HEAT AND MASS TRANSFER
IN FREEZING UNSATURATED SOIL

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in the
Department of Agricultural Engineering
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by
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Progressive freezing of unsaturated soil induces moisture migration from warm to cold regions. The water movement and freezing process are coupled and jointly influence the temperature field and the rate of heat transfer. The overall process with or without significant frost heaving is an important consideration in the fields of hydrology, engineering and agriculture. Efforts to understand the coupled heat and mass transfer processes during freezing of a soil are therefore important.

The primary objective of this study was to determine the validity of the Harlan model describing the coupled heat and moisture flow for the soil-water system in which the temperature is below freezing (Harlan, 1973). This involved both the obtaining of suitable experimental data and the development of a computer program for the numerical solution of the model equations. An overview discussion pertaining to this system is presented in order to establish the background understanding necessary to illustrate the development as well as the solution of the governing equations in the model.

Temperature and water-content profiles in an unsaturated soil subjected to temperature gradients with the cold-side temperature below freezing were measured in a horizontal column. The column was well insulated to ensure that one-dimensional heat transfer occurred. Measurements of moisture contents within the soil samples as a function of time were carried out by the gamma-ray attenuation method.
The results of these laboratory tests were compared with numerical solutions of the coupled heat and mass transfer equations. The model used is essentially that developed by Harlan, in which the major driving force causing moisture movement is assumed to be due to the existence of a total potential gradient created by the temperature gradient. The formulated differential equations were solved numerically by the finite difference method using the Crank-Nicholson scheme. The results are encouraging. The calculated values from the model agree very well with the experimental data for both temperature and moisture content profiles under different conditions imposed on the system. The conclusion is that a modified form of Harlan's model can be successfully applied to solve the problem of the coupled heat and mass transfer in soil during freezing.
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CHAPTER I

INTRODUCTION

Freezing and thawing of soils take place every winter over the major part of Canada. The influence of these phenomena on the thermal state and moisture condition in soil is of great importance to engineers, agriculturists, hydrologists and others. For example:

1. It is well known that freezing of soil produces frost heaves which lift the surface layer of the soil causing damage to engineering structures and pavements.

2. Accurate predictions of the temperature regime in time and space are required not only for ecological studies but also for engineering design, particularly in temperature-sensitive areas where freezing and thawing occur.

3. Hydrologists recognize that the effect of the state and amount of moisture in the surface layer of the soil on the infiltration process under freezing conditions is extremely important for accurate prediction of snowmelt runoff.

4. More recently, freezing and thawing problems of soil associated with the construction of cold-gas pipelines and hot-oil pipelines to transport liquified petroleum gas and crude oil from the arctic region to the southern parts of Canada and the United States have been widely discussed.

5. In the prairie provinces of Canada where rainfall is limited, agriculturists have observed carefully the
thermally-induced moisture redistribution in soil upon freezing and the subsequent infiltration process of snow-melt water during the thaw period in attempts to find methods of increasing soil moisture for crop production.

Many problems of man's engineering failures in cold climates associated with soil freezing and thawing are documented by Ferrians et al. (1969) and Muller (1947). Williams (1970) relates freezing and thawing problems of soil to hydrology. Gray and Norum (1968) discuss the effect of soil moisture on the infiltration process under frozen conditions. Pelton et al. (1968) review the influence of freezing and thawing on soil water.

In the past, numerous models have been proposed to describe the thermal regime of soil systems at temperatures below freezing. Most of the work has been directed toward the heat transfer process only. The calculations of the rate and depth of freezing and thawing neglect mass transfer by simply assuming that water in soil does not move. However, whether or not one is dealing with an open or closed system, freezing and thawing in fine-grained soils in nature are usually accompanied by considerable moisture redistribution. Nakano and Brown (1971, 1972) consider heat conduction only and present a numerical one-dimensional model for predicting soil temperatures in cold regions. Comparing the model results with measurements taken on a test area near Barrow, Alaska, they concluded that heat and mass transfer are the two major physical processes taking place in the area where freezing and thawing of soils occur. They stressed
that the effect of mass transfer is an important factor to be considered.

Experience and experiments indicate that as a soil cools below the freezing point, not only does the water in the frozen zone turn to ice but also the water which was not originally in the frozen zone moves into the frozen zone from the surrounding unfrozen soil and then freezes. The migration of water from warm to cold regions is continuous as long as the temperature gradient exists and external water supply is available. If the soil pores become filled with ice, ice lens formation can be expected to take place and the soil will heave.

Because the moisture migration and freezing process are coupled and jointly influence the temperature field and the rate of heat transfer; unless provision is made to properly account for the resulting heat transfer and modification to the thermal properties, the model proposed to deal with the freezing soil-water system is not physically consistent. Moreover, this migration of water, with or without significant frost heaving, is an important consideration in construction work and to the fields of hydrology and agriculture in both seasonal frost and permafrost regions. For example, during the cold season, as a result of the moisture migration, water accumulates and freezes near the soil surface layer as the cold wave, with temperatures below freezing, progresses downward in the soil. This phenomenon reduces the shear strength of the soil and creates a stability problem when the soil thaws and also is a factor
contributing to the reduction of the infiltration rate of a frozen soil.

The theory and experimental verification of isothermal moisture movement in saturated and unsaturated soil are well developed (Gray, 1970; Kirkham and Powers, 1972; Nielsen et al. 1972). Likewise, the physical law governing heat flow in soil systems, dependent on soil moisture content but independent of soil moisture movement, is well advanced (Jumikis, 1966; Luikov, 1966). Mathematical models describing simultaneous heat and mass transfer in porous materials for temperatures above freezing have been studied by many investigators (Philip and de Vries, 1957; Woodside and Kuzmak, 1958; Cary and Taylor, 1962a, 1962b; Hadas, 1968). However, although it has been apparent for many years that the soil moisture and thermal states of soil systems are coupled during freezing and thawing, and this phenomenon constitutes an important problem, there has been comparatively little attention given in the scientific literature to the development of a generalized theory defining heat and mass transfer processes under subfreezing conditions. The reason for this can be attributed to the complexity of the phenomenon and a lack in understanding of the phase change processes in soil during freezing and thawing.

During the last decade, as the result of the increased construction and development activities in the northern part of Canada and Alaska, the process of soil freezing has been a subject of many intensive studies. Substantial knowledge of the physics and thermodynamics of soil-water freezing has
been established. At present, with adequate computer capability, it is possible to model realistically the coupled thermal states and soil moisture of soil systems involving freezing and thawing and to allow the systematic mathematical treatment of the complicated problems such as:

(1) predictions of the temperature regime by considering water movement in frozen soils,

(2) thermally-induced soil-water redistribution involving a phase change upon freezing,

(3) snowmelt and rainfall infiltration into soils under frozen conditions, and

(4) frost heaving associated with soil freezing.

Recently, two types of models based on different mechanisms by which water is transported in frozen soils have been reported for describing the coupled heat and mass transfer in soils involving freezing and thawing. Harlan (1972, 1973) adopted the concept of the analogy between mechanisms of water transport in unsaturated soil and those in partially-frozen soil and proposed a simultaneous heat and mass transfer model for water movement in frozen soil. This model has been used as a basis for computer simulation of thermally-induced soil-water redistribution due to freezing and as well to simulate infiltration of snowmelt and rainfall into frozen soils. The mass transfer equation used in Harlan's model assumes that the major driving force causing mass movement is due to the existence of a potential gradient created by the temperature gradient. Bresler and Miller (1975), applying the capillary concept of soil freezing, pre-
sented a model to simulate the soil-water redistribution during freezing in an unsaturated soil. They introduced series parallel transport in frozen soil involving moving pore ice and unfrozen water based on the capillary sink mechanisms for extracting water from the frozen zone.

At present, the major limitation to the numerical simulation of heat and mass transfer in frozen soil is the lack of quantitative information to verify the proposed models. The main objective of this study was therefore to determine the validity of the Harlan model. This involved both the obtaining of suitable experimental data and the development of a computer program for the numerical solution of the model equations.

The mechanisms by which heat and moisture are transported in frozen soils, involving a change of phase, are highly complex. For example:

1. Water is transported simultaneously in its liquid and gaseous phase.
2. Heat flow occurs by conduction as well as convection.
3. The process of freezing or thawing takes place over a wide range of temperatures because liquid water and ice coexist in soils at temperatures well below 0°C (Williams, 1964; Jame, 1972).

In unfrozen soils, the effect of temperature on the soil property is small and can be neglected in practice; in frozen soil the effect of temperature on the physical properties of a soil is very large. The reason is that changes in
temperature change the interaction of water with the soil and also changes the ratio of the amount of liquid water to ice. The effect of temperature on the physical properties of frozen soil is thus similar to the combined effect of changes in the water content and temperature to the physical properties of unfrozen soils. When dealing with the freezing and thawing problem in soils, the effect of temperature on the properties of the frozen soil, therefore, must be understood and taken into consideration.

Chapter 2 contains a review of available literature pertinent to the study of the freezing and thawing problem in soils. The existing models and solutions as well as common parameters involved for the problem are discussed, primarily for obtaining up-to-date information for the present study analysis. In Chapter 3, experimental method and results are provided. The temperature and water content profiles in a horizontal soil column under different temperature gradients with the cold-side temperature below freezing were measured as a function of time. The soil column was insulated to insure that one-dimensional heat transfer occurred. The gamma radiation attenuation method was used to measure the moisture contents within the sample. Chapter 4 is devoted to the numerical simulation and its solution for the coupled heat and mass transfer in a freezing unsaturated soil. The model used is essentially that reported by Harlan (1973). The predicted temperature and moisture distributions obtained from the model along the column as a function of time were compared to the experimental results to test the validity
of Harlan's model and its accuracy for predicting heat and moisture movement. The results show close agreement between the predicted and measured values for both temperature and moisture content profiles under different conditions imposed on the system. Substantial differences were also observed between the temperature profile and the depth of freezing obtained from the model and those obtained by assuming water movement in soil does not occur and considering heat transfer only. This result demonstrates that the effect of mass transfer on the thermal state of soil is an important factor to be considered when dealing with freezing and thawing problems in soils.
CHAPTER II

REVIEW OF LITERATURE

2.1 The Freezing Temperature of Soil Water and Unfrozen Water in Frozen Soils

A property of water in porous materials is that it freezes at temperatures below 0°C; the magnitude of the freezing-point depression increases as the water content decreases. The reason all soil water does not freeze at a fixed temperature (e.g.; 0°C) is attributed to the forces with which water is retained in soils. Early studies of a freezing soil-water system were concerned only with the determination of the freezing point, that is, the temperature at which freezing commences in a soil sample.

In North America, Bouyoucos (1917, 1936) provided the foundation for modern investigations of the freezing phenomenon in earth materials, and found that frozen soil retains a fraction of its total water content in the unfrozen state. Since then, the existence of unfrozen water in frozen soils has been recognized and well established. In a wet soil, as much of the water exists under a relatively small tension force, it usually freezes at a temperature slightly below 0°C. As ice is formed, the freezing point of the unfrozen water decreases further below 0°C. There is no single freezing point temperature for water in soils and the amount of unfrozen water in a frozen soil varies with temperature.

A general equation defining the freezing-point depres-
sion for soil water has been derived by Low et al. (1968). The thermodynamic argument leads to the conclusion that, at the freezing temperature of a soil at a given water content, this water content may be taken as or regarded as equal to the unfrozen water content of that soil at the same temperature with the remaining portion of water being in the form of ice. This conclusion would appear to be an oversimplification of the process as the hysteresis effect in unsaturated soil systems would suggest the functional relationship between unfrozen water and temperature would be multivalued. However, the results of recent experiments support the single-valued relationship. Jame and Norum (1972) presented experimental results showing the relation between freezing-point depression and water content for two types of soils and compared them with the unfrozen water content curves of the same soils obtained by a calorimetric method. The results, shown in Figure 1, illustrate that the relationship between freezing-point depression and moisture content can be used to represent the relationship between the temperature and the unfrozen water content. The importance of this relationship is that the amount of unfrozen water in frozen soil may be determined from the negative temperature, independent of the total water content for a given soil.

Of the moisture present in clay, as much as one half may be in the liquid state at a temperature of -2°C (Williams, 1964). In some sands, the unfrozen water present at the same temperature would be one tenth or less of the total amount,
Type 1 soil: Soil with 50% silica flour and 50% clay

Type 2 soil: Soil with 50% silica flour and 50% clay

Figure 1 Relationship between freezing point depression and water content and relationship between unfrozen water content and subzero temperature (Jame and Norum, 1972)
the remainder being ice. Generally, the amount of unfrozen water present decreases with decreasing temperature and it increases with increasing temperature.

The amount of unfrozen water in a frozen soil is important as it affects the engineering properties of frozen soils, for example, soil strength, heat capacity and thermal conductivity. Also it is believed a major portion of water transported from warm to cold regions caused by thermal gradients takes place in the unfrozen adsorbed films (Harlan, 1973; Hoekstra, 1966). From recognition of the importance of the unfrozen water in frozen soil has evolved the need for methods for determining the water-ice phase composition of frozen soil throughout a wide range of temperatures which may be encountered in the field. During the past decade, several means of obtaining the unfrozen water content as a function of temperature have been investigated. These include direct and indirect methods.

The direct methods (see Jame, 1972; Anderson and Morgenstern, 1973) include: the diatometric method (Bouyoucos, 1936; Buehrer and Aldrich, 1946; Koopmans and Miller, 1966), the adiabatic calorimetric method (Williams, 1964), the heat capacity method (Anderson, 1966), the X-ray diffraction method (Anderson and Hoekstra, 1965), the calorimetric method (Nersesova, 1954; Yong and Warkentin, 1966; Jame, 1972), the nuclear magnetic resonance method (Wu, 1964), differential thermal analysis (Anderson and Tice, 1971), and the isothermal calorimetric method (Anderson and Tice, 1972). Among these methods, the use of Nuclear Magnetic Resonance
equipment and procedures is believed to have the greatest potential. With this method advantage is taken of the fact that the unfrozen water has a very narrow spectral line compared with that of ice.

Direct measurement of the unfrozen water in frozen soil is usually difficult and time consuming. The majority of the above-mentioned methods have primarily a scientific rather than practical use. For practical purposes, usually indirect methods are employed to estimate the unfrozen water content in a frozen soil.

Anderson and Tice (1972), using the isothermal calorimetric method, obtained phase composition curves for 11 representative soils having widely varying properties and characteristics (see Figures 2 and 3). They found that in most cases the data are well represented by a simple power equation of the form:

\[ W_u = \alpha T^\beta \] 

(2-1)

where \( W_u \) is the unfrozen water content on dry weight basis (g H\(_2\)O/g soil), \( T \) is the temperature below zero (°C), and \( \alpha \) and \( \beta \) are characteristic soil parameters. When the values of \( \alpha \) and \( \beta \), obtained for each of these 11 soils by a least squares regression of experimentally measured values of \( W_u \) and \( T \), were regressed against the specific surface area, \( S \), for each soil, it was found that

\[ \ln \alpha = 0.5519 \ln S + 0.2618 \] 

(2-2)

with a correlation coefficient of 0.90 and,
FIGURE 2  PHASE COMPOSITION CURVES FOR SIX REPRESENTATIVE SOIL AND SOIL CONSTITUENTS (Anderson and Tice, 1972)
FIGURE 3  PHASE COMPOSITION CURVES FOR FIVE REPRESENTATIVE SOILS AND SOIL CONSTITUENTS

(Anderson and Tice, 1972)
\[ \ln(-\beta) = -0.2640 \ln S + 0.3711 \] .... (2-3)

with a correlation coefficient of 0.86. Combining equations (2-2), (2-3) and (2-1), one obtains

\[ \ln W_u = 0.2618 + 0.5519 \ln S - 1.449 S^{-0.264} \ln T \] .... (2-4)

Equation (2-4) can be used to provide a good first approximation of the unfrozen water content of salt-free soils not subjected to overburden pressures at any temperature below 0°C. Table 1, provided by Anderson and Tice (1972), gives the specific surface areas of six representative soils, their experimental values of \( \alpha \) and \( \beta \) and the freezing point depressions calculated from equation (2-1) for three values of the liquid water content, \( W_u \).

Koopmans and Miller (1966), Williams (1968) and Jame and Norum (1972) have advocated the use of the soil water characteristic curve, which shows the water content as a function of soil water suction, for estimating the unfrozen water content. For a given sub-zero temperature, the soil water suction of a partially frozen soil can be expressed by the equation (Jame, 1972):

\[ \Delta P_f = \frac{L}{T_g} (T - T_o) \] .... (2-5)

where

\[ \Delta P_f = \text{soil water suction for partially frozen soil, expressed as the height of column of water, m,} \]

\[ L = \text{latent heat of fusion, 0.336 MJ/kg,} \]
Table I  
Calculated Freezing Point Depression Values for Six  
Representative Soils.  
(Anderson and Tice 1972)

<table>
<thead>
<tr>
<th>Soil</th>
<th>Specific Surface Area (m²/g)</th>
<th>Experimental Values</th>
<th>Freezing Point Depression, ΔT (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>α</td>
<td>β</td>
</tr>
<tr>
<td>1 Manchester very fine sand</td>
<td>0.016</td>
<td>0.0346</td>
<td>-0.048</td>
</tr>
<tr>
<td>2 Fairbanks silt</td>
<td>40</td>
<td>0.0481</td>
<td>-0.326</td>
</tr>
<tr>
<td>3 Kaolinite</td>
<td>84</td>
<td>0.2380</td>
<td>-0.360</td>
</tr>
<tr>
<td>4 Suffield silty clay</td>
<td>140</td>
<td>0.1392</td>
<td>-0.315</td>
</tr>
<tr>
<td>5 Hawaiian clay</td>
<td>382</td>
<td>0.3242</td>
<td>-0.243</td>
</tr>
<tr>
<td>6 Umiat bentonite</td>
<td>800</td>
<td>0.6755</td>
<td>-0.343</td>
</tr>
</tbody>
</table>
\[ T = \text{temperature, K,} \]
\[ T_0 = \text{normal freezing temperature of water, 273 K,} \]
\[ g = \text{gravitational acceleration, 9.81 m/s}^2. \]

Figure 4 illustrates the relation between the freezing point depression and the theoretical equilibrium soil water suction.

For an equal amount of liquid water in the soil, the pore water pressure for ice-free and partially frozen soil can be related as,

\[ \Delta P_f = n \cdot \Delta P_a \]

(2-6)

where \( \Delta P_a \) is the soil water suction for the unfrozen soil and \( n \) is an adjustment factor. From their experiments, Koopmans and Miller (1966) found that the value of \( n \) for wholly colloidal (SLS) soils was 1.0. For non-colloidal (SS) soils, the value was 0.45 which corresponded to the ratio of \( \delta_{iw}/\delta_{aw} \), where \( \delta_{iw} \) and \( \delta_{aw} \) are the surface tension of the ice-water interface and air-water interface respectively.

The water content for a given value of \( \Delta P_a \) can be obtained by using conventional suction-moisture content tests such as pressure membrane or pressure plate. Thus from a series of suction-moisture content determinations on the soil, the soil water suction for the partially frozen soil, \( \Delta P_f \), as a function of unfrozen water content can be constructed by using equation (2-6). Finally, use of equation (2-5) which relates freezing temperature to \( \Delta P_f \) enable determination of the unfrozen water content as a function of temperature, for the soil in question. From his experiments, Williams
SOIL WATER SUCTION (CM. OF WATER)

FREEZING TEMPERATURE (°C)

SOIL WATER SUCTION VERSUS TEMPERATURE BELOW FREEZING

( FROM EQUATION 2-5)
(1968) claimed that the observed suction-moisture content and temperature-unfrozen water content relationship permits prediction of unfrozen water content of a given soil at various negative temperatures down to -1°C, and often somewhat lower, without the need for the direct measurement.

2.2 THERMAL PROPERTIES OF SOIL

A knowledge of thermal properties of soils is necessary for predicting heat flow in soil. Two fundamental thermal properties of soil which govern heat transfer by conduction are its heat capacity and its thermal conductivity. Both properties depend on the content of water, ice and mineral components of the soil. When water changes to ice, its thermal conductivity increases by a factor of 4, its heat capacity decreases by a factor of ¼, and it releases enough heat to raise the temperature of an equal volume of most soil minerals by about 160°C. Because of this behavior, the water-ice phase composition of a frozen soil plays an important role in any thermal considerations of frozen and thawed earth material.

