26)=THETA(20)+(2.0/7.0)*(THETA(20)-THETA(21))
   T(23)=T(3)+(1.0/7.0)*(T(3)-T(4))
   T(24)=T(7)+(3.0/7.0)*(T(7)-T(8))
   T(25)=T(11)+(5.0/7.0)*(T(11)-T(12))
   T(26)=T(20)+(2.0/7.0)*(T(20)-T(21))
   CALL PRINTS(NP1, LCFG1, LCFG2, WC, THETA,
1 SI, T, NODE, TIME)
ENDIF
GO TO 100
ELSE
   DAY=DAY+1.0
   GO TO 100
ENDIF
END

* SUBROUTINES

* Some common parameters are calculated in COMPRM.

SUBROUTINE COMPRM(T, RO, DRODT, Y, U, ROL, DNOTT)
REAL T
DOUBLE PRECISION EXPORO, RO, DRODT, Y, U, ROL, DNOTT
EXPORO=DEXP(0.06374*(T-273.16)-(0.1634D-03)*(T-273.16)**2.0)
RO=(5.144D-03)*EXPORO
DRODT=(5.144D-03)*(0.06374-(0.3268D-03)*(T-273.16))*EXPORO
Y=9.81/(461.52*T)
U=0.6612*(T-229.0)**(-1.562)
ROL=RO/1000.0
DNOTT=(21.6D-06)*(T/273.16)**1.8
RETURN
END

* Subroutine SINI converts the gravimetric water content to suction.

SUBROUTINE SINI(WC, S115, S095, S135)
REAL WC
DOUBLE PRECISION S115, S095, S135
S115=((0.562/(1.15*WC-0.046))**((1.0/0.117)-1.0)**(1.0/1.13)/2.94
S095=((0.648/(0.95*WC-0.038))**((1.0/0.133)-1.0)**(1.0/1.15)/11.0
S135=((0.513/(1.35*WC-0.054))**((1.0/0.147)-1.0)**(1.0/1.17)/0.264
RETURN
END

* This subroutine does some manipulations for further calculations.

SUBROUTINE FINALP(A, B, C, D, E, F, G, H, BLANDA, P1, P2, 1 P3, P4, Q1, Q2, Q3, Q4)
REAL BLANDA
DOUBLE PRECISION P1, P2, P3, P4, P5, P6, P7, P8, P9, P10, P11,
1 Q1, Q2, Q3, Q4, Q5, Q6, Q7, Q8, Q9, Q10, Q11, Q12, Q13,
2 A, B, C, D, E, F, G, H
Q1=A*F
Q2=E*B
Q3=D*E
Q4=A*H
Q5=C*E
Q6=A*G
Q7=Q2-Q1
Q8=(Q4-Q3)*BLANDA/Q7
Q9=1.0+2.0*Q8
Q10= - Q8
Q11=(Q6-Q5)*BLANDA/Q7
Q12=2.0*Q11
Q13= -Q11
Q1=Q9
Q2=Q10
Q3=Q12
Q4=Q13
P1= Q7
P2=C*F
P3=B*G
P4=(P2-P3)*BLANDA/P1
P5=1.0+2.0*P4
P6=-P4
P7=F*D
P8=B*H
P9=(P7-P8)*BLANDA/P1
P10=2.0*P9
P11=-P9
P1=P5
P2=P6
P3=P10
P4=P11
RETURN
END

* This subroutine calculates the model coefficients for the bottom layer B.