2.2.A Heat Capacity

The amount of heat a volume of soil stores before its temperature rises a certain amount governs how fast a soil will increase in temperature as heat is applied to it. This quantity is called the heat capacity. The heat capacity can be based on the mass or on the volume. The mass specific heat C is defined as the joules of heat required
to raise one gram of soil one degree Celsius and has units of \( \text{J/g} \cdot ^\circ\text{C} \). The volumetric specific heat is defined as the amount of heat required to raise one cubic centimeter of soil one degree Celsius and has units of \( \text{J/cm}^3 \cdot ^\circ\text{C} \). The volumetric specific heat, \( C_p \), is equal to the mass specific heat multiplied by the density, \( \rho \), of the material.

Kersten (1949) has shown that the heat capacity of a soil, water and ice mixture can be calculated by proportion using the respective heat capacities of the components.

Assuming the mass specific heat of water and ice are 4.184 \( \text{J/g} \cdot ^\circ\text{C} \) and 2.1 \( \text{J/g} \cdot ^\circ\text{C} \) respectively, Kersten gave the following equations to calculate the mass specific heat of different soil-water (ice) mixtures:

\[
C_u = \frac{C_s + 4.184 \, W}{1 + W} \quad \text{.... (2-7)}
\]

\[
C_f = \frac{C_s + 2.1 \, W}{1 + W} \quad \text{.... (2-8)}
\]

where \( C_u \) and \( C_f \) are the mass specific heat in \( \text{J/g} \cdot ^\circ\text{C} \) for unfrozen and frozen soil respectively, \( C_s \) is the mass specific heat of dry soil and \( W \) is the moisture content based on dry weight. Similar equations are also provided by Jumikis (1966) and Aldrich (1956).

Kersten (1949) indicated that a value of \( C_s \) equal to 0.711 \( \text{J/g} \cdot ^\circ\text{C} \) represents an average value for most soils at temperatures near the freezing point, and that factors such as density, particle size and shape and mineral composition have very little, if any, effect on the heat capacity
of a soil. Johnson (1952) and Jumikis (1958) found that the mass specific heat of dry soil, minerals and rocks varies within narrow limits and that a value of approximately 0.836 \( \frac{J}{g\cdot \degree C} \) was an average value.

Equations (2-7) and (2-8) are for completely unfrozen and frozen soils. Since in most soils except coarse grained soils liquid water can co-exist with ice at temperatures well below 0°C, these equations need to be modified for calculating the mass specific heat of a partially-frozen soil. The equation used for this purpose is:

\[
C = C_s + 4.184 \, W \left(1 - \eta \right) + 2.1 \, W \frac{1 + \eta}{1 + W} \quad \text{.... (2-9)}
\]

where \( \eta \) represents the fraction of total water which is ice.

In most practical cases, the volumetric specific heat is required rather than the mass specific heat. The volumetric specific heat of a mixture can also be obtained by summing the values of the volumetric specific heat for each constituent, \( (C_p)_j \), weighted by their respective volume fraction \( \phi_j \); thus,

\[
C_p = \sum_{j=1}^{n} (C_p)_j \, \phi_j \quad \text{.... (2-10)}
\]

Most soil minerals, and ice have a value of \( C_p \) within 10 to 15 percent of \( 2.1 \, \frac{J}{cm^3 \cdot \degree C} \). Water, of course, has a volumetric specific heat of \( 4.184 \, \frac{J}{cm^3 \cdot \degree C} \).

For a soil-water mixture, if the dry density of the soil \( \gamma_d \) (mass of dry soil per unit volume, g/cm\(^3\)) is known,
the volumetric specific heat can be obtained by the equation:

\[ C_p = \gamma_d (C_s + 4.184 W_u + 2.1 W_i) \] .... (2-11)

where unfrozen water content \( W_u \) and ice content \( W_i \) are based on the dry weight of the soil.

Both equations (2-10) and (2-11) are suitable only for a constant phase composition. In frozen soils, where phase change is a common, gradual occurrence, the volumetric specific heat of a frozen soil should include a component to account for the latent heat of fusion. Thus, the term volumetric specific heat is not strictly applicable, and the term apparent volumetric specific heat, denoted by \( \bar{C}_p \), is employed for frozen soils (Williams, 1964; Anderson et al., 1973).

Neglecting the gas phase, a frozen soil-water mixture is regarded as consisting of two components (soil and water) and three phases - namely, a soil particle matrix, ice and the water that remains unfrozen. The volumetric specific heat of this system may be expressed as the sum of the volumetric specific heat of these three phases plus a term accounting for the latent heat involved in changing the proportion of unfrozen water to ice. Thus,

\[ \bar{C}_p = C_p + L \gamma_d \frac{\partial W_u}{\partial T} \] .... (2-12)

or

\[ \bar{C}_p = \gamma_d (C_s + 4.184 W_u + 2.1 W_i + L \frac{\partial W_u}{\partial T}) \] .... (2-13)

where \( L \) is the latent heat of freezing of soil water, J/g,
and \( \frac{\partial W_u}{\partial T} \) is the rate of change of unfrozen water content with temperature.

It has been known that the latent heat of fusion of soil water is less than that of pure bulk water and is equal to the difference between the partial specific enthalpies of the unfrozen water and ice (Anderson, 1966). The significance of the dependence of \( L \) on \( W_u \) has been investigated, and it has been found that a correction for this difference is significant only for temperatures below about \(-20^\circ C\) (Anderson et al., 1973). The conventional value of the latent heat of freezing of water, 333.4 J/g, is widely used in heat flow calculations in frozen ground.

2.2.B Thermal Conductivity

The thermal conductivity, \( \lambda \), defined as the quantity of heat which flows normal to a surface of unit area per unit time under a unit temperature gradient, has units of Watt/m \(^\circ C\). It is measured under either a steady-state or transient flow conditions.

For steady-state flow, a uniform temperature gradient is applied and the sample is allowed to condition thermally until constant heat-flow conditions are attained (Kersten, 1949; Woodside, 1957; Sass et al., 1971). The theory of the steady-state flow is simple, but maintaining a linear flow in the sample presents operational difficulties. It may take a long time to obtain constant heat-flow conditions, which may result in thermally-activated diffusion of water in either frozen or unfrozen unsaturated soils (Hutcheon, 1958). If this movement
occurs in a sample of finite thickness, water or ice accumu-
lates at the cold end and drying occurs at the warm end.

In frozen soils, the ice-water ratio is a function of temperature. This imposes additional difficulties in the measurement of the thermal conductivity by the steady-state method. When a sample is subjected to a temperature gradient, it does not have a constant ice-water ratio throughout its length. Since the thermal conductivities of ice and water are different, the thermal conductivity of the sample would also not be constant.

In the transient method, a long thin probe, containing an axial heater filament and a temperature sensor is inserted into the medium of unknown thermal conductivity. Heat is supplied to the filament at a constant rate, and the conductivity is determined by comparing the observed temperature rise with the appropriate radial heat conduction model (Woodside and Messmer, 1961; Wechsler, 1966; Penner, 1970). The use of the transient method for measuring thermal conductivity also has difficulties. The problem of induced moisture flow in an unsaturated soil system is similar to that encountered with the steady-state method but may be more critical as the temperature gradient next to the probe can be much greater than that usually occurring in the steady-state method. Woodside (1958) suggested that increasing the diameter of the probe and using low heat inputs would reduce the thermal gradients and thus decrease the induced moisture flow. Large-diameter probes are usually not sufficiently long to satisfy the requirement of a line heat source assumed for the development of the simple
theory describing their behavior.

In recognition of the difficulties associated with the different methods of measuring thermal conductivities, particularly in unsaturated soils, the line heat source probe technique was considered the preferred method. One advantage of the transient method, compared to the steady-state method, is that the thermal conductivity measurement is of short duration. This is a time-saving feature which also reduces the time that the sample is subjected to thermal gradient - the cause of thermally activated diffusion. What is more, the transient method is generally less expensive than the steady-state method and is simple to operate.

The most comprehensive treatment of the thermal conductivity of natural soils has been presented by Kersten (1949). He made a very extensive series of measurements, using a steady-state cylindrical heat flow method, by which he determined the dependence of the thermal conductivity of 19 soils on the mean temperature, density, and moisture content. His data are the most widely used in making ground heat flow calculations. For predicting the thermal conductivity of frozen and unfrozen soils, Kersten derived equations from his experimental data and claimed that for most conditions the following empirical relationships should enable the calculation of soil thermal conductivities to within 25%:

1. For fine-grained soils:

   \[
   \text{Unfrozen: } \lambda = A (0.9 \log W - 0.2) 10^{0.01Yd} \]

   \[
   \cdots \quad (2-13)
   \]
Frozen: $\lambda = A \{0.01(10)^{0.008}\gamma_d^B (W)\}$  \hspace{1cm} (2-14)

2. For coarse-grained soils:

Unfrozen: $\lambda = A (0.7 \log W + 0.4) 10^{0.013}\gamma_d^B$  \hspace{1cm} (2-15)

Frozen: $\lambda = A \{0.076(10)^{0.013}\gamma_d^B + 0.032(10)^{0.0146}\gamma_d^B (W)\}$ \hspace{1cm} (2-16)

Where $\lambda =$ the thermal conductivity of soil, Watt/m °C,
$W =$ the soil moisture content, percent by dry weight,
$\gamma_d =$ the dry density of soil, kg/m$^3$,
$A =$ 0.144133 (conversion factor), and
$B =$ 0.06242796 (conversion factor).

Soils with 50 percent or more of silt and clay sizes were defined as fine-grained, and those with less than 50 percent were defined as coarse-grained. For equations (2-13) and (2-14) to be applicable, the moisture content, $W$, should be equal or greater than 7 percent, and equations (2-15) and (2-16) are valid for moisture contents of 1 percent or more. Sanger (1963) has presented these equations in graphical form as shown in Figures 5 and 6.

De Vries (1952) reviewed some of the formula by which the thermal conductivity of soil might be estimated from a knowledge of the volume fractions and thermal conductivities of its constituents. An equation, originally derived by
FIGURE 5 DEPENDENCE OF THERMAL CONDUCTIVITY $\lambda$ ON DRY UNIT WEIGHT AND WATER CONTENT — FOR COARSE-GRAINED SOIL (SANGER, 1963)

CONVERSION FACTOR:

1 BTU/ft·hr·°F = 1.7296 WATT/m·°C

1 lb/ft$^3$ = 16.018463 kg/m$^3$
FIGURE 6 DEPENDENCE OF THERMAL CONDUCTIVITY $\lambda$ ON DRY UNIT WEIGHT AND WATER CONTENT — FOR FINE-GRAINED SOIL (SANGER, 1963)
Maxwell (1904) for the calculation of electrical conductivity and later used by Euken (1932) for thermal conductivity of a material made up of many substances, was applied by de Vries to soils. The equation is:

\[
\lambda = \frac{\sum_{j=1}^{n} \phi_j \lambda_j F_j}{\sum_{j=1}^{n} \phi_j F_j}
\]  

(2-17)

Where

- \( \lambda \) = the thermal conductivity of the system,
- \( j \) = the number of different kinds of particles in the system (\( j=1 \) is for the continuous medium in which other components are dispersed),
- \( \phi_j \) = the volume fraction of \( j \)-th kind of particles,
- \( \lambda_j \) = the thermal conductivity of \( j \)-th kind of particles, and
- \( F_j \) = the ratio of average temperature gradient in the \( j \)-th kind of particles to the average temperature gradient in a continuous medium.

The value for \( F_j \) was estimated by de Vries (1952) from the following expression:

\[
F_j = \frac{1}{3} \frac{3 \sum_{n=1}^{3} (1 + \frac{\lambda_j}{\lambda_1} - 1) \cdot g_n}{\sum_{n=1}^{3} (1 + \frac{\lambda_j}{\lambda_1} - 1) \cdot g_n}^{-1}
\]  

(2-18)

with \( F_1 = 1.0 \) and \( g_1 + g_2 + g_3 = 1 \), where \( g_1 \), \( g_2 \) and \( g_3 \) are depolarization factors.

The values for \( g_1 \), \( g_2 \) and \( g_3 \) depend on the relative lengths of the major and minor axes of the dispersed parti-
cles. Hence, for spherical particles $g_1 = g_2 = g_3 = 1/3$. De Vries (1952) compared the values of $\lambda$ predicted by equation (2-17) with experimental results obtained for numerous systems of spheres of various substances dispersed in fluid media. He arrived at the following semi-empirical conclusions.

1. Equation (2-17) provides good results for systems whose dispersed particles have smaller conductivities than that of the continuous medium. The computed values will be slightly larger than the true values, but the error will always be less than 10 percent.

2. When the ratio of the thermal conductivity of the dispersed particles to the thermal conductivity of the continuous medium is about 10, the equation will predict values that are too low, but by less than 10 percent.

3. When this ratio of the thermal conductivities (dispersed particles: medium) is of the order of 100, the predicted values are about 25 percent too low.

In using equation (2-17) to calculate the thermal conductivity of soil, de Vries assumed for the solid particles $g_1 = g_2 = 0.125$ and $g_3 = 0.750$, which corresponds to particles shaped like an ellipsoid of revolution. These values gave estimated thermal conductivities close to measured values. Woodside and Cliffe (1959) and Penner (1962) have also used equation (2-17) to predict the thermal conductivity of air dry and water saturated soils. They found good agreement between predicted and measured thermal conductivities for these two phase systems.

For unsaturated soil, de Vries considered water as the
continuous medium in which ellipsoids of air and solids were dispersed. Since the ratio of the thermal conductivities of the dispersed particles to that of the continuous medium were approximately 10 for the solid particles and 0.2 for air, according to de Vries's conclusions, equation (2-17) should have predicted thermal conductivities within 10 percent of the true magnitude. De Vries provided both the calculated and experimental values for the thermal conductivities of several samples of Healy clay and Fairbanks sand. An analysis of the data showed good agreement between the calculated and experimental values. The only instances when the difference between the two values was more than 10 percent were at low moisture contents.

The use of equation (2-17) for the calculation of the thermal conductivity of soil requires a knowledge of the conductivities of the soil constituents. The thermal conductivities of water and dry air are available in many physics-chemistry and engineering handbooks, and may be taken as 0.581 and 0.023 W/m °C for water and dry air respectively at temperature 0°C (Jumikis, 1966; Luikov, 1966). The value for the thermal conductivity of air in moist soil must be adjusted to account for latent heat transfer. A method derived by Krisher and Rohralter (as quoted in de Vries (1952)) may be used to make this determination. The adjusted value for moisture contents above the wilting point was 0.1004 W/m °C at temperature of 20°C. According to Van Wijk (1963) the thermal conductivity of the solid soil constituents of practically all mineral soils, with the notable exception of
sands, may be taken as 2.941 W/m·°C. The thermal conductivity of sand can be taken as that of pure quartz, given by Van Wijk as 8.82 W/m °C.

The influence of temperature on thermal conductivity of soil has been studied by Kersten (1949). He found that the thermal conductivities of most soils in the temperature range of 0°C to 30°C could be expected to increase slightly with an increase in temperature. In practice, the thermal conductivity of soil is considered to be relatively insensitive to temperature changes above 0°C, and therefore, is assumed to be constant in heat flow calculations. At temperatures below 0°C, where soils have a temperature-dependent ice content, the thermal conductivity of frozen soils cannot be assumed a constant.

Penner (1970) measured thermal conductivities of two frozen soils, Leda clay and Sudbury silt clay, in saturated conditions by means of the transient heat-flow method using a line heat source. The results of his studies, shown in Figure 7, clearly indicate the dependence of thermal conductivity on temperature. Lowering the freezing temperature of a saturated soil increases its ice content and reduces its water content, and because ice has a greater thermal conductivity than water the overall conductivity of the soil system is increased.

De Vries method of calculating the thermal conductivity of soil was applied to frozen soils by Penner (1970). In this calculation it was assumed that ellipsoids of soil
FIGURE 7 ESTIMATED AND MEASURED THERMAL CONDUCTIVITY FOR PARTIALLY - FROZEN SOIL (Penner, 1970)
solids and ice were dispersed in a continuous medium of unfrozen liquid water. Despite some criticism in applying this equation, the estimated values are in very good agreement with the measured values (see Figure 7).

Penner et al. (1975), using the transient heat flow method, determined the thermal conductivities of 10 fine-grained soils in unfrozen and frozen states. The measured values were in good agreement with Kersten's results obtained by the steady-state heat flow method. For most of the soils, they found that at low moisture contents the thermal conductivity of the unfrozen soil was higher than for the frozen soil. With increasing moisture content, the thermal conductivity of the frozen soil became progressively greater than that of the unfrozen soil. Figure 8 shows the thermal conductivity of one type of soil (with 54% clay and 46% silt) at various densities and moisture contents for three temperatures, i.e. 5, -5, and -15°C obtained by Penner et al. (1975). The change of thermal conductivity from the unfrozen state to the frozen state for the same type of soil is given in Figure 9. In the Figure the ratio of $\lambda_2/\lambda_1$ and $\lambda_3/\lambda_1$, where $\lambda_1$ is the unfrozen thermal conductivity at +5°C and $\lambda_2$ and $\lambda_3$ are the frozen thermal conductivities at -5 and -15°C respectively, are less than 1 at low moisture contents and increase to values greater than 1 at the higher levels of saturation.

Kersten (1949) also observed that at low moisture contents the thermal conductivity of an unfrozen soil was greater than its value when frozen. He reported that at
FIGURE 8 TEMPERATURE VERSUS THERMAL CONDUCTIVITY - FOR SOIL WITH 54% CLAY AND 46% SILT
(Penner et al., 1975)
\( \lambda_1 \), THERMAL CONDUCTIVITY AT 5°C
\( \lambda_2 \), THERMAL CONDUCTIVITY AT -5°C
\( \lambda_3 \), THERMAL CONDUCTIVITY AT -15°C

- \( \gamma_d = 1.563 \text{g/cm}^3 \), \( W = 19.2\% \)
- \( \gamma_d = 1.567 \text{g/cm}^3 \), \( W = 14.7\% \)
- \( \gamma_d = 1.387 \text{g/cm}^3 \), \( W = 5.6\% \)

**FIGURE 9** RATIO OF \( \lambda_2/\lambda_1 \) AND \( \lambda_3/\lambda_1 \) AS A FUNCTION OF SATURATION PERCENTAGE FOR SOIL WITH 54% CLAY AND 46% SILT (Penner et al., 1975)
moisture contents less than six percent for sandy soil and less than ten percent for fine-grained soil the thermal conductivity in the frozen state is lower than in the unfrozen state. Figure 10, taken from Kersten (1949), shows the ratio of the thermal conductivity at -4°C to the thermal conductivity at +4°C plotted as a function of moisture content for three soils; Lowell sand, Romsey sandy loam and a Fairbanks silt. The reduction of thermal conductivity in the frozen state at low moisture content is believed to be due to the location of ice within the soil matrix. Before freezing, water forms a bridge between soil particles due to surface tension and provides an effective path for heat conduction. During freezing, some of the bridge water is removed. The ice crystals are thought to partially fill the voids between soil particles; the wide conductivity path between particles is removed during the phase change. At high moisture contents, a larger number of pores are filled with ice resulting in an overall increase in thermal conductivity.

Mickley (1951) and Gemant (1952) have also attempted to treat the thermal conductivity of granular material analytically, as well as experimentally, by considering the combined thermal properties of their constituents. Mickley (1951) suggested a model for approximation of thermal conductivity of soil mass by considering different combinations of the thermal conductivities of solid matter, water and air. Gemant (1952) derived a formula for thermal conductivity of soil which considers the thermal conductivity of water and solid matter, the dry density of the soil, and the moisture content.
FIGURE 10 RATIO OF THERMAL CONDUCTIVITY AT -4°C TO +4°C AS A FUNCTION OF MOISTURE CONTENT FOR SEVERAL SOILS (Kersten 1949)
of the soil.

As mentioned in the preceding discussion, many formulas have been proposed to account for the thermal conductivity of an aggregate in terms of its constituents. Some are very cumbersome, and none has a completely satisfactory theoretical rationale. The major problem arises when the constituent thermal conductivities differ by several orders of magnitude, such as in an unsaturated condition where soil contains appreciable volumes of air and highly conducting mineral grains. In a saturated soil, the thermal conductivities of the different media differ by less than a factor of 20. It has been verified experimentally (Sass et al., 1971; Woodside and Messmer, 1961) that under these conditions no formula is more successful than using a simple weighted geometric mean:

\[ \lambda = \lambda_1^{\phi_1} \cdot \lambda_2^{\phi_2} \cdot \lambda_3^{\phi_3} \cdots \lambda_n^{\phi_n} = \prod_{i=1}^{n} \lambda_i^{\phi_i} \]

where \( \lambda_i \) is the constituent thermal conductivity and \( \phi_i \) is its respective volume fraction.
2.3 MODELS OF HEAT TRANSFER IN FROZEN SOILS

The temperature regime of the ground affects the biological systems both above and below ground. Accurate predictions of the temperature regime in time and space are required not only in ecological studies but also in engineering design, particularly in the temperature-sensitive area where freezing and thawing occur, and the subsequent impact of engineering works to the environment. The problem of thermal flow in frozen soils has been the subject of many studies, most of them have been directed toward the calculation of the rate and depth of freezing and thawing. A resume of some of these studies is presented in subsequent discussions.

2.3.1 Empirical Method

Heat can be transferred in soil by conduction, by convection, by mass flow of water, and by the evaporation and condensation of water. If soil moisture is considered as a static phenomenon, heat conduction is believed to be the major method of heat transfer in soil. Although the basic laws of heat conduction are known (Jumikis, 1966), and the corresponding governing differential equations are developed (Luikov, 1966), the solution for those equations which involve a change of phase is difficult and complicated. For most practical applications, empirical methods for the prediction of temperature and the freezing and thawing depth of soil are still widely used.

Many empirical methods (Casagrande, 1931; Shannon, 1944; U.S. Corps of Engineers, 1946, 1954, 1961) have been
presented which relate the depth of frost penetration in soil to the accumulated degree-days of temperature below 0°C. The algebraic sum of these daily values over the freezing season is called the freezing index.

The degree-day corrections are based entirely on air temperatures, although the effects of such climatic variables as radiation and cloud cover enter indirectly into the relationships (U.S. Corps of Engineers, 1954). Empirical correction factors have also been determined for various types of surfaces, which make it possible to convert an air-temperature index to a surface temperature index (U.S. Corps of Engineers, 1946). However, the effects of several factors such as soil type, thermal conductivity, and soil water content are not included in these factors. Thus, empirical methods for prediction of soil temperature, or frost penetration, either ignore potentially important variables in the heat transfer process, or treat them in a very indirect manner.

2.3.2 Freezing of Coarse-Grained Soil

Numerous models have been proposed to describe the thermal regime of soil in which temperature is below freezing. In the classic methods, it is assumed that the water in soils does not move and that it freezes at the freezing point of water (0°C) to form a freezing front which advances through the soil. Mathematically, it is a moving boundary problem.

The first published discussion of the freezing and thawing problem was given by Stefan (1890). Actually, the first important exact solution of this problem was determined
by Franz Neumann and presented in lectures in the 1860's. However, the first publication (Weber, 1901) of these lectures did not appear until 1912. The problem, hence, is commonly referred to as the Stefan or Neumann problem.

In treating the freezing and thawing of a soil water system as a moving-boundary problem, it is assumed that all the water in the soil freezes at 0°C. However, this assumption is not usually valid because in most soils a certain fraction of the soil water remains liquid at temperatures below 0°C. The existence of unfrozen water in frozen soils has been generally recognized. Only in coarse-grained materials, such as sands and gravels, does all the soil water change phase in situ at a fixed temperature close to 0°C. This type of soil may be treated, for practical purposes, as being either completely frozen or completely thawed.

2.3.2. A Stefan's Model

In the Stefan's model for computing the depth of frost penetration as a function of time, it is assumed that the variation of temperature from the top of ground surface to the freezing front is linear and that the temperature remains constant below the frost line. Figure 11 shows the thermal condition assumed in the Stefan's model.

According to the assumptions, the continuity equation at a point on the freezing front requires that

\[ \frac{\lambda_f (T_s - T_o)}{x} = L \gamma dW \frac{dx}{dt} \quad \ldots \quad (2-20) \]
FIGURE 11  THERMAL CONDITIONS ASSUMED FOR THE STEFAN'S MODEL
Where
\[ \lambda_f = \text{the thermal conductivity of frozen soil}, \]
\[ T_s = \text{the temperature at ground surface (below freezing)}, \]
\[ T_0 = \text{the freezing temperature of water (0°C)}, \]
\[ L = \text{the latent heat of fusion}, \]
\[ \gamma_d = \text{the dry density of soil}, \]
\[ W = \text{the water content by dry weight}, \]
\[ x = \text{the depth of frost penetration, and} \]
\[ t = \text{time}. \]

Therefore, the depth of frost penetration is
\[
x = \sqrt{\frac{2 \lambda_f (T_s - T_0)}{L \gamma_d W}} \quad \ldots \quad (2-21)
\]

The term \( \int (T_s - T_0) \, dt \), if expressed in degree-days, is called the freezing index.

Because of the simplifying assumptions involved in its development and the fact that the volumetric heat capacity of the soil mass is neglected, the depth of frost penetration by the Stefan's model is usually overestimated.

2.3.2.B Neumann's Model

Neumann provided a more rigorous analysis for the freezing and thawing problem in soil. Neumann's model was developed for a homogeneous, isotropic, semi-finite body. It is assumed that the initial temperature, \( T_{i} \), of the soil is positive and constant. Then, by a sudden lowering of the surface temperature to a new constant and freezing value, \( T_s \), the cooling process is inaugurated. In the formulas, Neumann
gives two partial differential equations to consider not only the frozen part but also the unfrozen part of the soil underneath the frost boundary. Figure 12 shows the temperature profile for Neumann's model. These equations are:

(1) for the frozen part of the soil, \(0 < x < \xi\):

\[
\frac{\partial^2 T_1}{\partial x^2} = \frac{1}{\alpha_1} \frac{\partial T_1}{\partial t} \quad \ldots \quad (2-22)
\]

and

(2) for the unfrozen part of the soil, \(x > \xi\):

\[
\frac{\partial^2 T_2}{\partial x^2} = \frac{1}{\alpha_2} \frac{\partial T_2}{\partial t} \quad \ldots \quad (2-26)
\]

where \(T\) is temperature, \(t\) is time, \(\xi\) is the depth of frost penetration, \(\alpha\) is the thermal diffusivity, \(x\) is the distance from the ground surface, and the subscripts \(1\) and \(2\) correspond to the frozen and unfrozen regions respectively.

The thermal diffusivity, \(\alpha\), is defined as

\[
\alpha_i = \frac{\lambda_i}{(C_p)_i} \quad i = 1, 2
\]

where \(\lambda\) is the thermal conductivity and \(C_p\) is the volumetric specific heat.

The following boundary conditions are used to solve equations (2-22) and (2-23)

(1) The initial conditions:

at \(x \geq 0, t = 0\)

\[
T_1 (x, t) = T_2 (x, t) = T_i \quad \ldots \quad (2-24)
\]
\[
\frac{\partial^2 T_1}{\partial x^2} = \frac{1}{\alpha_1} \frac{\partial T_1}{\partial t}
\]

\[
\frac{\partial^2 T_2}{\partial x^2} = \frac{1}{\alpha_2} \frac{\partial T_2}{\partial t}
\]

FIGURE 12 TEMPERATURE PROFILE FOR NEUMANN'S MODEL
(2) The fixed boundary conditions:

at \( x = 0, \ t > 0 \)
\[ T_1 (x, t) = T_s \]

at \( x \to \infty, \ t > 0 \)
\[ T_2 (x, t) = T_i \] \hspace{1cm} .... (2-25)

at \( x = \xi, \ t > 0 \)
\[ T_1 (x, t) = T_2 (x, t) = T_o \]

The heat balance at the freezing front, where \( x = \xi \), requires that

\[
\lambda_1 \frac{\partial T_1}{\partial x} \bigg|_{x=\xi} - \lambda_2 \frac{\partial T_2}{\partial x} \bigg|_{x=\xi} = L \gamma W \frac{\partial \xi}{\partial t} \] \hspace{1cm} .... (2-26)

Neumann provided the exact solutions for the equations (2-22) and (2-23) using the boundary conditions given in equations (2-24) to (2-26) as follows (Jumikis, 1966):

\[ \xi = m \sqrt{t} \] \hspace{1cm} .... (2-27)

\[ T_1 = T_s + (T_o - T_s) \frac{m}{G(\frac{2}{a_1 t})} \] \hspace{1cm} .... (2-28)

\[ T_2 = T_1 - (T_1 - T_o) \frac{m}{\left[ 1 - G\left(\frac{x}{2 \sqrt{a_2 t}}\right) \right]} \] \hspace{1cm} .... (2-29)
where the parameter $m$ is determined from the following transcendental function:

\[
\frac{LY_d W}{2} \int_\pi^\pi \frac{m}{\lambda_1} (T_o - T_s) e^{\frac{4a_1}{m}} G\left(\frac{m}{2\lambda_1}\right) - \frac{m^2}{\lambda_2} (T_1 - T_o) e^{\frac{4a_2}{m}} G\left(\frac{m}{2\lambda_2}\right)
\]

and $G(X)$ is the Gauss's error integral, defined as,

\[
G(X) = \frac{2}{\int_\pi^\pi} \int_0^X e^{-\eta^2} d\eta
\]

Neumann's theory is an excellent mathematical treatment of the freezing and thawing problem. However, the solution provided is only valid for the specified boundary conditions which are seldom satisfied in natural systems. Recently, since numerical techniques for solving the partial differential equation have become popular, the Neumann's solution is often used as a test of accuracy for the numerical solution in the moving-boundary problem.

Neumann's theory has been applied by Berggren (1943) and later in a modified form by Aldrich (1956) for predicting the temperature distribution in frozen soil. Aldrich (1956) developed the following solution for the depth of frost pene-
tration into a semi-infinite soil mass with uniform properties and assuming at initial instant the mass was isothermal:

\[ \xi = \beta \sqrt{\frac{48 \lambda F}{L \gamma_d W}} \]  

(2-31)

Where \( \beta \) = a correction coefficient (dimensionless),
\( \lambda \) = the thermal conductivity (W/cm °C),
\( F \) = the freezing index (°C - days),
\( L \) = the latent heat of fusion (J/g),
\( \gamma_d \) = the dry density of soil (g/cm³),
\( W \) = the water content by dry weight (g H₂O/g of water), and
\( \xi \) = the depth of frost penetration (cm).

The thermal conductivity \( \lambda \) in equation (2-31) is taken as the mean value of the thermal conductivities of the frozen soil \( \lambda_2 \) and the unfrozen soil \( \lambda_1 \), ie.,

\[ \lambda = \frac{1}{2} (\lambda_1 + \lambda_2) \]  

(2-32)

The correction coefficient \( \beta \) depends on the thermal properties of both the frozen and unfrozen soils. Values for \( \beta \) given by Aldrich (1956), are shown in Figure 13. The thermal ratio \( R \) is defined as the ratio of the temperature above 0°C to the temperature below 0°C, and can be expressed as

\[ R = \frac{(T_i - T_o) t}{F} \]  

(2-33)
FIGURE 13 CORRECTION COEFFICIENT $\beta$ FOR EQUATION (2-31)

(Aldrich, 1956)
where $T_i$ is the initial temperature (above $0\degree C$), $T_o$ is the freezing point of water, $0\degree C$, $t$ is time in days and $F$ is the freezing index, $\degree C \cdot$ days.

The dimensionless fusion parameter, $\mu$, listed in Figure 13 is determined from the expression

\[
\mu = \frac{(C_\rho) \cdot F}{L_\gamma_d W_t} \quad \text{(2-34)}
\]

where $C_\rho$ is the volumetric specific heat ($J/cm^3\degree C$), and is taken as the mean value of the volumetric specific heat of the frozen soil $(C_\rho)_1$ and the unfrozen soil $(C_\rho)_2$, i.e.,

\[
C_\rho = \frac{1}{2} \left[ (C_\rho)_1 + (C_\rho)_2 \right] \quad \text{(2-35)}
\]

Besides the models mentioned above, numerous other attempts have also been made to solve the moving-boundary problem (Portnov, 1962; Goodman, 1964; Sikarskie and Boley, 1965). Exact solutions are only available for some simple cases. Most of the efforts have been directed toward approximate methods of solution and with the advent of digital computers it has become possible to solve the governing differential equation numerically for many different boundary conditions.

2.3.3 Freezing of Fine-Grained Soils

In fine-grained materials, such as silts and clays, the ice and liquid water can coexist at temperatures well below $0\degree C$. The unfrozen water content decreases roughly exponentially with decreasing temperatures below $0\degree C$, and hence the thermal conductivity and the apparent specific heat of
the partially frozen material vary with changes of temperature. Upon freezing, the thermal conductivity of soil increases and the apparent specific heat decreases. In most fine-grained soils the values of the variables remain reasonably constant at temperatures below about -6°C to -8°C.

Errors are introduced to the heat flow calculations if the presence of water in frozen soils and the changes in the thermal properties with temperature are ignored. The magnitudes of the resulting errors are not easily estimated. For a simple case, Williams (1972) showed that the error is about 20 percent in a depth of freeze calculation. The example chosen did not represent any extreme situation so Williams (1972) concluded that in depth of freezing or depth of thaw calculations involving the assumption that all the water in the soil freezes at 0°C, errors between 10 and 30 percent are to be expected in most cases.

The behaviors of coarse-grained and fine-grained soils to freezing and thawing are sufficiently different to require two distinct mathematical formulations to describe the different processes in the two soil types. As mentioned previously, the mathematical description of the freezing-thawing problem in coarse-grained soils is commonly referred to as a moving boundary with phase change. In contrast to the moving boundary problem, the freezing problem associated with fine-grained soils has received less attention. Important contributions have been made by Lukianov and Golovko (1957). They have developed the heat conduction equation for soils with fine pores, in which some water remains unfrozen at the
freezing point to form a transient freezing zone. The equation given by Lukianov and Golovko (1957), describing one-dimensional heat flow is:

\[
\frac{\partial}{\partial x} \left[ \lambda(x, t, T) \frac{\partial T}{\partial x} \right] - \left[ C_P(x, t, T) \frac{\partial T}{\partial x} \right] - L \frac{\partial G(T)}{\partial T} \frac{\partial T}{\partial t} = 0
\]

\hspace{1cm} \text{\ldots (2-36)}

Where \( \lambda \) = the thermal conductivity, 
\( T \) = temperature, 
\( C_P \) = the volumetric specific heat, 
\( L \) = the latent heat of fusion, 
\( G(T) \) = the ice content (outside freezing zone \( G = 0 \)), 
\( x \) = distance, and 
\( t \) = time.

Applying the equation (2-36) and using the experimental unfrozen water content curve, Nakano and Brown (1971) computed the temperature profile for Barrow silt by the finite difference method, and compared the calculated data to the values computed by using the Neumann's exact solution under the assumption that all water contained in the soil freezes at 0°C. Figure 14 shows the results of the computation for the case of \( t = 24 \) hr. and under the following initial and boundary conditions:

\begin{align*}
(a) \quad t = 0, \ x & \geq 0, \quad T(x, t) = T_i = 4°C \\
(b) \quad t > 0, \ x = 0, \quad T(x, t) = T_s = -4°C \\
(c) \quad t > 0, \ x = 2000 \ (\text{cm}), \quad T(x, t) = T_i = 4°C
\end{align*}
Figure 14 Temperature Profile for Barrow Silt Calculated at $t = 24$ HR Under the Conditions:

- $t = 0 \quad X > 0 \quad T(X, t) = T_{11} = 4^\circ C$
- $t > 0 \quad X = 0 \quad T(X, t) = T_{1T} = -4^\circ C$
- $t > 0 \quad X = 2000 \quad T(X, t) = T_{T1} = 4^\circ C$

(Nakano and Brown, 1971)
The temperature profile computed by equation (2-36) and the experimental unfrozen water content curve is smoother than that computed by using the Neumann's exact solution. The maximum difference between the two temperature profiles is about 0.8°C locally. If the freezing depth is defined as the distance from the surface to the freezing point (0°C), the difference in the calculated freezing depth for these two methods is about 30 percent (6 cm). In view of these effects, it is clear that the unfrozen water which exists under natural conditions in most frozen fine-grained soils plays an important role in the thermal regime involving phase change.

If no soil moisture movement occurs, the freezing in fine-grained soils can be treated numerically as long as the unfrozen water content curve of the material is provided. However, freezing in fine-grained soils is generally accompanied by migration of liquid water towards the freezing plane, resulting in the formation of ice lenses that may develop to a considerable thickness, particularly if the freezing occurs slowly. Consequently, the heat transferred by moisture flow and the changes of the thermal properties of soil produced by the redistribution of water (and hence ice) affect the thermal calculations of a freezing soil. Assuming water in the soil does not move and considering heat conduction only, Nakano and Brown (1971, 1972) have presented a numerical one-dimensional model for predicting temperature distributions in cold region soils. They presented data and modeling results for a test area near Barrow, Alaska. It is significant that Nakano and Brown (1972) observed that heat and mass transfer
are the two major physical processes taking place in arctic tundra soils. They stressed that the effect of mass transfer is an important factor to be considered.

Recently several investigators have embarked on projects to develop coupled heat and mass transfer models for soil-water systems during freezing and thawing; notably Kennedy and Lielmezs (1973), Harlan (1971, 1973), Guymon and Luthin (1974), Bresler and Miller (1975).
2.4 Water Movement in Freezing Soil-Water Systems

Water movement in porous material is a complex phenomenon. Soil water moves in response to gradients in the soil-water potential. The various types of potential gradients which could result in moisture transfer in soil have been summarized by Winterkorn (1958) as follows:

1. Hydrostatic potential;
2. Potential due to the hydration energy of ions, related to heat of wetting;
3. Potential due to the osmotic energy of ions;
4. The capillary potential (suction) due to the surface tension of water and the size and geometry of the soil pores;
5. Applied electric potentials;
6. Thermal gradients; and
7. Vapor pressure potentials.

In natural systems, none of these potentials act alone, thereby resulting in a complicated physical phenomenon. Water movement may occur in either or both the liquid and vapor state and in each phase as mass movement or diffusive flow.

2.4.1 Unsaturated Flow Under Isothermal Condition

Under isothermal conditions, soil moisture flow in the liquid phase is given by the modified Darcy's law:

\[ V = -K(\theta, T) \frac{\Delta \phi}{\Delta X} \]  

\[ \text{.... (2-37)} \]
Where \( V \) = water flux, \\
\( K (\theta, T) \) = hydraulic conductivity, and \\
\( \frac{\Delta \phi}{\Delta X} \) = potential gradient.

The hydraulic conductivity, \( K (\theta, T) \), is a function of temperature \( (T) \) and moisture content \( (\theta) \). The magnitude of \( K (\theta, T) \) is determined by the physical characteristics of the soil, the properties of the fluid, and the interaction between the soil and the fluid. The potential gradient, \( \Delta \phi/\Delta X \), is the driving force and depends on the capillary, osmotic, pressure and gravitational components of the total potential.

Substituting equation (2-37) into the continuity equation results in the transfer potential distribution equation. The equation, expressed in vector notation, for unsaturated flow in soil-water systems under isothermal conditions is given as:

\[
V \cdot [K(\theta) \nabla \phi] = \frac{\partial \theta}{\partial t} \quad \ldots \quad (2-38)
\]

where \( V \cdot \) is the divergence operator, \( V \) is the gradient operator and \( t \) is time. For a specific set of initial and boundary conditions for the system, the continuity equation can be solved by analytical or numerical techniques in terms of the transfer potential. Once the transfer potential distributions are known, it is possible to compute the flux rate.
2.4.2 Moisture Movement Under Anisothermal Conditions
With Temperature Above Freezing

Moisture movement in porous media under temperature gradients has been studied by many workers. Most of them have dealt with soil water systems in which the temperatures were above freezing. Invariably, it was noted that soil moisture moved from the warmer to colder areas of the soil sample. The magnitude of the moisture transfer depended on the temperature gradient and the initial moisture content.