SUBROUTINE PRM115(WC, SI115, T115, BLANDA, TET115, P1, P2, P3, P4,
1 Q1, Q2, Q3, Q4)
REAL POR115, PA115, TET115, BLANDA, T115, RH115, AB
DOUBLE PRECISION DNOTT, RO, DRODT, Y, U, ROL, CE115,
1 X115, C1V115, C2V115, DVP115, SK115, UK115, XX115,
2 W115, TK115, HV115, CSI115, CSIT15, SIK115, SIKT15,
3 CTT115, CTSI15, TTK115, TSIK15, A115, B115, CI115,
4 D115, E115, F115, G115, H115, P1, P2, P3, P4,
5 Q1, Q2, Q3, Q4, SI115
TET115=0.046+0.562/(1.0+(DABS(2.94*SI115))**1.13)**0.117
POR115=0.577
PA115=POR115-TET115
CALL COMPRM(T115, RO, DRODT, Y, U, ROL, DNOTT)
CE115=(0.253*(DABS(SI115))**0.133)/(1.0+(DABS(2.94*SI115))**1.13)
1 **1.12
RH115=DEXP(SI115*Y)
X115=Y*(POR115-TET115)
C1V115=ROL*RH115*(X115-DABS(CE115))
C2V115=(RH115/1000.0)*(PA115)*(DRODT-(RO*SI115*9.81)/(461.52*T115
1 **2))
DVP115=DNOTT*((PA115-0.03)/(1.0-0.03))**1.5
SK115=((1.0D-7)*9.94D-04)/U
IF(WC.EQ.0.274) THEN
AB = 16.0
ELSEIF(WC.EQ.0.318) THEN
AB = 18.0
ELSEIF(WC.EQ.0.366) THEN
AB = 19.0

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ENDIF
UK115=SK115*(1.0/(1.0+(DABS(2.94*SI115))*1.13)**0.117)**AB
XX115=DVP115*ROL*Y*RH115
W115=(DVP115*RH115*DRODT)/1000.0
TK115=(1.3+ALOG10(TET115/POR115)*1.16)*0.7
HV115=(2.45D+06)*((1.0-POR115)*0.904+(2.5D+06)*((1.0-POR115)*0.096+
1 4.18D+06*TET115
CSI115=DABS(CE115)+C1V115
CSIT15=C2V115
SIK115=UK115+XX115
SIKT15=W115
CTT115=(HV115/1000.0)+(2.48D+06)*C2V115
CTSI15=(2.48D+06)*C1V115
TTK115=(TK115/1000.0)+(2.48D+06)*W115
TSIK15=(2.48D+06)*XX115
A115=CSI115
B115=CSIT15
C115=SIK115
D115=SIKT15
E115=CTSI15
F115=CTT115
G115=TSIK15
H115=TTK115
CALL FINALP(A115, B115, C115, D115, E115, F115, G115, H115, BLANDA,
1 P1, P2, P3, P4, Q1, Q2, Q3, Q4)
RETURN
END

* This subroutine calculates the model coefficients for the loose layer (L).

SUBROUTINE PRM095(WC, SI095, T095, BLANDA, TET095, P1, P2, P3, P4,
1 Q1, Q2, Q3, Q4)
REAL POR095, PA095, TET095, BLANDA, T095, RH095, AB, WC
DOUBLE PRECISION DNOTT, RO, DRODT, Y, U, ROL, CE095,
1 X095, C1V095, C2V095, DVP095, SK095, UK095, XX095,
2 W095, TK095, HV095, CSI095, CSIT95, SIK095, SIKT95,
3 CTT095, CTSI95, TTK095, TSIK95, A095, B095, C095,
4 D095, E095, F095, G095, H095, P1, P2, P3, P4,
5 Q1, Q2, Q3, Q4, SI095
TET095=0.038+0.648/(1.0+(DABS(11.0*SI095))*1.15)**0.133
POR095=0.651
PA095=POR095-TET095
CALL COMPRM(T095, RO, DRODT, Y, U, ROL, DNOTT)
CE095=-(1.57*(DABS(SI095))*0.153)/(1.0+(DABS(11.0*SI095))*1.15)
1 **1.13
RH095=DEXP(SI095*Y)
X095=Y*(POR095-TET095)
C1V095=ROL*RH095*(X095-DABS(CE095))
C2V095=(RH095/1000.0)*(PA095)*(DRODT-(RO*SI095*9.81)/(461.52*T095 + 1 **2))
DVP095=DNOTT*((PA095-0.03)/(1.0-0.03))*1.5
SK095=((2.66D-06)*9.94D-04)/U