In a soil sample initially at an uniform temperature and moisture content, vapor pressure changes were found to occur in response to a temperature gradient. Hence, vapor pressure gradients were considered as the driving force for moisture flow under temperature gradients in nonfreezing soil water systems. It was found, however, that the amount of observed moisture transfer exceeded values calculated from the simple vapor diffusion equation based on Fick's law. In an attempt to account for this difference, Smith (1943) proposed that moisture movement from hot to cold occurs partly in liquid phase. In addition to changing the vapor pressure of water, a temperature gradient would also induce a suction gradient due to changes in surface tension, thus causing a thermocapillary flow directed toward the cooler areas. However, this hypothesis was not supported by data that became available later by investigations using salt tracer techniques (Gurr et al., 1952; Kuzmak and Sereda, 1957).

Conceptually, water in soils at moisture contents
less than saturation can be visualized as occupying wedge-shaped volumes interconnected by thin liquid films existing in clay platelets and on soil particle surfaces (Kemper, 1960). Liquid transfer between wedge-shaped volumes and therefore through soil in general must take place through these films. Because the properties of these adsorbed films do not change significantly with temperature above 0°C, liquid transfer under temperature gradients in soil is assumed to be insignificant for most field and laboratory situations (Harlan, 1974).

To account for the higher observed vapor fluxes, Philip and de Vries (1957) postulated a "series parallel" mechanism for moisture flux in soil under temperature gradients. They assumed that liquid and vapor continuities in soil are disrupted since water occurs as "islands" in the neck of pores between solid particles. When a temperature gradient is imposed, water vapor condenses on one side of these "islands" and evaporates from the other. As a result, liquid flow will occur across the "islands", thus enhancing the vapor flow. Furthermore, Philip and de Vries (1957) argued that the magnitude of the temperature gradient in air voids exceeded the over-all temperature gradient in the system by a factor of 2 or 3, which would also induce vapor transport. As expected, the "series parallel" theory predicts a much higher vapor flux and is in better agreement with experimental observations than the simple vapor diffusion theory. The concept of stepwise transfer of moisture by vapor diffusion and liquid flow has been supported by Woodside and Kuzmak (1958) and Woodside and Cliffe (1959). The existence of larger
temperature gradients in the air voids was experimentally measured by these investigators on a large scale model.

The "series parallel" theory proposed by Philip and de Vries has a sound theoretical basis and predicts moisture fluxes of the correct order of magnitude. However, the flux equation developed by this theory is limited in application because of the large number of parameters involved and the difficulty in measuring them. More recently, the problem of nonisothermal diffusion of water vapor in soil has been approached by using the theory of irreversible thermodynamics (Taylor and Cary, 1964; Luikov, 1966; Groenevelt and Bolt, 1969). The irreversible thermodynamic approach, based on an accepted theoretical consideration, is more general than the theory of Philip and de Vries, and does not invoke any model or mechanism. Cary (1963) applied this theory satisfactorily to vapor transport under a temperature gradient across an air gap.

2.4.3 Water Movement in Frozen Soils

The movement of moisture in soil under temperature gradient with the cold-side temperature below freezing is much more complex than above freezing systems as several of the many transfer potentials may be present. The mechanism of water transport in freezing soil-water systems, accompanied by a change of phase, is complicated by the simultaneous transfer of heat and water; the latter occurs in both liquid and vapor phases. Dirksen and Miller (1966) have shown that the process of water movement in soil is considerably altered by the presence of an ice phase. In general, the freezing
process induces both heat and moisture transfer from warm to cold areas.

Experience and experiments indicate that as a soil cools below the freezing point not only does the water in the frozen zone turn to ice but also the water which was not originally in the frozen zone moves into the frozen zone from the surrounding unfrozen soil and then freezes (Dirksen, 1964; Ferguson et al., 1964). This migration of water is continuous as long as the temperature gradient exists and an external water supply is available. If the soil pores become filled with ice, ice lens formation can be expected to take place and the soil will heave.

The moisture migration and freezing process are coupled and jointly influence the temperature field and the rate of heat transfer. Unless provision is made to properly account for the resulting heat transfer and modification to the thermal properties, the model proposed to deal with the freezing soil-water system is not physically consistent. Moreover, this migration of water, with or without significant frost heaving, is an important consideration in construction works and to the fields of hydrology and agriculture in both seasonal frost and permafrost regions. For example, from a hydrologic point of view, the moisture distribution at snowmelt time may significantly affect the capacity of soil to infiltrate water.

The mechanism that causes the attraction of water from the unfrozen zone into the frozen zone while freezing occurs in a soil-water system has been a subject of contro-
versy for a long time. Jumikis (1966) concluded that the modes of moisture transportation upon freezing are: vapor transport, film-capillary transport, film transport, and the combination of vapor and film transportation. Vapor diffusion occurs when the voids are relatively large and there is no continuous soil moisture in liquid form in the voids. The driving pressure is the vapor pressure difference between the partial vapor pressure at the warmer end and the partial vapor pressure in the region of the soil system where ice exists. The moisture migration in the vapor phase takes place in the direction along the drop of the thermal gradient. If a soil is completely saturated, moisture migration can not take place in the vapor phase. If the packing of the soil particles is very dense, moisture transfer in the vapor phase is ineffective.

When the packing of the soil particles is such that the voids are occupied by the capillary water which is interconnected through the soil system by the film water on the surface of the soil particles, a movement of film-capillary soil moisture from warm areas to the freezing isothermal surface takes place. Under these conditions, the driving force is the capillary pressure gradient along the warm end to the curved surface, or menisci, at the freezing ice lenses, plus the flow pressure (molecular, viscous, or both) caused by molecular motion of the warmer particles of water to the cold front.

In a soil in which the soil particles are densely and closely packed to the extent that the soil particles are so close to each other that the moisture around and bet-
ween them forms uninterrupted liquid films throughout the entire soil system, and depending upon the texture of the soil, the film transport mechanism becomes more effective than the capillary transport. Similarly, moisture transport in the vapor phase is insignificant compared with the movement of liquid. In film transport, the driving pressure is the pressure difference between the warm regions and the cold regions caused by the thermo-viscous flow of the film moisture and other potentials. These may be the result of differences in density of moisture at different temperatures, or differences in electrolyte concentration at different elevations in the soil system. The film moisture moves parallel to the soil particle surface after overcoming the shearing resistance of the liquid.

Depending upon the texture and gradation of the soil, the degree of packing of the soil particles, and the presence of a multilayered soil system, a combination of the various soil moisture transport mechanisms may exist simultaneously upon freezing. In reporting results on moisture transfer in freezing soil, Jumikis (1966) pointed out that it is essential to report also the porosity of the soil, because for each degree of packing there is a different moisture transport mechanism in action.

2.4.3.A Experimental Works

Dirksen (1964) performed experiments of measuring water-content profiles as a function of time in an unsaturated soil column subjected to temperature gradients with the cold-
side temperature below freezing. The columns were sliced at the indicated times and the total water content of each slice was determined gravimetrically. The test results obtained from a New Hampshire silt are presented in Figures 15 and 16. The results clearly show that the presence of a freezing face induces substantial moisture transfer. From his experiments, Dirksen (1964) also observed that not only moisture flow took place from unsaturated unfrozen soil to the freezing front but also the total water and ice content behind the freezing front continued to increase with time over an extensive region. The changes inside the frozen soil were so great and so rapid that they could not be explained by thermal vapor diffusion. The magnitude of vapor transport calculated from the equation for vapor diffusion given by Philip and de Vries (1957) showed that it was too small by a factor of at least 1000. With this evidence, Dirksen and Miller (1966) concluded that during freezing of the soil all the water entering the frozen soil from the unfrozen region did not freeze at the freezing front but at least part moved appreciable distances into the frozen soil, and that the migration of water takes place mainly as liquid flow. Frozen soil actively extracts water from the unsaturated unfrozen soil as a result of the potential gradient set up by a decrease of pore water pressure in the unfrozen water films.

The importance of liquid transport from warm to cold regions as a consequence of temperature gradients during freezing of a soil-water system was also observed by Hoekstra
FIGURE 15 TIME SEQUENCES OF FREEZING OF UNSATURATED SOIL COLUMN (Dirksen, 1964)
Fig. 16. Time sequences of freezing of unsaturated soil column (Dirksen, 1964)

- Temperature gradient: 1.38°C/cm
- Dry density: 1.60 g/cm³
- Porosity: 36.8%
(1966) and Cary and Mayland (1972). Hoekstra conducted experiments similar to those of Dirksen, in which the water content of a soil sample, 11.5 cm in diameter and 15.2 cm long, were measured as a function of time by the non-destructive gamma-ray attenuation method. His results showing the water content and temperature versus time at a distance 7.5 cm from the cold plate (temperature -10°C) are given in Figure 17. It can be seen that the water content initially decreased due to the migration of water toward the frozen zone. The minimum water content is when the sample reached 0°C. As soon as ice formed, the water content increases. From the results it is obvious that the water content increases after the soil is frozen.

Hoekstra (1966) presented the observed changes of water content profiles at different times within the sample as shown in Figure 18. From the areas under the curves, he determined the amount of moisture flow at a certain location in the sample. For example, the amount of water that passed through the cross section approximately 4 cm from the cold plate between 140 and 160 minutes is represented by shaded area A; likewise, the amount of water that passed through a cross section at 12.5 cm from the cold plate in the same time interval is proportional to the shaded area B. Flow rates as high as $0.63 \times 10^{-4}$ cm/s were measured in frozen soil in response to the imposed thermal gradients. Since vapor transport of water alone could not explain the high rate of moisture transfer, Hoekstra pointed out that water transport through the films of unfrozen water is probably highly signi-
FIGURE 17 WATER CONTENT AND TEMPERATURE VERSUS TIME AT 7.5 cm FROM THE COLD PLATE – COLD PLATE TEMPERATURE -10°C (Hoekstra, 1966)
FIGURE 18 WATER CONTENT PROFILES AT DIFFERENT TIME (MINUTES)

(Hoekstra, 1966)
ficant. In a series of soil column experiments, Hoekstra (1966) observed that the magnitudes of moisture flow in frozen and unfrozen soil were of the same order. With this evidence, he concluded that moisture flow in frozen soil appears to be as significant as flow in the unfrozen soil when freezing takes place. Figure 19 shows the relationship between rate of flow of water per unit temperature gradient and average temperature below 0°C for Fairbanks silt. The rate of flow can be seen to decrease with a decrease in temperature. This implies that the temperature of the system places a physical restraint upon the mobility of water in a partially frozen soil.

Cary and Mayland (1972) proposed a set of phenomenological equations describing both water and salt movement in unsaturated frozen ground. These equations were tested in a series of experiments in which temperatures ranging over the soil profiles varied from -0.5 to -5°C. Water and salt redistribution in a silt loam were followed for six weeks. It was found, in agreement with earlier investigators, that the dominant water flow occurred along a pressure gradient in the unfrozen water interface. A typical flux observed was $1 \times 10^{-5}$ cm/day at an average matric potential of -1.0 MN/m². Cary and Mayland (1972) pointed out the equations such as these are applicable only when ice lensing does not occur; otherwise established flow paths are disrupted and flow is drastically and unpredictably reduced.

Observations of the behavior of soil-water systems have shown liquid water to exist as films adsorbed on the
FIGURE 19 RATE OF FLOW IN FROZEN SOIL AS A FUNCTION OF TEMPERATURE BELOW 0°C
(Hoekstra, 1966)
surface of soil particles in equilibrium with ice at temperatures far below 0°C. The unfrozen water content and hence the thickness of the adsorbed films has been shown to depend mainly on temperature and except for very dry soil to be nearly independent of the total water content, that is, liquid water and ice (Anderson and Koekstra, 1965; Low et al., 1968; Williams, 1968; Jame and Norum, 1972). The thickness of the liquid films decreases from 50 angstroms or more at 0°C to about 9 angstroms at -5°C and 3 angstroms at liquid nitrogen temperature (about -200°C) (Anderson, 1968).

The mobility of the unfrozen water films in a partially-frozen soil has been reported by Hoekstra and Chamberlain (1964). Anderson (1968) has also pointed out that these unfrozen liquid films are continuous and behave in a liquid-like manner; only below about -80°C do the properties of liquid water in the interfacial regions approach those of the solid state.

Because the unfrozen water content of a frozen soil decreases directly with temperature below 0°C, a thermal gradient in a frozen soil therefore can be considered to be acting in an analogous manner to a water content gradient in unfrozen soil. Liquid transfer is expected to occur from areas of higher water content to those of lower water content, i.e., from the warm to the cold side, at a rate dependent on the magnitude of the thermal gradient, the temperature of the system, and the surface or conducting area. Flow is confined primarily to the unfrozen water films. As mentioned previously, vapor transport in frozen soil under temperature gradients may
occur but was found to be several orders of magnitude lower than liquid moisture transfer due to hydraulic mechanisms (Dirksen, 1964). Since the liquid water content in frozen soil is independent of total water content, the migration of water should be continuous as long as the temperature gradient exists and an external water supply is available. No equilibrium moisture content distribution would be expected to be reached in the frozen soil. If the soil pores become filled with ice, ice lenses will form and the soil will heave. The frozen soil tends to act, therefore, like a sink. The formation of an ice lens may disrupt the continuity of the unfrozen water films, and thus the migration of moisture toward the cold side will be affected significantly.

2.4.3.B Harlan's Model

Adopting the concept of the analogy between mechanisms of water transport in unsaturated soil and those in partially-frozen soil, Harlan (1972, 1973) developed a model for water movement in frozen soil which was used subsequently as a basis for computer simulation of thermally-induced soil-water redistribution due to freezing as well as the infiltration of snowmelt and rainfall into frozen and partially-frozen soils.

In Harlan's model, the driving force for mass transport is the total potential gradient created by the temperature gradient at the frozen-unfrozen soil boundary. Since the thickness of adsorbed films in frozen soil decrease directly with temperature, the hydraulic conductivity should also decrease with temperature below 0°C. The flow is assumed to
be adequately described by application of the Darcy law used for flow in porous media. Mass flux is therefore given as the product of the potential gradient and hydraulic conductivity. As the amount of unfrozen water in a frozen soil is determined mainly by the magnitude of the negative temperature and independent of the total water content, mass conservation is necessary so that the negative divergence of liquid flow is taken to be the rate of ice accumulation. Latent heat released by ice accumulation produces a positive divergence of heat flow, completing coupling between mass and heat transport mechanisms during freezing of a soil-water system.

In frozen soil, ice, unfrozen water and vapor coexist at a certain temperature below 0°C. According to the condition of phase equilibrium and on the assumptions that water vapor behaves as an ideal gas, and that ice formed in the soil pores has the property of bulk ice, i.e., at atmospheric pressure, the resultant energy state, or soil-water potential of a frozen soil at a certain temperature can be expressed by the Gibbs free energy $\psi$ (Jame, 1972) namely:

$$\psi = \frac{RT}{M} \ln \left( \frac{P_{\text{ice}}}{P^o_T} \right) \quad \ldots \quad (2-39)$$

Where $R = \text{the ideal gas constant}$, $T = \text{the absolute temperature of the system}$, $M = \text{the molecular weight of water}$, $P_{\text{ice}} = \text{the vapor pressure of pure bulk ice at temperature } T$, and $P^o_T = \text{the vapor pressure of supercooled water at temperature } T$. 
Values for the vapor pressure of supercooled water and vapor of pure bulk ice at a given temperature below $0^\circ$C are fixed and can be found in physical tables such as the Smithsonian Physical Table (1961).

In much the same manner as the hydraulic conductivity of an unsaturated soil is related to the soil-water pressure head, the hydraulic conductivity of a partially-frozen soil can be related to the energy state of the soil-water-ice system. Although the hydraulic conductivity relationship should be similar for frozen and unfrozen materials, they are not necessary identical (Harlan, 1973). To indicate the possible order of magnitude of the hydraulic conductivity in frozen soils, Harlan (1974) presented values for a frozen Fairbanks silt for different soil-water potentials (see Figure 20). These conductivities were calculated from observed rates of flow in a frozen soil at different temperatures below $0^\circ$C as reported by Hoekstra (1966) and based on the assumption that fluid flow in frozen soil obeys Darcy's law. Actual values for the hydraulic conductivity of frozen soil are expected to extend over several orders of magnitude, depending not only upon temperature and soil surface area, but also upon the concentration of dissolved materials in the unfrozen solution and the presence of ice lenses in the soil-water system. Williams and Burt (1974) discuss a method for measuring the hydraulic conductivity of frozen soils and show the variability of the hydraulic conductivity as a function of temperature for a frozen silt.
FIGURE 20  CALCULATED HYDRAULIC CONDUCTIVITY AS A FUNCTION OF WATER POTENTIAL FOR FROZEN FAIRBANKS SILT

( Harlan, 1974 )
Harlan presented the model of coupled heat and mass transfer in a partially frozen soil and a finite difference numerical scheme for the solution. Using the same analogy between mechanisms of water movement in unfrozen and frozen soil as proposed by Harlan, Guymon and Luthin (1974) presented a one-dimensional model of heat and mass transport for arctic soil based on an equivalent quasi-linear variational functional for the Darcy equation and heat conduction equation including convection components. Guymon and Luthin's model was solved by a finite element analog.

2.4.3.C Capillary Sink Model

In contrast to Harlan's model, Bresler and Miller (1975) proposed the capillary sink model for defining water transport in frozen soil based on the capillary concept of soil freezing. The concept of the capillary model in freezing soil-water systems has been widely used to explain aspects of frost heaving in terms of the behavior of ice-water inter- faces in saturated soil.

Everett (1961) provided a relationship between capillary pressure and temperature. Following his idea, Miller (1963) believed that there exists a capillary pressure between ice and water in a soil just as there is one between air and water and that the soil water characteristic curves which show water content as a function of pore water pressure can be used to predict unfrozen water content of a frozen soil as a function of temperature and pore pressure. The results obtained in studies of saturated soil by Koopmans and
Miller (1966) demonstrated that an ice-water interface in non-colloidal (SS) soils behaved in a manner analogous to the behavior of an air-water interface in the same soil. Conversely, the theory does not apply to wholly colloidal (SLS) soils.

Miller (1972, 1973) extended the capillary theory to freezing of unsaturated soils, in which air-water, ice-water and air-ice interfaces exist. Figure 21 illustrates an equilibrium configuration of the three interfaces at the surface of a flat mineral particle having an adsorbed film of water. For the air-water-ice system to be in equilibrium the following conditions are required:

1) The freezing point of water, in the absence of solutes, obeys the general form of the Clapeyron equation. When the freezing point depression, \( \Delta T \), is small, its value can be calculated by the expression:

\[
\Delta T = \frac{(V_w P_w - V_i P_i)}{(\Delta H_f/T)}
\]  

(2-40)

Where \( P_w \) = the pore water pressure (negative in unsaturated soils),

\( P_i \) = the ice pressure,

\( V_w \) = the specific volume of water,

\( V_i \) = the specific volume of ice,

\( \Delta H_f \) = the latent heat of phase transition, and

\( T \) = the absolute temperature.

The pore water pressure is taken as that value measured by a
FIGURE 21 AN EQUILIBRIUM CONFIGURATION OF AIR-ICE, AIR-WATER AND ICE-WATER INTERFACES AT SURFACE OF A FLAT MINERAL PARTICLE HAVING AN ADSORBED WATER FILM (Miller, 1973)
tensiometer and does not represent the actual fluid pressure within an adsorbed water film.

(2) The shapes of three interfaces should be governed by the Kelvin equation for the pressure discontinuity at a curved phase boundary. For the air-water interface,

$$P_a - P_w = \frac{2\gamma_{aw}}{\gamma_{aw}}$$

where $P_a$ is the pressure of the soil air, $\gamma_{aw}$ is the surface tension of the air-water interface, and $\gamma_{aw}$ is the mean curvature of the interface. Since the soil air is assumed to remain at atmospheric pressure, i.e., $P_a = 0$ (gauge), therefore,

$$P_w = \frac{-2\gamma_{aw}}{\gamma_{aw}}$$

For the ice-water interface,

$$P_i - P_w = \frac{2\gamma_{iw}}{\gamma_{iw}}$$

where $\gamma_{iw}$ is the surface tension of the ice-water, $\gamma_{iw}$ is the mean radius of curvature of the interface, taken to be positive when centered on the ice side of the interface.

For the air-ice interface,

$$P_i - P_a = \frac{2\gamma_{ai}}{\gamma_{ai}}$$
where $\delta_{ai}$ is the surface tension of the air-ice interface, $\gamma_{ai}$ is the mean radius of curvature, taken to be positive when centered on the ice side of the interface. It is assumed that the curvature of the air-ice interface in soil pores changes rapidly through condensation or sublimation when there are exposed areas of adsorbed film water very close by.

(3) Air-water, ice-water, and air-ice interfaces meet at a point, i.e., point P in Figure 21, and are mutually tangent at that point. This requires that:

$$\delta_{ai} = \delta_{aw} + \delta_{iw} \quad \ldots \quad (2-44)$$

The ratio of $\delta_{aw}$ to $\delta_{iw}$, obtained by Koopmans and Miller (1966) based on the experimental results, is equal to 2.2. Thus, from equation (2-44), it follows that:

$$\delta_{aw} : \delta_{iw} : \delta_{ai} = 2.2 : 1 : 3.2$$

Actual surface tension values provided by Hesstvedt (1964) are: $\delta_{iw} = 30$ mN/m and $\delta_{aw} = 72$ mN/m.

To satisfy condition (1), (2), and (3), the apparent contact angle, $\phi$, between the air-ice interface and the particle surface must have a value given by the following expression (Miller, 1973):

$$\phi = \cos^{-1} \left[ \frac{(\Delta H_f/T) \Delta T - (V + 1 - \delta_{iw}/\delta_{aw}) P_w}{(\Delta H_f/T) \Delta T - (V + 1 + \delta_{iw}/\delta_{aw}) P_w} \right]$$

$$\ldots \quad (2-45)$$

which gives $\phi$ as a function of the freezing point depression,
ΔT, and the pore water pressure $P_w$. If $P_w$ is held constant, a decrease in $ΔT$ causes the ice pressure $P_i$ to increase [see equation (2-40)] and $\phi$ to decrease [see equation (2-45)]. This demonstrates that both the ice pressure and the apparent contact angle $\phi$ in a soil pore ought to vary with changes in pore water pressure and temperature. The ice pressure in a freezing soil-water system is not necessarily at atmospheric pressure as it was assumed in Harlan's model. The assumption that pore ice is at atmospheric pressure and has the same Gibbs free energy as bulk ice at the same temperature has been used by many scientists [for example see Edlefsen and Anderson (1943), Hoekstra (1966) and Harlan (1971)]. Before Miller's capillary model of soil freezing was introduced, this assumption seemed to be the only way that the freezing point depression of water in moist soil could be reconciled with the Clapeyron equation (Jame, 1972). According to Miller's calculation (1972), the ice pressure is at atmospheric pressure only when the apparent contact angle, $\phi$, is 68 degrees. If $\phi$ is greater than 68 degrees, the ice pressure will be intermediate between the air pressure and the pore water pressure, i.e., less than atmospheric pressure, and if $\phi$ is less than 68 degrees, the ice pressure is greater than atmospheric pressure.

Applying the capillary theory of air-water-ice equilibrium in a single crevice formed between uniform cylindrical particles in orthogonal array, Miller (1973) observed that if pore water pressure is held constant, two critical temperatures, $T^*$ and $T^{**}$, will exist when the temperature is reduced below 0°C. At a temperature above $T^*$, stable
ice can not exist in the unsaturated pore because there is no combination of values of ice pressure, pore water pressure and temperature that will be compatible with pore geometry while simultaneously satisfying equilibrium conditions (1) and (2) as described previously. In the interval $0^\circ C > T > T^*$, therefore, the condition of state of water and ice will be as shown at the top of Figure 22.

When the temperature reaches $T^*$, an ice body in the form of a cylinder, inscribed beneath the air-water meniscus and between adjacent particles as illustrated at the right side of Figure 22, can satisfy the equilibrium conditions. In the range between $T^*$ and $T^{**}$, air, ice, and water can co-exist at equilibrium, with the ice content increasing as temperature decreases. An example of such a stable ice body is shown at the bottom of Figure 22.

The rate of change of ice volume with decreasing temperature increases when the temperature approaches $T^{**}$ and becomes infinite at that temperature. The critical temperature $T^{**}$ expresses a limit at which it becomes impossible to simultaneously satisfy equilibrium conditions if an air-ice interface is present with the air at atmospheric pressure. Consequently, when the temperature falls below $T^{**}$, the un-filled pore will spontaneously and irreversibly fill with ice if liquid water is available.

Both temperatures $T^*$ and $T^{**}$ are dependent upon the pore water pressure and the pore geometry. In principle, a similar situation would occur in unsaturated pores in soil upon freezing. When the cold wave progresses into the soil,
the indicated equilibrium ice content begins to rise after passage of the $T^*$ isotherm, and then jumps to pore saturation when the temperature reaches $T^{**}$. To the extent that pores in the wake of those isotherms fail to achieve equilibrium ice content, they constitute unsatisfied and active sinks for water, and will tend to energetically extract water from the only available source, the unfrozen soil.

Based on the capillary sink mechanism for extracting water from the frozen zone, Bresler and Miller (1975) introduced series-parallel moisture transport during freezing unsaturated soil. In unfrozen soil, series-parallel mechanisms involve liquid and vapor phases, whereas, in frozen soil, series-parallel transport involves moving pore ice and unfrozen liquid water. Pore ice will move with the same linear velocity as an ice lens grows in the frozen zone by reverting to film water on one side of the particles and back to ice on the other side depending on the pore water pressure and temperature at each location. The ice transport component is considered to be necessary and will interact strongly with liquid transport as a result of shear at the phase boundary. Since in the region near the freezing front, the moisture transport process appears too chaotic in the presence of active unsatisfied sinks, a detailed simulation of moisture redistribution in this region is very difficult, if not impossible. For practical purposes, Bresler and Miller (1975) presented a simplified model for the simulation of soil-water redistribution during freezing an unsaturated soil based on the capillary theory of soil freezing. The coupled
heat and mass transfer equations of their model were solved by the finite difference method.

2.4.4 Summary

To summarize, the mechanisms by which water is transported in freezing soil-water systems are highly complex, involving simultaneous transfer of heat and liquid flow. The nature of these mechanisms within the soil-water system is at present imperfectly understood. To date there is little supporting evidence from either field or laboratory investigation to validate any of the proposed models discussed previously for describing the coupled heat and mass transfer in soil involving freezing and thawing. It is known that mathematical modeling is futile if the physical laws governing the processes are not known or are misrepresented. For this reason the continued development of physical based mathematical models in conjunction with complete and well-designed observation programs in the field or laboratory are the greatest requirement for solving freezing and thawing problems in soil. Therefore one of the objectives of this research program was to determine experimentally the effect of heat and mass transfer on the freezing of soil so as to provide evidence for the development and/or validation of appropriate mathematical models.
2.5 COMPUTER SIMULATION OF HEAT AND MASS TRANSFER IN A PARTIALLY FROZEN SOIL

From the foregoing discussed models of heat and mass transfer involving freezing and thawing in soil, it is clear that two systems of simultaneous equations which express the interrelationships among the laws of heat and fluid flow and the characteristics of the fluid and the medium involved are required to describe the transfer processes. Since analytical solutions to nonlinear, partial differential equations associated with this problem are either impossible, or excessively cumbersome, the usual approach is to use numerical solutions.

The choice of the numerical method depends on the problem under consideration. The most common methods for this type of problem are finite-difference and finite-element methods. In the finite-difference method, the governing differential equation is converted directly to an algebraic equation by replacing derivatives in finite difference form and solving it numerically. This method is easy to understand and simple to program. However, there is an inherent limitation to it, namely the region of the problem must be divided into a regular grid, i.e., squares or rectangles. Thus, most real boundaries of soil layers or of structures in or on the soil must be approximated and the approximation may cause significant errors in the calculation.

The finite-element method involves, by using variational techniques, the finding of a functional which when
minimized is equivalent to the basic differential equation plus associated initial and boundary conditions. The solution of the equivalent variational problem can then be found approximately by numerical methods. The principal advantage of this method, because of the use of triangular-shaped elements, is the accuracy and efficiency with which complicated geometrical boundaries can be treated.

Although advantageous for two-dimensional problems, especially if complex geometries are involved, the finite-element method possesses little if any advantage over the well known finite-difference method for one-dimensional problems. Emery and Carson (1971) compared the overall computation times of these two methods for the case of a one-dimensional diffusion equation. They found that the finite element formulation required several times as many calculations as the finite-difference formulation. For one-dimensional analysis, the finite-difference method is in common use.

Two different forms are distinguished in the finite-difference method, ie., explicit and implicit forms. Each form has different schemes depending on how the derivatives are replaced by the finite differences. Since both heat and mass transfer equations are basically a type of diffusion equation, a simple diffusion equation with homogeneous material properties is employed to discuss various numerical schemes used to treat the freezing and thawing problem in soil.

For the governing differential equation

\[
\frac{\partial U}{\partial t} = \alpha \cdot \frac{\partial^2 U}{\partial x^2}
\]

\[\ldots\] (2-46)
let

\[ U^n_i = U(x, t) = U(i \Delta x, n \Delta t) \]

where \( a \) = diffusivity,
\( \Delta x \) = the grid spacing,
\( \Delta t \) = the time step,
\( x \) = distance coordinate,
\( t \) = time, and
\( \beta = a \Delta t / (\Delta x)^2 \).

In the following discussion, grid-points involved for the derivation of the finite difference equation in the scheme are shown in the respective diagram. Symbols ⬜ in the diagrams indicate the known values and ⬝ are for the unknown values to be calculated.

(a) The explicit form:

(i) Forward difference scheme

The finite difference equation for the governing partial differential equation is

\[ \frac{U^{n+1}_i - U^n_i}{\Delta t} = \alpha \cdot \frac{(U^n_{i+1} - 2U^n_i + U^n_{i-1})}{(\Delta x)^2} \]

or
\[ u_{i+1}^n = \beta u_{i-1}^n + (1 - 2\beta) u_i^n + \beta u_{i+1}^n \quad \ldots \quad (2-47) \]

The forward difference scheme, though simple to program, has same drawbacks. As can be seen from equation (2-47), \( u_{i+1}^n \) depends only on \( u_{i-1}^n \), \( u_i^n \), and \( u_{i+1}^n \). Referring to Figure 23, only those values of \( U \) within the pyramid-shaped area A can have any influence on the value of \( u_{i-1}^n \), whereas it is known that the solution \( U(x, t) \) of the governing differential equation depends also on the values of \( U \) both in A and in B for times earlier than time level \( n+1 \).

Figure 23 Limitation of the forward difference scheme

The major drawback of this scheme is the stability problem. The stability criterion for the forward difference method requires that \( 0 < \beta \leq \frac{1}{2} \). This requirement places an undesirable restriction on the time step as it must be chosen small enough to guarantee a stable solution. For problems extending over large values of time, this could result in an excessive amount of computation time. This scheme is therefore considered to be inefficient for practical computations. Nevertheless, this method has been used by Dempsey (1970) and Ho et al. (1970) to study the transient temperature distribution involving freezing and thawing in road pavements. On
the basis of comparisons between predicted and observed data, Ho et al. (1970) concluded that their program could be used for thermal pavement design in frost regions.

(ii) Alternating-direction scheme (Saul'yev method)

Advance to time level \( n+1 \) by proceeding in the positive \( x \)-direction with the following finite difference equation,

\[
\frac{u_{i+1}^n - u_i^n}{\Delta t} = \alpha \cdot \frac{(u_{i-1}^{n+1} - u_{i+1}^{n+1} - u_i^{n+1} + u_i^n)}{(\Delta x)^2}
\]

ie.,

\[
u_{i}^{n+1} = \frac{(\beta u_{i-1}^{n+1} + (1 - \beta) u_{i}^{n} + \beta u_{i+1}^{n})}{(1 + \beta)}
\]

and then advance to time level \( n+2 \) by proceeding in the negative \( x \)-direction over the same region with the following finite difference:
\[
\frac{u_i^{n+2} - u_i^{n+1}}{\Delta t} = \alpha \cdot \frac{(u_{i-1}^{n+1} - u_i^{n+1} - u_{i+1}^{n+1} - u_{i+1}^{n+2})}{(\Delta x)^2}
\]

or

\[
u_i^{n+2} = \frac{[ \beta u_{i-1}^{n+1} + (1 - \beta) u_i^{n+1} + \beta u_{i+1}^{n+2} ]}{(1 + \beta)}
\]

The alternating-direction procedure is then repeated for successive pairs of time-steps. Note that \(u_{i-1}^{n+1}\) in equation (2-48) and \(u_{i+1}^{n+2}\) in equation (2-49) will be known either from computations at the preceding grid point or from a boundary condition.

The alternating-direction explicit method possesses unconditional stability while retaining much of the programming simplicity of the forward difference method. This method has been used in a number of papers involving freezing and thawing in soil (Doherty, 1970; Gold et al., 1972; Lachenbruch, 1970). One of the disadvantages of this method is that it may give rise to serious errors when used on systems where a sharp contrast in material properties of neighboring layers occurs. Furthermore, the truncation error for this method is large, as even for a homogeneous system with uniform grids, relatively short time-step must be used to obtain useful accuracy.

(b) the implicit form

The implicit method overcomes the difficulties associated with the explicit method, but at the expense of a
somewhat more complicated calculation procedure. It consists of representing the derivative with respect to x by a finite-difference form evaluated at the advanced point of time level n+1, instead of at time level n as in the explicit method. Two different forms of this method are commonly used; namely the backward-difference and the Crank-Nicholson form.

(i) Backward-difference scheme

\[
\frac{U_{i}^{n+1} - U_{i}^{n}}{\Delta t} = \alpha \cdot \frac{(U_{i-1}^{n+1} - 2U_{i}^{n+1} + U_{i+1}^{n+1})}{(\Delta x)^2}
\]

Rearranging, the equation becomes

\[
-\beta U_{i-1}^{n+1} + (1 + 2\beta) U_{i}^{n+1} - \beta U_{i+1}^{n+1} = U_{i}^{n}
\]

\[
\ldots \quad (2-50)
\]

(ii) Crank-Nicholson scheme
The finite difference form of the governing partial differential equation i.e., equation (2-46), is

\[
\frac{U_i^{n+1} - U_i^n}{\Delta t} = \frac{\alpha}{2(\Delta x)^2} \left[ (U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}) + (U_{i-1}^n - 2U_i^n + U_{i+1}^n) \right].
\]

That is

\[
-\beta U_{i-1}^{n+1} + 2(1 + \beta) U_i^{n+1} - \beta U_{i+1}^{n+1} = \beta U_{i-1}^n + 2(1 - \beta) U_i^n + \beta U_{i+1}^n \quad \ldots \quad (2-51)
\]

Implicit methods involve the solution, at each time-step, of a system of linear algebraic equations, and thus require somewhat more calculations per time-step than do explicit methods. However, stability of the implicit methods is unconditional and truncation error is small enough to allow the use of much larger time-steps. Furthermore, the system of linear equations resulting at each time step of the implicit methods is a tridiagonal matrix. A system of linear equations can be solved by a Gaussian elimination method; but with a tridiagonal matrix, the solution can be obtained more efficiently by a specific technique (see Appendix A) and can save a lot of computational time. The total computational time required to achieve a solution may be significantly less than what would be required by explicit methods.

Since the Crank-Nicholson scheme of equation (2-51) requires only slightly more computations per time-step than
the backward-difference method of equation (2-50), and produces a significantly smaller truncation error, the Crank-Nicholson method is, therefore, highly recommended and has been widely used (Nakano and Brown, 1971; Harlan, 1973; Bresler and Miller, 1975).
CHAPTER III

EXPERIMENTAL METHOD AND RESULTS

The temperature and water-content profiles in soils under different temperature gradients with the cold-side temperature below freezing were measured as a function of time and distance from the cold face in soil samples placed in a horizontal, cylindrical tube. The soil column was insulated to ensure that one-dimensional heat transfer occurred. Measurements of the moisture contents within the sample were obtained using the gamma radiation attenuation method. All temperature were recorded by thermocouples.

3.1 EXPERIMENTAL MATERIAL AND THERMAL UNIT

The soil material used in the study was a #140 mesh silica flour (Hoskin Scientic Ltd., Montreal), with a particle size distribution as:

<table>
<thead>
<tr>
<th>Sieve Size</th>
<th></th>
<th>% Finer Than</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>Diameter (mm)</td>
<td>(by dry weight)</td>
</tr>
<tr>
<td>100</td>
<td>0.149</td>
<td>99.8</td>
</tr>
<tr>
<td>140</td>
<td>0.106</td>
<td>98.6</td>
</tr>
<tr>
<td>200</td>
<td>0.074</td>
<td>92.4</td>
</tr>
<tr>
<td>270</td>
<td>0.055</td>
<td>81.6</td>
</tr>
<tr>
<td>325</td>
<td>0.044</td>
<td>71.2</td>
</tr>
</tbody>
</table>

The necessary bulk of soil, previously conditioned to the required moisture content, was packed into a lucite tube: 30 cm in length and 10 cm in diameter. To achieve an uniform density throughout each sample, the soil was packed in twelve layers, each approximately 2.5 cm in thickness.
The average dry density of the soil sample was approximately 1.33 g/cm³ and the porosity was 0.49.

Hollow brass circulation plates were placed at both ends of the soil column and the unit was sealed with wax so that no water could flow into or out of the system. Twelve copper-constantan thermocouples were inserted into the center of the soil sample at 2.5 cm intervals for temperature measurements (see Figure 24).

Details of the construction of the thermal unit, with the prepared soil column in position, are illustrated in Figure 25. The prepared soil column, surrounded by 10 cm layer of styrofoam, was positioned inside a 32 cm diameter copper cylinder, open at both ends. The gap between the styrofoam and the copper cylinder was packed with rock wool. The copper cylinder was covered with 2 cm of rock wool for insulation and the whole unit was placed horizontally on the top of a lathe bed.

At each end of the sample, two loops of circulating copper tube were placed tightly inside the perimeter of the copper cylinder. Liquid in the hot and cold temperature-controlled baths was circulated through loops of copper tubing as well as through the hollow brass circulating plates at either end of the insulated soil column. This arrangement (see Figure 25) resulted in the same overall temperature gradient in the outer copper cylinder as in the soil column, thus providing reasonable assurance of one-dimensional heat transfer in the soil sample.

Anti-freeze solution was used as the circulation liquid. The hot and cold liquids, conditioned to the desired tempera-
Figure 24: A prepared soil column
FIGURE 25 THE THERMAL APPARATUS
tures were circulated to the thermal unit by immersion pumps located in the hot and cold temperature-controlled baths. A COLORA Minicryostates Model KKS served as one of the temperature-controlled baths used in this experiment. The other one was a MR-3262A constant temperature bath from Blue M Electric Company.

The thermocouple reference was maintained at 0°C by a ZEREF Model 136C ice point reference from Mectron Ltd. The outputs of the thermocouple potentials were monitored by a DANA 5900 digital multimeter having a resolution of one microvolt on the 0.1 V range.
3.2 EXPERIMENTAL PROCEDURE

To start each experiment, the soil column was first brought to the desired initial temperature. This was done by setting the two temperature-controlled baths at the same temperature and circulating liquid to the unit. Usually it took about ten hours to cool the soil column from room temperature to an initial temperature of 5°C. Gamma radiation intensities taken before cooling the sample and after it had reached the initial temperature showed that no detectable moisture redistribution occurred in the column during the cooling period.