IF(WC.EQ.0.274) THEN
  AB = 16.0
ELSEIF(WC.EQ.0.318) THEN
  AB = 18.0
ELSEIF(WC.EQ.0.366) THEN
  AB = 19.0
ENDIF
UK095=SK095*(1.0/(1.0+(DABS(11.0*SI095))**1.15)**0.133)**AB
XX095=DVP095*ROL*Y*RH095
W095=(DVP095*RH095*DRODT)/1000.0
TK095=1.1+ALOG10(TET095/POR095)*0.994
HV095=(2.45D+06)*(1.0-POR095)*0.904+(2.5D+06)*(1.0-POR095)*0.096+
  1.418D+06*TET095
CSI095=DABS(CE095)+C1V095
CSIT95=C2V095
SIK095=UK095+XX095
SIKT95=W095
CTT095=(HV095/1000.0)+(2.48D+06)*C2V095
CTS195=(2.48D+06)*C1V095
TTK095=(TK095/1000.0)+(2.48D+06)*W095
TSIK95=(2.48D+06)*XX095
A095=CSI095
B095=CSIT95
C095=SIK095
D095=SIKT95
E095=CTS195
F095=CTT095
G095=TSIK95
H095=TTK095
CALL FINALP(A095, B095, C095, D095, E095, F095, G095, H095, BLANDA,
  P1, P2, P3, P4, Q1, Q2, Q3, Q4)
RETURN
END

* This subroutine calculates the model coefficients for dense layer (D).

SUBROUTINE PRM135(WC, SI135, T135, BLANDA,TET135, P1, P2, P3, P4,
  Q1, Q2, Q3, Q4)
REAL POR135, PA135, TET135, BLANDA, T135, RH135, AB, WC
DOUBLE PRECISION DNOTT, RO, DRODT, Y, U, ROL, CE135,
1 X135, C1V135, C2V135, DVP135, SK135, UK135, XX135,
2 W135, TK135, HV135, CSI135, CSIT35, SIK135, SIKT35,
3 CTT135, CTSI35, TTK135, TSIK35, A135, B135, C135,
4 D135, E135, F135, G135, H135, P1, P2, P3, P4,
5 Q1, Q2, Q3, Q4, SI135
TET135=0.054+0.513/(1.0+(DABS(0.264*SI135))**1.17)**0.147
POR135=0.504
PA135=POR135-TET135
CALL COMPRM(T135, RO, DRODT, Y, U, ROL, DNOTT)
CE135=(-0.019*(DABS(SI135))**0.173)/(1.0+(DABS(0.264*SI135))
1 **1.17)**1.15
RH135=DEXP(SI135*Y)
X135=Y*(POR135-TET135)
C1V135=ROL*RH135*(X135-DABS(CE135))
C2V135=(RH135/1000.0)*((PA135*(DRODT-(RO*SI135*9.81)))/461.52*T135
1 **2))
IF(PA135.GE.0.03) THEN
DVP135=DNOTT*((PA135-0.03)/(1.0-0.03))**1.5
ELSE
DVP135=0.0
ENDIF
SK135=((6.23D-9)*9.94D-04)/U
IF(WC.EQ.0.274) THEN
AB = 17.0
ELSEIF(WC.EQ.0.318) THEN
AB = 19.0
ELSEIF(WC.EQ.0.366) THEN
AB = 23.0
ENDIF
UK135=SK135*(1.0/(1.0+(DABS(0.264*SI135))**1.17)**0.147)**AB
XX135=DVP135*ROL*Y*RH135
W135=DVP135*RH135*DRODT/1000.0
TK135=1.42+ALOG10(TET135/POR135)*1.25
HV135=(2.45D+06)*(1.0-POR135)*0.904+(2.5D+06)*(1.0-POR135)*0.096+
1 4.18D+06*TET135
CSI135=DABS(CE135)+C1V135
CSIT35=C2V135
SIK135=UK135+XX135
SIKT35=W135
CTT135=(HV135/1000.0)+(2.48D+06)*C2V135
CTSI35=(2.48D+06)*C1V135
TTK135=(TK135/1000.0)+(2.48D+06)*W135
TSIK35=(2.48D+06)*XX135
CALL FINALP(A135, B135, C135, D135, E135, F135, G135, H135, BLANDA,
1      P1, P2, P3, P4, Q1, Q2, Q3, Q4)
RETURN
END

* This subroutine puts the corresponding initial values of temperature and suction for
* each node.

SUBROUTINE INITIA(NP1, LCFG1, LCFG2, WC, TINI, SI, T,
1      NODE)
REAL WC, T(26)
INTEGER I, NP1, LCFG1, LCFG2, NODE(26)
DOUBLE PRECISION S115, S095, S135, SI(26)
DO 20 I=1,NP1
      NODE(I)=I
20 CONTINUE
DO 30 I=2,NP1
      T(I)=TINI
30 CONTINUE
CALL SINI(WC, S115, S095, S135)
IF(LCFG1.EQ.1) THEN
DO 40 I=2,5
      SI(I)= -S115
40 CONTINUE
ELSEIF(LCFG1.EQ.2) THEN
DO 50 I=2,5
      SI(I)= -S095
50 CONTINUE
ELSEIF(LCFG1.EQ.3) THEN
DO 60 I=2,5
      SI(I)= -S135
60 CONTINUE
ENDIF
IF(LCFG2.EQ.1) THEN
DO 70 I=6,9
      SI(I)= -S115
70 CONTINUE
ELSEIF(LCFG2.EQ.2) THEN
DO 80 I=6,9
   SI(I) = -S135
80 CONTINUE
ENDIF
DO 90 I=10,NP1
   SI(I) = -S115
90 CONTINUE
RETURN
END

* This subroutine calculates the new temperature and suction.

SUBROUTINE NEWSIT(WC, LCFG1, LCFG2, SI, T, BLANDA, N, NP1,
1     THETA, SINEW, TNEW)
REAL T(26), TNEW(26), BLANDA, THETA(26), WC
DOUBLE PRECISION P1, P2, P3, P4, Q1, Q2, Q3, Q4, SI(26), SINEW(26)
INTEGER I, N, NP1, LCFG1, LCFG2
DO 10 I=2,5
   IF(LCFG1.EQ.1) THEN
      CALL PRM115(WC, SI(I), T(I), BLANDA, THETA(I),
1         P1, P2, P3, P4, Q1, Q2, Q3, Q4)
   ELSEIF(LCFG1.EQ.2) THEN
      CALL PRM095(WC, SI(I), T(I), BLANDA, THETA(I),
1         P1, P2, P3, P4, Q1, Q2, Q3, Q4)
   ELSEIF(LCFG1.EQ.3) THEN
      CALL PRM135(WC, SI(I), T(I), BLANDA, THETA(I),
1         P1, P2, P3, P4, Q1, Q2, Q3, Q4)
   ENDIF
   SINEW(I) = P1*SI(I) + P2*SI(I+1) +
1      P2*SI(I-1) + P3*T(I) + P4*T(I-1) +
2      T(I+1) + P4*T(I-1) +
   TNEW(I) = Q1*T(I) + Q2*T(I+1) + Q2*T(I-1) +
1      Q3*SI(I) + Q4*SI(I+1) +
2      Q4*SI(I-1)
10 CONTINUE
DO 20 I=6,9
   IF(LCFG2.EQ.1) THEN
      CALL PRM115(WC, SI(I), T(I), BLANDA, THETA(I),
1         P1, P2, P3, P4, Q1, Q2, Q3, Q4)
   ELSEIF(LCFG2.EQ.2) THEN
      CALL PRM135(WC, SI(I), T(I), BLANDA, THETA(I),
1         P1, P2, P3, P4, Q1, Q2, Q3, Q4)
   ENDIF
   SINEW(I) = P1*SI(I) + P2*SI(I+1) +
1 \quad P2*SI(I-1)+P3*T(I)+P4*
2 \quad T(I+1)+P4*T(I-1)
3 \quad TNEW(I)=Q1*T(I)+Q2*T(I+1)+Q2*T(I-1)+
1 \quad Q3*SI(I)+Q4*SI(I+1)+
2 \quad Q4*SI(I-1)