When the soil column attained a uniform initial temperature, the temperature at one end of the column was maintained at the initial temperature while the other end of the column was cooled to and then kept at a constant low temperature by resetting the constant temperature bath. Gamma radiation intensities and thermocouple potentials were recorded periodically to determine moisture contents and temperatures within the soil column.

Each test was continuous for 72 hours. At the termination of each experiment the soil container was removed from the apparatus and the soil column was promptly forced out of the tube and sliced into transverse sections of 1 to 1.5 cm thickness by an electric saw. The soil sections were weighed and put in an oven at 105°C for three days to determine the gravimetric water content.
3.3 MOISTURE CONTENT MEASUREMENT - GAMMA RAY ATTENUATION METHOD

Measurements of the moisture contents within the soil sample as a function of time and distance from the cold face were carried out by the gamma-ray attenuation method. The procedure followed was similar in principle to that used by Gurr (1962). The technique allowed the determination of the moisture content at any given position along the column without disturbing the soil. The theory and technique of measuring moisture contents by the gamma-ray attenuation method are well known (Gardner, 1965).

The arrangement of the equipment, the source, and the detector is shown in Figure 26. The source of gamma radiation was 200 millicuries of Cs$^{137}$ that was contained in a 20 cm x 20 cm x 20 cm lead block. The collimated gamma rays were monitored by a solid sodium iodide (NaI) crystal 2.5 cm in diameter. The gamma rays were collimated through 2mm diameter holes in the lead block containing the Cs$^{137}$ source and the 5 cm x 20 cm x 20 cm lead shield in front of the NaI crystal.

The probe used was a Nuclear-Chicago Model. Next to the NaI crystal was a photomultiplier tube which was mechanically attached and optically coupled to the crystal. The tube operated on a high voltage of 900 - 1600 volts D.C. The output of the scintillation detector is related to the voltage applied to the phototubes of the detector. The starting potential of the detector is the voltage at which the detector first begins to detect radiation. As the applied voltage is increased a region is reached where any further
FIGURE 26 SCHEMATIC DIAGRAM OF γ - RADIATION FOR MEASURING THE WATER CONTENT OF SOIL
increase in the voltage makes no appreciable difference to the count rate. This range of voltage is known as the plateau. The voltage at which this plateau begins is known as the threshold of the detector. For good results the operating voltage should be at the mid-point of the plateau. This was found to be 1250 volts. The high voltage was supplied by a ORTEC Model 446 high voltage power supply.

A signal from the photomultiplier tube is fed into a transistorized preamplifier which converts the output current pulses from the photomultiplier into voltage pulses and amplifies these pulses so that they are suitable for the pulse height analyzer. The preamplifier operates on a 10 volt D.C. power source.

The housing for the detector probe is a cylinder about 35 cm in length. This cylinder encloses all the principal parts of the detector assembly, ie. the NaI crystal, the photomultiplier tube and the preamplifier, and has electrical cables at the end leading to the high and low D.C. voltage sources and the pulse analyzer.

The pulse height analyzer used was a ORTEC Model 406A Single Channel Analyzer which sorted the pulses from the scintillation detector according to amplitude, passing those lying between two preselected limits to the Scaler-timer and discriminating against those of higher or lower energies. Those two limits define a 'window' or energy band, which was centered on the peak voltage produced by the Cs$^{137}$ source. By using this procedure the pulse height analyzer excluded scattered and background radiations. Cs$^{137}$ emits beta par-
articles, becoming Barium$^{137}$ which in turn emits gamma rays at 0.662 Mev. The base line and window width on the pulse height analyzer for this study was set to accept gamma radiation of 0.662±0.036 Mev. A ORTEC Model 434 digital ratemeter was used as the Scaler-timer which accumulated and stored pulses from the pulse height analyzer in digital form. The ratemeter totalized pulses during a precise preset time period.

A lathe bed was used to support the soil column, the source and the detector. Figure 27 and 28 show the experimental apparatus. The source holder and the detector placed 40 cm apart, were mounted on a carriage which could be moved along the lathe bed. The height and position of the platforms on which the source holder and the detector rested were adjustable, so that the collimated holes in the source and the detector could be aligned. The soil sample with its thermal insulation material was positioned horizontally between the source and the detector in such a way that the collimated gamma rays passed through the center of the soil sample when the source and the detector were moving back and forth along the soil column. To avoid interference due to condensation of water vapor on the copper cylinder of the thermal insulation unit, openings of dimension 5 cm x 36 cm were provided on both sides of the copper cylinder. The openings were only open while conducting the moisture measurements. Thus the gamma rays only penetrated through the styrofoam insulation layer, the soil container and the soil sample. The intensity of gamma radiation was measured as a function of time at 1 cm intervals along the soil column.
Figure 27  Experimental Apparatus for Freezing Test (Front View)
Figure 28 Experimental Apparatus for Freezing Test (Side View)
The basic equation describing the passage of primary monoenergetic radiation through a homogeneous material is given as:

\[ I = I_0 \exp (-\mu \rho x) \] \hspace{1cm} \text{(3-1)}

Where

- \( I \) = the intensity of the beam (counts/sec),
- \( I_0 \) = the radiation intensity with no interference (counts/sec),
- \( \mu \) = the mass absorption coefficient (cm²/g),
- \( \rho \) = the density of the material (g/cm³),
- \( x \) = the thickness of the material (cm).

For this study in which gamma rays passed through the styrofoam insulation layer, the soil container and the soil sample, equation (3-1) can be rewritten as:

\[ I = I_0 \exp \left[ -(\mu_{st} \rho_{st} x_{st} + \mu_{c} \rho_{c} x_{c} + \mu_{s} \rho_{s} d + \mu_{w} \theta d) \right] \] \hspace{1cm} \text{(3-2)}

where the subscripts \( st, c, s, w \), are for styrofoam, soil container, dry soil and water respectively, \( \theta \) is the volumetric water content, cm³/cm³, and \( d \) is the diameter of the soil sample, cm.

The attenuation of gamma radiation through a standard plastic material (subscript \( P \)) is given as:

\[ I_p = I_0 \exp (-\mu_{p} \rho_{p} x_{p}) \] \hspace{1cm} \text{(3-3)}

Dividing equation (3-2) by equation (3-3) and taking logarithms yields:
\[
\ln \left( \frac{I}{I_p} \right)_o = \mu_p \rho_p x_p - \left( \mu_{st} \rho_{st} x_{st} + \mu_c \rho_c x_c \right) + \mu_s \rho_s d + \mu_w \theta_o d \quad \text{(3-4)}
\]

In equation (3-4) the term \( \left( \frac{I}{I_p} \right)_o \) represents the count ratio of the rate at the start of the test and \( \theta_o \) is the initial water content. For any time, \( t \), the equation can be written as:

\[
\ln \left( \frac{I}{I_p} \right)_t = \mu_p \rho_p x_p - \left( \mu_{st} \rho_{st} x_{st} + \mu_c \rho_c x_c \right) + \mu_s \rho_s d + \mu_w \theta d \quad \text{(3-5)}
\]

Subtracting equation (3-5) from equation (3-4) gives

\[
\ln \left( \frac{I}{I_p} \right)_o - \ln \left( \frac{I}{I_p} \right)_t = \mu_w (\theta - \theta_o) d 
\quad \text{...... (3-6)}
\]

and it follows that

\[
\theta = \frac{\ln \left( \frac{I}{I_p} \right)_o - \ln \left( \frac{I}{I_p} \right)_t}{\mu_w d} + \theta_o \quad \text{...... (3-7)}
\]

The volumetric water content at each location in the sample at time \( t \) during the freezing process can be computed directly from equation (3-7). In applying the equation for this purpose, it is assumed that the structure of the solid soil matrix remains unchanged during the run, and that the mass absorption coefficient \( \mu \) for water and ice are the same. The first assumption is valid for a soil that does not shrink or swell. In freezing of a soil, if the soil pores become filled with ice as the result of moisture migration, frost
heaving might occur causing changes in the dry density. Under this circumstance, the moisture content measurement by the gamma-ray attenuation method fails. The second assumption is based on the assumption that the gamma radiation probably does not differentiate between ice and unfrozen water and hence it is unlikely that the value of $\mu_w$ depends on the phase composition of water in the frozen soil.

The count rate $I_p$ was taken on a 25.4 cm plastic bar before and after taking each count rate through the soil column. The rate through the soil at each location was then divided by the properly adjusted count rate through the plastic bar. This procedure served as a check on the stability of the electronic system during each measurement and eliminated the effect of fluctuations in the strength of the source.

For each measurement, five 20-second counts were taken. The average of these five readings was used in the calculation.

To solve equation (3-7), the value of the mass absorption coefficient of water, $\mu_w$, is needed. The procedure used to obtain this coefficient was to measure the radiation intensity through different thicknesses of water. This was done by placing a plastic channel having seven compartments, each with the dimension of 3 cm in thickness and 10 cm in depth, between the source and the detector probe. The compartments were filled with water one at a time and the radiation intensity was measured. The attenuation of gamma radiation is given as:

$$I = I_o \exp \left[ - (\mu_c \rho_c x_c + \mu_w \rho_w x) \right] \quad \ldots \quad (3-8)$$
where the subscripts c and w refer to the plastic container and water respectively, and x is the thickness of water.

Dividing equation (3-8) by equation (3-3), and taking the logarithm gives:

\[ \ln \left( \frac{I}{I_p} \right) = \mu_p \rho_p x - \mu_c \rho_c x_c - \mu_w \rho_w x \]  \hspace{1cm} \text{.... (3-9)}

or

\[ \ln \left( \frac{I}{I_p} \right) = A - \mu_w \rho_w x \]  \hspace{1cm} \text{.... (3-10)}

where A is a constant.

A plot of \( \ln \left( \frac{I}{I_p} \right) \) versus the thickness of the water, x, yields a straight line with the slope being the value of the product \( \mu_w \rho_w \). Figure 29 shows results obtained from one test. A straight line was fitted to the points by the least square method to obtain value of \( \mu_w \rho_w \). Assuming \( \rho_w \) was equal to unity, the average measured mass absorption coefficient of water, \( \mu_w \), for five tests is 0.083785 ± 0.00021 cm\(^2\)/g. This value is close to the theoretical value of 0.0855 cm\(^2\)/g given by Grodstein (1957). The same procedure was used to measure the mass absorption coefficient of the dry soil used in this study. The value was found to be 0.074024 ± 0.0008 cm\(^2\)/g.
FIGURE 29  DETERMINATION OF THE MASS ABSORPTION COEFFICIENT OF WATER
3.4 RESULTS AND DISCUSSION

Tests were conducted using average temperature gradients of 1°C/cm (cold end -10°C, warm end +20°C) and 1/3°C/cm (cold end -5°C, warm end +5°C) on samples having initial moisture contents of 5, 10, 15, and 20 percent by dry weight.

Measurements of radiation intensity taken at 1 cm intervals along the column revealed that the soil was uniformly packed. Assuming the moisture content was constant throughout the soil column it was found that the dry density of the soil at any point was between 1.28 g/cm³ and 1.39 g/cm³ with 86% of the values falling within ± 0.0302 g/cm³ of the mean.

To check if the heat transfer in the soil column was one-dimensional, the temperature at the midpoint of the soil column was measured when the ends were maintained at 5.0°C with an ambient temperature of 25°C. The midpoint temperature under these conditions was 5.4°C. An additional check was made by measuring, for each test, the temperatures at the outer edge of the soil column and the center of the soil column midway between the ends. The maximum difference in temperatures was 0.3°C. The difference could be a result of heat loss through the insulation, incorrect positioning of the thermocouple, or a difference in the thermal conductivities of the soil container and the soil sample.

In total, more than twenty freezing trials were conducted with the results being reproducible. The results from some of the tests are shown in Figure 30 to 36. From the results obtained in the test program it was found:
FIGURE 31 SOIL MOISTURE AND SOIL TEMPERATURE DISTRIBUTIONS; (INITIAL SOIL MOISTURE CONTENT 15.00% ; TEMPERATURE GRADIENT = 1/3 °C/CM.) (TEST NO. 8)
Figure 32 Soil moisture and soil temperature distributions; (initial soil moisture content 10.08%; temperature gradient = \(1/3\) °C/cm.) (Test No. 9)
Figure 33: Soil moisture and soil temperature distributions. (Initial soil moisture content 19.92 %; temperature gradient ~ 1 °C/cm.)
FIGURE 34  SOIL MOISTURE AND SOIL TEMPERATURE DISTRIBUTIONS; (INITIAL SOIL MOISTURE CONTENT 15.45%; TEMPERATURE GRADIENT = 1 °C/CM.)
(TEST NO. 13)
FIGURE 35
SOIL MOISTURE AND SOIL TEMPERATURE DISTRIBUTIONS; (INITIAL SOIL MOISTURE CONTENT = 9.92 %; TEMPERATURE GRADIENT = 1 °C / CM.)

DISTANCE FROM COLD END (CM.)

% WATER (ICE) CONTENT (BY DRY WT.)

TEMPERATURE °C
1. Due to the low moisture content in the unfrozen regions and the short experimental period, ice lenses were not observed and frost heaving did not occur.

2. The moisture contents measured by the gamma radiation technique and those determined by the gravimetric method were in close agreement both in frozen and unfrozen regions. As mentioned previously, if frost heaving occurs in the soil, the gamma radiation attenuation method could not be used to measure the soil moisture content because by using the method one assumes that the soil matrix remains unchanged.

3. The moisture content of the soil close to the cold plate did not increase substantially as observed by Dirksen (1964) and Hoekstra (1966) (see Figures 15, 16, and 18). In his experiments, Hoekstra found that a small layer of ice had formed directly under the cold plate which caused the sharp increase in water contents in the proximity of the cold plate. He claimed that the ice lens was probably formed by sublimation of the water vapor. In the present study when the sample was examined at the end of each run, no ice layer was found directly under the cold plate.

4. An extremely sharp discontinuity in the moisture profile exists at the freezing front. Behind the freezing front the water (ice) content is substantially higher than the initial moisture content, while the moisture content in front of the freezing front is much lower. The moisture content profiles in the unfrozen soil were found to be relatively uniform at any given time. The moisture content profiles in
the unfrozen region obtained by Hoekstra (1966) (see Figure 18) show a sharply decreasing moisture content near the frozen soil.

5. The moisture content at any point within the frozen part of the soil column, with the exception of that zone immediately adjacent to the freezing front, did not increase substantially with time. These observations also are contradictory to the results reported by Dirksen (1964) and Hoekstra (1966). These differences in findings are attributed to the fact that different types of soil were used in the experiments. For the sample used in the study, the amount of unfrozen water at soil temperature below -1°C was very small, about 2% by dry weight and the amount changes very little with a decrease in soil temperature (Jame and Norum, 1972). As the rate of water transport in the frozen region was very slow, the change of water content in that area could not be detected in a short time period.

6. Different temperature conditions imposed on soil columns having the same initial moisture content affects the shape of the moisture distribution profiles. In comparing Figures 31 (Test No. 8) and 34 (Test No. 13), in which the initial soil moisture content were 15% and 15.45% respectively, it is quite evident that there is a general tendency for the soil moisture content within the frozen zone to increase to the freezing front under a temperature gradient of 1°C/cm (-10°C at cold end and +20°C at warm end) as in the case of Test No. 13, whereas in the case of Test No. 8 where the temperature gradient was 1/3°C/cm (-5°C at cold end and +5°C
at warm end) the moisture content within the frozen zone was relatively constant. This characteristic reflects the effect of the rate of advance of the freezing front into the soil on the shape of the moisture content profile; the longer the freezing front became stationary at a certain position, the greater the amount of water would accumulate near the freezing front.

7. Under a given temperature gradient, the higher the initial soil moisture content, the deeper the freezing front penetrated into the soil. For the temperature gradient of 1°C/cm (-10°C at cold end and +20°C at warm end), the depth of freezing at different times for initial moisture contents 19.92%, 9.92%, and 5.59% were as follows:

<table>
<thead>
<tr>
<th>Time (hours)</th>
<th>19.92%</th>
<th>9.92%</th>
<th>5.59%</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3.3</td>
<td>3.4</td>
<td>3.4</td>
</tr>
<tr>
<td>4</td>
<td>5.3</td>
<td>5.2</td>
<td>5.2</td>
</tr>
<tr>
<td>6</td>
<td>6.7</td>
<td>6.7</td>
<td>6.6</td>
</tr>
<tr>
<td>12</td>
<td>9.5</td>
<td>9.0</td>
<td>8.2</td>
</tr>
<tr>
<td>24</td>
<td>12.5</td>
<td>11.0</td>
<td>9.2</td>
</tr>
<tr>
<td>72</td>
<td>14.5</td>
<td>12.3</td>
<td>9.5</td>
</tr>
</tbody>
</table>

Figure 37 shows the temperature profiles of these three tests. It can be seen from the Figure that in the early stages of cooling the temperature profiles as well as the depth of freezing
for the three samples were almost the same. However, as time progressed the rate of advance of the freezing front in the samples having the lower moisture content becomes slower than in the samples with higher moisture content.

8. A preliminary phenomenological analysis of the experimental results indicated that the processes of heat transfer and moisture migration are coupled in a very complex fashion. A complete mathematical model describing simultaneous heat and mass transfer involving a phase change is needed to explain the behavior of this complex phenomenon. Efforts to develop and solve such a model are presented in the next chapter.
Figure 37: Temperature distributions with different water content.
CHAPTER IV

NUMERICAL SIMULATION OF COUPLED HEAT AND MASS TRANSFER IN A FREEZING UNSATURATED SOIL

A mathematical model describing one-dimensional heat and moisture transfer in a horizontal soil column resulting from the application of a sub-freezing temperature was solved numerically by the finite difference method. The model is essentially that reported by Harlan (1971, 1973). This model was chosen over the Bresler-Miller model because the latter is used primarily for ice lens modelling. The current study did not consider cases where ice lensing would occur. The predicted temperature and moisture distributions along the soil column as a function of time were compared to the experimental results to test the validity of Harlan's model and its accuracy for predicting heat and mass transfer.

4.1 CONCEPT OF THE MODEL

The concept of Harlan's model is described in Section 2.4.3.B. The model requires the solution of two equations, one for heat transfer and another for moisture transport. The model is based on the following assumptions:

1. The porous media are nondeformable. Various changes in soil matrix, such as those due to swelling, frost heave, and expansion of water volume on ice lens formation in the soil, are negligible.

2. Convective heat transfer associated with movement
of the gaseous phase is small and its effect on net heat transfer is negligible.

3. All processes are single valued; i.e. hysteresis is not present in relationships such as the soil water characteristic curve.


5. The amount of unfrozen liquid water in a partially frozen soil is determined by temperature only. Dissolved salts have a negligible effect on the amount of unfrozen water.

6. Moisture movement takes place in the liquid phase. Vapor movement is small and can be neglected.

The basic equations used in the model are given below. Details of the derivation of these equations were presented by Harlan (1971, 1973).

Heat transfer equation:

$$\frac{\partial}{\partial x} \left[ \lambda (x, T, t) \frac{\partial T}{\partial x} \right] - C_p L \frac{\partial (V_x T)}{\partial x} = \frac{C_p}{\partial t} \frac{\partial T}{\partial t}$$

(4.1)

Where

- $\lambda$ = thermal conductivity, W/cm°C,
- $T$ = temperature, °C,
- $x$ = position coordinate, cm,
- $t$ = time, seconds,
- $C_p$ = the mass specific heat of water, J/g °C,
- $\rho_L$ = the density of water, g/cm³,
- $V_x$ = the fluid flow velocity in x direction, cm/s,

and
The apparent volumetric specific heat, incorporating the latent heat of fusion, is estimated by the equation,

\[
C_p = \sum_{i=1}^{n} (C_p)_i \phi_i - \rho_s \frac{\partial \theta_s}{\partial t} \quad \ldots \quad (4-2)
\]

Where \((C_p)_i\) = the volumetric specific heat of \(i\)-th constituent, \(J/cm^3 \degree C\),

\(\phi_i\) = the volumetric fraction of \(i\)-th constituent,

\(L\) = the latent heat of fusion, \(J/g\).

\(\rho_s\) = the density of ice, \(g/cm^3\), and

\(\theta_s\) = the volumetric ice fraction, \(cm^3/cm^3\).

Moisture transfer equation:

\[
\begin{align*}
\frac{\partial}{\partial x} \left[ K (x, m, T, \Psi) \frac{\partial \phi}{\partial x} \right] &= \frac{\partial \phi_u}{\partial t} + \frac{\rho_s}{\rho_l} \frac{\partial \theta_s}{\partial t} \ldots \quad (4-3)
\end{align*}
\]

Where \(K\) = the soil hydraulic conductivity, \(cm/s\),

\(\phi\) = the total soil water potential, \(cm\),

\(\Psi\) = \(\Psi + Z\),

\(Z\) = elevational head, and

\(\theta_u\) = volumetric liquid water fraction, \(cm^3/cm^3\).

The fluid flow velocity, \(v_x\), is given as,

\[
v_x = -K \frac{\partial \phi}{\partial x} \quad \ldots \quad (4-4)
\]

In the derivation of the equations, the components due
to thermal, osmotic, and chemical forces were assumed to be negligible.

The two transport equations with associated auxiliary equations are solved for prescribed boundary conditions and porous media characteristics. Since analytical solutions to these nonlinear partial differential equations are unavailable, numerical techniques must be employed. The solution of the model yields temperature, water and ice contents at various times during freezing and thawing of soils.

The second term in equation (4-1) is the convective heat transfer associated with liquid water movement. The presence of this term in Harlan's model requires more iterations between the heat and mass transfer equations for a numerical solution and thus substantially increases computer costs. Although this component of heat transfer in soil has been acknowledged, due to the complexities in obtaining solutions, method of formulating equations of heat transfer in soil very often assume heat conduction is the dominant mode of heat transfer and convective heat transfer is often ignored or assumed negligible (Bresler and Miller, 1975; Outcalt, 1976; Aguirre-Puent and Fremond, 1976).

The possible effects on the accuracy of the calculations caused by omitting convective heat transfer in problems of soil freezing and thawing have been a concern to researchers in this field. Nixon (1975) examined the role of convective heat transfer in the thawing of frozen soils. He provided a solution for a one-dimensional thawing problem which accounts for convective heat transfer associated with the migration of
melt water into soils. The equation he used was the same as equation (4-1). The solutions to the problem demonstrate that convective heat transfer plays a very minor role in determining the rate of thaw. Nixon concluded that effects of unidimensional convective heat transfer in the thawed zone may be ignored in most practical engineering computations without fear of incurring errors of more than a few percent.

Based on Nixon's findings and an attempt to minimize computer costs, the convective heat transfer term was eliminated from equation (4-1) in the analyses. In effect, this change will not significantly affect the results in cases where the velocity of liquid water is very slow and the convective heat transfer is insignificant compared to the heat transferred by conduction. The heat transfer equation, obtained by combining equations (4-1) and (4-2), thus, becomes

\[
\frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) = \rho C_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial t} \left( \rho C_p \frac{\partial T}{\partial \theta} \right) \quad \ldots \quad (4-6)
\]

Where

\[
\rho C_p = \sum_{i=1}^{n} (\rho C_p)_i \phi_i
\]

For the case of one-dimensional horizontal fluid flow, the gravitational potential, \( Z \), is constant. By introducing the soil-water diffusivity, \( D \), defined as

\[
D = K \frac{\partial \psi}{\partial \theta_u} \quad \ldots \quad (4-7)
\]
the moisture transfer equation becomes

$$\frac{\partial}{\partial x} (D \frac{\partial \theta}{\partial x}) = \frac{\partial \theta}{\partial t} + \frac{\rho_s}{\rho} \frac{\partial \theta_s}{\partial t}. \quad \ldots \quad (4-8)$$

Equation (4-8) is a simpler form of the flow equation which can be readily solved by numerical methods. The soil-water diffusivity, with units of cm²/s, is a function of the moisture content in unfrozen soil-water systems. The physical property of the soil-water diffusivity has been a subject of intensive studies in the field of soil physics (Kirkham and Powers, 1972).

Equations (4-6) and (4-8) were solved numerically by the finite difference method. The boundary conditions used in the solutions were:

$$T = T_1 \quad x = 0 \quad t \geq 0 \quad \ldots \quad (4-9)$$

$$T = T_2 \quad x = L \quad t \geq 0 \quad \ldots \quad (4-10)$$

$$\frac{\partial \theta}{\partial x} = 0 \quad x = 0 \quad t \geq 0 \quad \ldots \quad (4-11)$$

$$\frac{\partial \theta}{\partial x} = 0 \quad x = L \quad t \geq 0 \quad \ldots \quad (4-12)$$

where $T_1$ and $T_2$ are the specified temperatures at ends of the soil column, and $L$ is the length of the soil column. Both $T_1$ and $T_2$ may be time dependent. Equations (4-11) and (4-12) imply that the system is closed with regard to liquid water transport so that no water flows into or out of the system.

The initial conditions are

$$T = T_0 \quad 0 \leq x \leq L \quad t = 0 \quad \ldots \quad (4-13)$$
\[ \theta_s = (\theta_s)_0 \quad 0 \leq x \leq L \quad t = 0 \quad \ldots \quad (4-14) \]

\[ \theta_u = (\theta_u)_0 \quad 0 \leq x \leq L \quad t = 0 \quad \ldots \quad (4-15) \]

where \( T_0, (\theta_s)_0 \) and \( (\theta_u)_0 \) are the known values of temperature and ice and liquid water contents respectively along the soil column at \( t = 0 \). Those values can be either constants or functions of \( x \). The total volumetric water content, \( \theta \), expressed as the equivalent liquid water content, is defined as

\[ \theta = \theta_u + \frac{\rho_s}{\rho_l} \theta_s \quad \ldots \quad (4-16) \]
4.2 NUMERICAL SOLUTION

To solve the problem numerically, equations (4-6) and (4-8) were first expressed in the implicit finite difference form. The method used was the well-known Crank-Nicholson scheme [see Section 2.5.B (ii)]. For the purpose of this study, the space-time domain \((x, t)\) of interest is subdivided into a rectangular grid system with variable space and time increments. Very fine space-increments were used in the region near the freezing front. Small time steps were needed at the initial stages when the freezing front penetrated into the soil column rapidly. Figure 38 shows the arrangement of the grid points for deriving the finite difference equations. Each point in the network is designated as \((i, n)\) indicating that this point is located at the coordinates \(x_i\) and \(t^n\), which are given as

\[
x_i = \sum_{p=2}^{i} \Delta x_p \quad i = 2, 3, \ldots, I
\]
\[
t^n = \sum_{r=1}^{n} \Delta t^r \quad r \geq 1
\]

and \(t^0 = 0\), where \(\Delta x\) and \(\Delta t\) are the space and time increment respectively. The grid point \(I\) occurs at the cold end of the soil column, i.e. \(x = 0\) and the warm end of the column is at \(I\), where \(x = L\). The points, \(x_0\) and \(x_{I+1}\), have been extended beyond the physical boundaries of the system to facilitate the treatment of boundary conditions (4-11) and (4-12).

The finite difference form used to approximate equation
(A) RECTANGULAR GRID FOR CRANK-NICHOLSON METHOD

(COLD END) FREEZING FRONT WARM END

(B) SPATIAL NODES

FIGURE 38 ARRANGEMENT OF GRID POINTS
(4-6) is

\[
\frac{1}{\lambda \Delta x_i + \Delta x_{i+1}} \left[ \lambda \left( \frac{\Delta T_{i+1} - \Delta T_i}{\Delta x_i + \Delta x_{i+1}} \right) \right] \frac{\lambda^{n+\frac{1}{2}}}{\lambda^{i+\frac{1}{2}}}
\]

\[
+ \left( \frac{T_{i+1}^n - T_i^n}{\Delta x_i + \Delta x_{i+1}} \right) - \frac{1}{2} \lambda^{i+\frac{1}{2}} \left[ \frac{T_{i+1}^{n+1} - T_{i+1}^n}{\Delta x_i + \Delta x_{i+1}} \right]
\]

\[
+ \left( \frac{T_i^n - T_{i-1}^n}{\Delta x_i} \right) = \rho_i^{n+\frac{1}{2}} \left( \frac{T_{i+1}^{n+1} - T_i^n}{\Delta t} \right)
\]

\[
- \rho (\theta_{s_i}^{n+1} - \theta_{s_i}^n) / \Delta t^{n+1}
\]

\[
\ldots \ldots \text{(4-17)}
\]

Rearranging equation (4-17) gives

\[
\frac{\lambda^{n+\frac{1}{2}}}{\left( \Delta x_i + \Delta x_{i+1} \right) \Delta x_{i+1}} \left( T_{i+1}^{n+1} - T_{i+1}^n + T_{i+1}^n - T_i^n \right)
\]

\[
- \frac{\lambda^{i+\frac{1}{2}}}{\left( \Delta x_i + \Delta x_{i+1} \right) \Delta x_i} \left( T_i^{n+1} - T_{i-1}^n + T_i^n - T_i^n \right)
\]

\[
= \rho_i^{n+\frac{1}{2}} \left( \frac{T_{i+1}^{n+1} - T_i^n}{\Delta t} \right) - \rho (\theta_{s_i}^{n+1} - \theta_{s_i}^n) / \Delta t^{n+1}
\]

\[
\ldots \ldots \text{(4-18)}
\]

or

\[
\beta T_{i-1}^{n+1} + (-\alpha - \beta - r) T_i^{n+1} + \alpha T_{i+1}^{n+1} = \beta T_i^n
\]

\[
+ (\alpha + \beta - r) T_i^n - \rho (\Delta S_i)
\]

\[
\ldots \ldots \text{(4-19)}
\]
Where

\[ a = \frac{\Delta t^{n+1} \cdot \alpha^{n+\frac{1}{2}}}{(\Delta x_i + \Delta x_{i+1}) \cdot \Delta x_i} \]

\[ \beta = \frac{\Delta t^{n+1} \cdot \beta^{n+\frac{1}{2}}}{(\Delta x_i + \Delta x_{i+1}) \cdot \Delta x_i} \]

\[ r = C\rho_i^{n+\frac{1}{2}} \]

and

\[ \Delta S_i = \theta_{n+1,si} - \theta_{n,si} \]

The use of the subscript \( i \) and superscript \( n \) in the equations denotes that the function is evaluated at the point \( (i, n) \) in the network. Values of \( \lambda_{i+\frac{1}{2}}^{n+\frac{1}{2}}, \lambda_{i-\frac{1}{2}}^{n+\frac{1}{2}} \) and \( C\rho_i^{n+\frac{1}{2}} \) can be obtained by

\[ \lambda_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{4} (\lambda_{i+1}^{n+1} + \lambda_i^{n+1} + \lambda_{i+1}^n + \lambda_i^n) \quad \cdots \quad (4-20) \]

\[ \lambda_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{4} (\lambda_i^{n+1} + \lambda_{i-1}^{n+1} + \lambda_i^n + \lambda_{i-1}^n) \quad \cdots \quad (4-21) \]

and

\[ C\rho_i^{n+\frac{1}{2}} = \frac{1}{2} (C\rho_{i}^{n+1} + C\rho_i^n) \quad \cdots \quad (4-22) \]

For the solution of (4-19) to be realized, the change of ice content \( \Delta S_i \) in the time interval \( \Delta t^{n+1} \) has to be determined first. The procedure for obtaining the estimated and
the improved values of $\Delta S_i$ will be described later.

All terms of $T^n_i$ ($i = 1, 2, \ldots, I$) in equation (4-19) are known from the previous time step. By introducing the boundary conditions,

$$T^n+1_1 = T_1$$
$$T^n+1_l = T_2$$

equation (4-19) becomes a set of $(I - 2)$ nonlinear equations with $(I - 2)$ unknowns. The solution of this set of equations can be obtained by means of the iteration method.

For actual computation the following iterative method was used in this study. First the values of $\lambda^n+1_i$ and $C_p^n+1_i$ ($i = 2, 3, \ldots, I - 1$), were evaluated for the first estimated values of $T^n+1_i$ ($i = 2, 3, \ldots, I - 1$), indicated as $T^n+1(1)$. Equation (4-19), thus, became a set of linear equations, and any of the standard methods for solving a linear system could be used. Since the resulting system of finite difference equations was essentially tridiagonal, i.e. all the elements of the corresponding matrix vanished except those on three diagonals, a special version of the Gauss elimination procedure known as Thomas tri-diagonal algorithm was particularly convenient for solving this system. A description of the Thomas tri-diagonal algorithm is given in Appendix A.

By solving (4-19), a new set of values, $T^n+1_i(2)$, was obtained. The values of $\lambda^n+1_i$ and $C_p^n_i$ were then reevaluated by a new value $T^n+1_i(3)$, defined as
The finite difference form used to approximate equation (4-8) is

\[
\frac{1}{2 \left( \Delta x_i + \Delta x_{i+1} \right)} \left\{ \frac{1}{2} \left( n^{n+1}_{i+\frac{1}{2}} \right) \left[ \frac{\left( e^{n+1}_{u_{i+1}} - e^{n+1}_{u_i} \right)}{\Delta x_{i+1}} \right] + \frac{1}{2} \left( n^{n+1}_{i-\frac{1}{2}} \right) \left[ \frac{\left( e^{n+1}_{u_i} - e^{n+1}_{u_{i-1}} \right)}{\Delta x_i} \right] + \left( \frac{e^n_{u_{i+1}} - e^n_{u_{i-1}}}{\Delta x_i} \right) \right\} = \frac{\rho_s}{\rho} \left( \frac{e^{n+1}_{s_{i+1}} - e^n_{s_i}}{\Delta t^{n+1}} \right) \quad \ldots \quad (4-24)
\]

Rearranging equation (4-24) gives

\[
\beta_1 e^{n+1}_{ui-1} + \left( -\alpha_1 - \beta_1 - 1 \right) e^{n+1}_{ui} + \alpha_1 e^{n+1}_{ui+1} = -\beta_1 e^n_{ui-1} + \left( \alpha_1 + \beta_1 - 1 \right) e^n_{ui} - \alpha_1 e^n_{ui+1} + \frac{\rho_s}{\rho} \cdot \Delta S_i \quad \ldots \quad (4-25)
\]

\[
T_i^{n+1}(3) = \frac{1}{2} \left( T_i^{n+1}(1) + T_i^{n+1}(2) \right) \quad \ldots \quad (4-23)
\]

The final values of $T_i^{n+1}$ were determined by repeating iterations until the old and new values of $T_i^{n+1}$ were sufficiently close. A similar procedure was applied for each time increment, starting with the initial condition where $t = 0$. 

The finite difference form used to approximate equation (4-8) is

\[
\frac{1}{2 \left( \Delta x_i + \Delta x_{i+1} \right)} \left\{ \frac{1}{2} \left( n^{n+1}_{i+\frac{1}{2}} \right) \left[ \frac{\left( e^{n+1}_{u_{i+1}} - e^{n+1}_{u_i} \right)}{\Delta x_{i+1}} \right] + \frac{1}{2} \left( n^{n+1}_{i-\frac{1}{2}} \right) \left[ \frac{\left( e^{n+1}_{u_i} - e^{n+1}_{u_{i-1}} \right)}{\Delta x_i} \right] + \left( \frac{e^n_{u_{i+1}} - e^n_{u_{i-1}}}{\Delta x_i} \right) \right\} = \frac{\rho_s}{\rho} \left( \frac{e^{n+1}_{s_{i+1}} - e^n_{s_i}}{\Delta t^{n+1}} \right) \quad \ldots \quad (4-24)
\]

Rearranging equation (4-24) gives

\[
\beta_1 e^{n+1}_{ui-1} + \left( -\alpha_1 - \beta_1 - 1 \right) e^{n+1}_{ui} + \alpha_1 e^{n+1}_{ui+1} = -\beta_1 e^n_{ui-1} + \left( \alpha_1 + \beta_1 - 1 \right) e^n_{ui} - \alpha_1 e^n_{ui+1} + \frac{\rho_s}{\rho} \cdot \Delta S_i \quad \ldots \quad (4-25)
\]
Where
\[ \alpha_i = \frac{\Delta t^{n+1} \cdot D^{n+\frac{1}{2}}_{i+\frac{1}{2}}}{(\Delta x_i + \Delta x_{i+1}) \cdot \Delta x_{i+1}} \]
\[ \beta_i = \frac{\Delta t^{n+1} \cdot D^{n+\frac{1}{2}}_{i-\frac{1}{2}}}{(\Delta x_i + \Delta x_{i+1}) \cdot \Delta x_i} \]

The finite difference equation (4-25) is solved implicitly for \( \theta^n_{ui} \) by using the estimated values of \( \Delta S_i \) and taking into account the appropriate initial and boundary conditions in each particular case. Values of \( D^{n+\frac{1}{2}}_{i+1} \) and \( D^{n+\frac{1}{2}}_{i-1} \) are determined by:

\[ D^{n+\frac{1}{2}}_{i+\frac{1}{2}} = \frac{1}{4} (D^{n+1}_{i+1} + D^{n+1}_{i} + D^{n}_{i+1} + D^{n}_{i}) \]
\[ D^{n+\frac{1}{2}}_{i-\frac{1}{2}} = \frac{1}{4} (D^{n+1}_{i} + D^{n+1}_{i-1} + D^{n}_{i} + D^{n}_{i-1}) \]

The boundary conditions to be satisfied at \( t > 0 \) are (4-11) and (4-12). In finite difference form these conditions become:

\[ \frac{\theta^n_{u2} - \theta^n_{uo}}{2\Delta x_2} = 0 \quad \text{for } i = 1 \]

that is

\[ \theta^n_{uo} = \theta^n_{u2} \quad \ldots \quad (4-26) \]

and

\[ \frac{\theta^n_{uI+1} - \theta^n_{uI-1}}{2\Delta x_I} = 0 \quad \text{for } i = I \]
A set of I nonlinear equations (for \( i = 1, 2, \ldots, I \)) with I unknowns can be formed by substituting equation (4-26) and (4-27) into (4-25). Since the system of finite difference equations is implicit and tridiagonal, the technique and procedure used to solve the system is exactly the same as the one described previously for solving equation (4-19).

As it can be seen from equations (4-6) and (4-8), the heat transfer equation and the mass transfer equation are coupled mathematically through the term \( \Delta S_i \), e.g. the change of ice content \( \Delta S_i \) in equation (4-19) and (4-25). To obtain a solution to the problem, the solution, therefore, must be iterated between these two equations. This is done by using the first estimated values of \( \Delta S_i \) to determine the temperature distribution \( T \) from equation (4-19) and the liquid water content \( \theta_u \) from equation (4-25) for the particular time step. Theoretically, if the estimated \( \Delta S_i \) are the correct values, the calculated liquid water content \( \theta_u \) in the freezing zone should be equal to the liquid water content of the frozen soil \( \theta_u' \) determined at the predefined temperature \( T \) by using the relationship between unfrozen water content and temperature below freezing for this soil. Otherwise, the estimated values of \( \Delta S_i \) can be adjusted according to the difference of \( \theta_u \) and \( \theta_u' \) to obtain a better second estimate values of \( \Delta S_i \). The iterative process is then repeated until suitable values of
\( \Delta S_i \) are found such that \( \theta_u \) approach \( \theta_u' \). It is not necessary that \( \theta_u \) be equal to \( \theta_u' \) for the particular time step. Rather, a prescribed iterative criteria can be set so that the difference between \( \theta_u \) and \( \theta_u' \) does not exceed an acceptable value. The most recent computed values of \( T \) and \( \theta_u \) apply for the time level \( t^{n+1} \). The ice content for that time level, \( \theta_s^{n+1} \), of course, is

\[
\theta_s^{n+1} = \theta_s^n + \Delta S_i
\]

The solution is therefore advanced from time level \( t^n \) to \( t^{n+1} \). The values of \( T \), \( \theta_u \), and \( \theta_s \) at time level \( t^{n+1} \) then become known ones and can be used to obtain values at time level \( t^{n+2} \). The process is repeated until the final time is reached.