20 \text{ CONTINUE}
\begin{align*}
\text{DO } 30 \text{ I}=10, N \\
\quad \text{CALL } \text{PRM115}(\text{WC, SI(I), T(I), BLANDA, THETA(I),} \\
\quad \text{P1, P2, P3,P4, Q1, Q2, Q3, Q4})
\quad \text{SINEW(I)}=P1*SI(I)+P2*SI(I+1)+
\quad \text{P2*SI(I-1)+P3*T(I)+P4*}
\quad \text{T(I+1)+P4*T(I-1)}
\quad \text{TNEW(I)}=Q1*T(I)+Q2*T(I+1)+Q2*T(I-1)+
\quad \text{Q3*SI(I)+Q4*SI(I+1)+}
\quad \text{Q4*SI(I-1)}
\end{align*}

30 \text{ CONTINUE}
SINEW(NP1)=SINEW(N)
TNEW(NP1)=TNEW(N)
THETA(NP1)=0.046+0.562/(1.0+(DABS(2.94*SINEW(NP1)))**1.13)**0.117
RETURN
END

* This subroutine prints the corresponding values of temperature and volumetric water
* content for 15, 45, 75 and 135 mm depths.

SUBROUTINE PRINTS(NP1, LCFG1, LCFG2, WC, THETA, SI, T, NODE,
1 \quad \text{TIME})
REAL T(26), WC, THETA(26), DEPTH
INTEGER NP1, I, NODE(26)
DOUBLE PRECISION SI(26)
WRITE(6,500)THETA(23),THETA(24),THETA(25),
1 \quad \text{THETA(26),T(23), T(24), T(25),T(26)}
PRINT 500, THETA(23),THETA(24),THETA(25),
1 \quad \text{THETA(26),T(23), T(24), T(25),T(26)}
500 \quad \text{FORMAT}(1X,F6.3, 3X,F6.3,3X, F6.3, 3X, F6.3,3X, F8.3,3X,F8.3,
1 \quad 3X,F8.3,3X, F8.3)
\text{RETURN}
END
APPENDIX D

Data

Experimental data used in this study are provided in a floppy disk attached. Files were created in EXCEL for Windows 95 v. 7.0. The list of the files and their contents are:

<table>
<thead>
<tr>
<th>File name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>reten.xls</td>
<td>soil-water characteristic data</td>
</tr>
<tr>
<td>sencal.xls</td>
<td>mini-gypsum block calibration data</td>
</tr>
<tr>
<td>27avgmt.xls</td>
<td>water content vs time data (27.4% IWC)</td>
</tr>
<tr>
<td>32avgmt.xls</td>
<td>water content vs time data (31.8% IWC)</td>
</tr>
<tr>
<td>36avgmt.xls</td>
<td>water content vs time data (36.6% IWC)</td>
</tr>
<tr>
<td>27avgtt.xls</td>
<td>temperature vs time data (27.4% IWC)</td>
</tr>
<tr>
<td>32avgtt.xls</td>
<td>temperature vs time data (31.8% IWC)</td>
</tr>
<tr>
<td>36avgtt.xls</td>
<td>temperature vs time data (36.6% IWC)</td>
</tr>
</tbody>
</table>