If the initial estimated value of \( \Delta S_i \) differs substantially from the correct value, the iterative criteria may not converge properly. Oscillations occur in the solution even though the implicit finite difference scheme used in the numerical procedure is stable for all values of \( \Delta x \) and \( \Delta t \). To avoid this problem, the change of ice content due to the heat transfer only for this time interval was determined first at the beginning of each time step and the value was used as the initial estimate of \( \Delta S_i \). This is done by assuming the water in the soil does not move and using the heat transfer equation

\[
\frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) = C_p \frac{\partial T}{\partial t}
\]
where
\[
C_p = C_p + L_p \frac{\partial u}{\partial T}
\]
to determine the temperature distribution for time level \(t_{n+1}\).

The corresponding liquid water content for the calculated temperature was then obtained from the relationship between the unfrozen water content and temperature for the soil. The change of ice content due to the heat transfer only is then the difference between the liquid water content at time level \(t_n\) which is already known from the previously time step and the computed liquid water content at time level \(t_{n+1}\). The method used for determining the apparent volumetric specific heat \(C_p\), appearing in the above equations was discussed in Section (2.2.A). \(\frac{\partial u}{\partial T}\) in the equation is the rate of change of unfrozen water content with temperature and can be evaluated from the slope of the unfrozen water content versus temperature curve.

For the purpose of this study, the soil column was dissected into a series of grid points using small grid-spacings near the cold end and expanding the grid-spacing with increasing distance from the cold end. In the area close to the freezing front, soil properties undergo substantial changes due to phase changes. To obtain accurate estimates of the soil properties in the region of the freezing front the grid spacing was decreased by increasing the number of grid points in the zone. Figure 39 illustrates the manner in which this was achieved. Figure 39 (A) shows the initial designated grid points denoted as A, B, C, ..., F, G for a
(A) INITIAL ORIGINAL SPACING OF GRID POINTS

FREEZING FRONT AT $t = t_1$

(B) GRID POINTS FOR $t = t_1$

FREEZING FRONT AT $t = t_2$

(C) GRID POINTS FOR $t = t_2$

FIGURE 39 ARRANGEMENT OF GRID POINTS NEAR THE FREEZING FRONT
certain portion of the soil column. Supposing that at time 
t_1 the freezing front was located between nodes C and D, for this case, new grid points were added among nodes B, C, D, and E as shown in Figure 39 (B). Values of temperatures, liquid water and ice contents at the added nodes required for the calculations were obtained from the known values at nodes B, C, D, and E assuming the magnitudes of the variables varied linearly between nodes. When the freezing front advanced to the position between nodes D and E at time t_2, grid points between nodes B and C were removed and new nodes were added between nodes E and F as shown in Figure 39 (C). Similarly, as the freezing front moved to the position between nodes E and F, grid points between nodes C and D were eliminated and new nodes were placed among nodes D, E, F, and G.

The numerical calculations were carried out on an IBM 360 digital computer.
4.3 SOIL PROPERTIES

The following list includes the relevant properties of the soil material used in this study.

(i) **Unfrozen Water Content of the Frozen Soil**

Experimental investigations, using the calorimetric method, were conducted to determine the phase composition of water at temperatures below freezing for the soil used in this study. The experimental results as well as complete details of the experimental method are given by Jame (1972). Because water contents obtained from direct measurements were expressed as percent on dry weight basis, it is necessary to convert them to the volumetric liquid fraction for use with the model. This is done by multiplying the water contents with the conversion factor \( \gamma_d \), where \( \gamma_d \) is the dry density of the soil.

It was noted from the experimental results that most of the water in the soil changes phase in a very small temperature range (about 0.25°C). To ensure that accurate estimates of the soil properties can be obtained near the freezing front requires the use of extremely refined space-grid. The latent heat contribution of one or more nodes may be missed entirely if the grid spacing is so fine that the phase plane moves across an entire nodal volume in one time step, and hence, the iteration formulation may not converge properly. To ensure that this does not happen, the time-steps have to be severely shortened, and numerical stability problems will arise. In order to overcome these stability problems a relatively larger freezing range (about 0.5°C) was chosen for the compu-
tation to replace the actual measured values. The selected curve, expressing the liquid water content as a function of temperature used in the calculation, together with the experimental data are shown in Figure 40. The curve is composed of four linear equations, each applicable over a given range of temperature. Choosing a slightly larger freezing range may cause a small loss of accuracy in predicted depth of freezing, however, the maximum error contributed from this factor was less than one centimeter in this study.

As it is assumed that the relationship between unfrozen water content and temperature can be used to represent the relationship between moisture content and its corresponding freezing temperature, the unfrozen water content versus temperature curve shown in Figure 40 also serves as the criterion for deciding whether the soil is in frozen or unfrozen state. For instance, if the calculated temperature $T$ of a grid point having a specified total moisture content falls below the freezing temperature $T_f$ corresponding to this moisture content as given from the curve, the grid point is regarded as in the frozen state. In actual computation, every node was scanned at each time step to determine whether it was frozen or unfrozen. The freezing front was assumed to be positioned midway between two adjacent nodes when one node was in the frozen state and the other one unfrozen.

(ii) Thermal Conductivity

Direct measurements were made to determine the thermal conductivities of the unfrozen soil at different moisture con-
\[ \theta_u = 0.49 + 2.2T \]
for \( 0 > T \geq -0.1 \)

\[ \theta_u = 0.325 + 0.55T \]
for \(-0.1 > T \geq -0.5 \)

\[ \theta_u = 0.0583 + 0.0167T \]
for \(-0.5 > T \geq -2 \)

\[ \theta_u = 0.025 - \]
for \( T \leq -2 \)

EXPERIMENTAL DATA (Jame and Norum, 1972)

CURVE USED IN THE COMPUTATION

FIGURE 40 UNFROZEN WATER CONTENT VERSUS TEMPERATURE CURVE
tents by means of a transient flow probe and/or diffusivity methods. The results of the measurements and details of the methods used are presented in a special report prepared by Jame (1977). An analysis of the data showed that there was a very good agreement between the experimental values and those predicted by the theoretical model proposed by de Vries (see Section 2.2.B). The de Vries method was therefore adopted to determine the thermal conductivity values required in the model.

The equation used is of the form:

\[
\lambda = \frac{\sum_{j=1}^{n} F_j \phi_j \lambda_j}{\sum_{j=1}^{n} F_j \phi_j} \quad \ldots \quad (4-28)
\]

where \( \lambda \) is the soil thermal conductivity, \( j \) is the number of different kinds of particles, \( \lambda_j \), \( \phi_j \) and \( F_j \) are the thermal conductivity, volumetric content and weighting factor respectively for the \( j \)-th component.

Equation (4-28) is based on the assumption that soil consists of a continuous medium, usually air for dry soil and water for moist soil, with other components dispersed in the continuous medium. The weighting factor \( F_1 \) for the continuous medium, designated as the \( j=1 \) component, is always equal to unity. Other values of \( F_j \) are calculated from

\[
F_j = \frac{1}{3} \sum_{n=1}^{3} \left[ 1 + \frac{\lambda_j - 1}{\lambda_1} q_n \right]^{-1} \quad \ldots \quad (4-29)
\]

with
\[ g_1 + g_2 + g_3 = 1 \]

where \( g_n \) is a depolarization factor depending on the shape of the component.

In this study, the value of \( \lambda_j \) for the soil particle, e.g. silica flour, was taken as that of pure quartz, given by de Vries (1963) as 8.54 W/m \( ^\circ \)C. The value of \( \lambda_j \) for the air-filled pores, as reported by Wierenga et al (1969), was taken to be \( \lambda_a + \lambda_v \), where \( \lambda_a \) is the thermal conductivity of the air and \( \lambda_v \) accounts for the latent heat transfer in the vapor phase across the gas-filled pore. A value of 0.025 W/m \( ^\circ \)C was used for \( \lambda_a \). For water contents above 0.2 cm\(^3\)/cm\(^3\), the air in the soil pores was considered water saturated and a value of 0.0736 W/m \( ^\circ \)C was used for \( \lambda_v \). For a liquid water content less than 0.2 cm\(^3\)/cm\(^3\), values of \( \lambda_v \) were assumed to decrease linearly from 0.0736 W/m \( ^\circ \)C to zero at oven-dryness. Other values of \( \lambda_j \) used were 0.573 and 2.176 W/m \( ^\circ \)C for water and ice respectively.

Water was considered to be the continuous medium for this study. Values of \( g_n \) for the soil particles were taken equal to 0.125, 0.125, and 0.75, which corresponds to particles having a shape of an ellipsoid of revolution. In accordance with Wierenga et al. (1969), values of \( g_1 \) and \( g_2 \) for air particles were assumed to decrease linearly from 0.333 in water saturated soil to 0.105 at a soil-water content of 0.2 cm\(^3\)/cm\(^3\). Below this water content \( g_1 \) and \( g_2 \) were assumed to decrease linearly to a value of 0.015 at oven-dryness.

The thermal conductivity for the unfrozen soil calculated from
de Vries equation by using the listed values are compared to the measured values in Figure 41.

Values of \( q_n \) used for ice in the frozen soil were taken as that of the soil particles. This is to assume that ellipsoids of ice are dispersed in the soil-water system where water is regarded as the continuous medium. It was noted from the results that the thermal conductivities of the frozen soil computed from this arrangement were too small especially when large ice contents are present. A correction factor therefore was needed to increase the calculated values for the thermal conductivity of the frozen soil. The correction factor used in this study was assumed to be a function of ice content following the form,

\[
A = 1 + \alpha \theta_s \quad \text{(4-30)}
\]

where \( A \) is the correction factor, \( \theta_s \) is the ice content and \( \alpha \) is a coefficient.

Kersten (1949) and Penner et al. (1975) all noted that for most soils at low moisture contents, the thermal conductivity in the unfrozen state was higher than that in the frozen state. With an increase in moisture content, the thermal conductivity of frozen soil becomes progressively greater than that of unfrozen soil. The reason for the reduction of thermal conductivity upon freezing at low moisture content, along with the experimental results obtained by Kersten (1949) and Penner et al. (1975), have been discussed in Section (2.2.B). Before freezing, water forms a bridge between soil particles and pro-
FIGURE 41 RELATIONSHIP BETWEEN THERMAL CONDUCTIVITY AND MOISTURE CONTENT FOR SOIL IN THE UNFROZEN STATE

EXPERIMENTAL VALUES (Jame, 1977)

CALCULATED FROM DE VRIES EQUATION
(CURVE USED IN THE COMPUTATION)

MOISTURE CONTENT (BY DRY WEIGHT), %

THERMAL CONDUCTIVITY, WATT/m °C
vides an effective path for heat conduction. During freezing, the ice crystals are thought to partially fill the voids between soil particles and some of the bridge water is removed, which apparently impedes the heat transfer. For soil at higher water content, because the ice fills the pores more completely, the ice matrix is continuous and some heat flow paths can bypass the liquid interface. As ice has a higher thermal conductivity than water, this leads to an overall increase in thermal conductivity.

From his experiments, Kersten (1949) pointed out that at moisture contents less than 6 percent for sandy soil and less than 10 percent for fine-grained soil, the thermal conductivity of the soil in the frozen state is lower than that in the unfrozen state. The value of the correction factor used for increasing the thermal conductivity of the frozen soil obtained from de Vries' model was therefore chosen in such a way that the computed results showing the ratio of the thermal conductivity in the frozen state, $\lambda_f$, to that in the unfrozen state, $\lambda_u$, for the soil at different moisture contents compared favorably with the values reported by Kersten (1949). It was found that a value of $\alpha$ equal to 2 gave the best results. The calculated relationship between $\lambda_f/\lambda_u$ and moisture content is shown in Figure 42, where the value of $\lambda_f$ used for the computation was taken at $-2^\circ C$. Results obtained by Kersten (1949) and Penner et al. (1975) are also presented in the Figure for comparison.

Figure 43 shows the dependence of the thermal conductivity of frozen soil on temperature for various moisture con-
A: LOWELL SAND (Kersten, 1949)
B: ROMSEY SANDY LOAM (Kersten, 1949)
C: FAIRBANKS SILT (Kersten, 1949)
D: SOIL WITH 54% CLAY AND 46% SILT (Penner et al., 1975)
E: SILICA FLOUR (SOIL USED IN THIS STUDY)

FIGURE 42 RATIO OF $\lambda_f/\lambda_u$ VERSUS MOISTURE CONTENT CURVE
FIGURE 43  DEPENDENCE OF THERMAL CONDUCTIVITY ON TEMPERATURE FOR THE SOIL IN THE FROZEN STATE AT DIFFERENT MOISTURE CONTENT
tents. The curves show that in the temperature range 0 to -0.5°C the thermal conductivity increases with decreasing temperature except for those soils having very low moisture contents. This is understandable because large amounts of water freeze to ice within this temperature range as can be seen from the unfrozen water content versus temperature curve shown in Figure 40. The substantial increase of ice content leads to the overall increase in the thermal conductivity. It is also expected that the thermal conductivity of all samples independent of moisture content level off at -2°C because below this temperature there is very little phase change. At temperatures between -0.5 and -2°C, the thermal conductivity decreases slightly as the temperature is lowered except at high moisture contents. This appears to contradict the results obtained by Penner et al. (1975), which showed the overall increase in thermal conductivity with decreasing temperature as indicated in Figures 8 and 9. However, the reduction of thermal conductivity caused by decreasing the temperature in a frozen soil was also observed in the experimental results obtained by Gilley and Allred (1976). They measured the thermal conductivity of a frozen Hubbard loamy sand by using the transient probe method. The measured values at -2.5°C and -15.5°C were 1.46 and 1.16 W/m°C respectively for a moisture content of 7.1%, and 1.74 and 1.35 W/m°C respectively for a moisture content of 16.6%. The reduction of thermal conductivity with decreasing temperature for a frozen soil probably can be attributed to the decrease of liquid water content in soil. Upon freezing, heat transfer from grain to grain still
occurs through the film of liquid water. With decreasing
temperature the film thickness decreases and the motion of the
molecules is restricted, which reduces the heat transfer.
For high moisture contents, as the ice fills the pores more
completely, the ice matrix is continuous. The reduction of
heat transfer through liquid water is thus balanced by the
increase of heat transfer through the ice matrix in the soil.

As a matter of fact, the thermal conductivity values,
shown in Figure 43, for the frozen soil used in this study
compared favorably with measured values obtained by Gilley
and Allred (1976).

(iii) Heat Capacity

As discussed in Section (2.2.A), the volumetric spe-
cific heat of the soil-liquid-ice mixture, \( C_p \), can be estimated
by the expression

\[
C_p = \sum_{i=1}^{n} (C_p)_i \phi_i
\] .... (4-31)

where \( (C_p)_i \) and \( \phi_i \) are the volumetric specific heat and volume
fraction respectively for the \( i \)-th component. If the dry den-
sity of soil, \( \gamma_d \), is known, the equation can be expressed as

\[
C_p = \gamma_d (C_s + 4.184 W_u + 2.10 W_i)
\] .... (4-32)

where \( C_s \) is the mass specific heat of soil, \( W_u \) and \( W_i \) are
the liquid water and ice content respectively, based on the
dry weight of the soil. Equation (4-32) assumes that the
mass specific heat of water and ice are equal to 4.184 and
2.10 J/g °C. The value of $C_s$, 0.837 J/g °C, was obtained from direct measurement by means of the calorimetric method. Details of the method were given by Jame (1972).

The apparent volumetric specific heat, $C_p$, which includes a term to account for the latent heat of fusion was calculated by the equation,

$$C_p = C_p' + L \rho L \frac{\partial \theta}{\partial T} \quad \ldots \quad (4-33)$$

where $L$, the latent heat of freezing of soil water, was taken at 333.4 J/g and $\rho_L$, the density of soil water, was equal to unity. $\frac{\partial \theta}{\partial T}$ is the rate of change in unfrozen water content with temperature. Its value corresponds to the slope of the unfrozen water content curve at the specified temperature $T$ (see Figure 40).

(iv) Soil-Water Diffusivity

Experimental equipment was not available to permit direct measurements of the soil water diffusivity. Hence, a trial and error method was adopted to approximate these values.

The soil was regarded as a Gardner soil, which is a soil having a soil-water diffusivity defined by the expression;

$$D (\theta) = D_1 \exp \left[ \beta (\theta - \theta_1) \right] \quad \ldots \quad (4-34)$$

where $D_1$ is the diffusivity at moisture content $\theta_1$ and $\beta$ is an empirical constant. Three sets of the measured diffusivity values provided by Elrick (1963), Nielsen (1966) and Whisler
et al. (1968) were used as a guide to determine the values of $D_1$ and $\beta$. The soil materials used by those investigators were similar to the one used in this study. Values of $D_1$ and $\beta$ were thus chosen within the range of the measured values. The selected soil-water diffusivity used in the model for the computation was determined in such a way that it would provide a better agreement between numerical and experimental results for different initial and boundary conditions imposed on the system. The selected diffusivity for the unfrozen soil, together with the measured values are shown in Figure 44.

For the soil in the frozen state, the quantity of liquid water is greatly reduced by the presence of ice. In his model, Harlan (1973) assumed that the hydraulic conductivity for a given liquid water content would be the same in the frozen, as in the unfrozen material. The procedure advocated by Harlan was first adopted in this study, that is to assume that at the same liquid water content the soil-water diffusivities for both ice-free and partially frozen soils were equal. Comparing the moisture distribution profiles obtained from the numerical results based on this assumption to those obtained from the actual measurements indicated that too much water (ice) was accumulated behind the freezing front and in the unfrozen region the water content decreased too sharply toward the frozen face. A possible reason for this difference was believed to be due to the fact that the method used by Harlan did not permit the effects of the ice on the water movement to be taken into account. Obviously, the presence of the ice in the soil will disrupt the established flow paths, and hence
**CURVE USED FOR CALCULATION**

**EXPERIMENTAL DATA**
- ○ ADELAIDE DUNE SAND (Elrick, 1963)
- × COLUMBIA SILT LOAM SOIL (Nielsen, 1966)
- ▲ HAYDEN SANDY LOAM (Whisler et al., 1968)

**FIGURE 44  SOIL-WATER DIFFUSIVITY FOR THE SOIL IN THE UNFROZEN STATE**
reduce the flow rate. In this study, an impedance factor, assumed to be a function of total ice content, was therefore introduced to reduce the diffusivity value for the soil in the frozen state. As there is no experimental data in the literature to substantiate this concept or procedure, the value of the impedance factor was chosen from one of the tests in such a way that the numerical results would compare favorably with the experimental results. The selected value, decreased exponentially from 1.0 for ice-free condition to 0.03 at ice content of 5% and to 0.001 at ice content equal to or more than 20%, was used in all tests in this study.
4.4 RESULTS AND DISCUSSION

Three experimental tests presented in the previous chapter were chosen for the simulation analysis to check the reliability of the proposed model as well as the developed numerical technique to solve it. These include:

(1) Test No. 8 (shown in Figure 31),
(2) Test No. 9 (shown in Figure 32),
(3) Test No. 13 (shown in Figure 34).

The initial moisture contents and the imposed temperature conditions on the soil columns of these three cases are given as follows:

<table>
<thead>
<tr>
<th>Test No.</th>
<th>Initial moisture Content (by dry weight)</th>
<th>Initial Temperature</th>
<th>Cold-end Temperature</th>
<th>Warm-end Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. 8</td>
<td>15%</td>
<td>+4.5°C</td>
<td>-5.9°C</td>
<td>+4.25°C</td>
</tr>
<tr>
<td>No. 9</td>
<td>10.08%</td>
<td>+5.0°C</td>
<td>-5.3°C</td>
<td>+5.0°C</td>
</tr>
<tr>
<td>No. 13</td>
<td>15.45%</td>
<td>+20°C</td>
<td>-10°C</td>
<td>+20°C</td>
</tr>
</tbody>
</table>

In the calculations, the following convergence criteria for iteration were used:

For the heat transfer equation:

\[
\frac{|T_{\text{new}} - T_{\text{old}}|}{T_{\text{old}}} \leq 0.01
\]

For the mass transfer equation:
where $T$ is the temperature, $\theta_u$ is the volumetric liquid water content, and the (new) and (old) are referring to the new calculated value and the old estimated value respectively.

One iteration between the heat and mass equations was carried out in this study.

Some difficulties were encountered in simulating the temperature conditions at the cold end. In conducting the experiment, the desired sub-freezing temperature was suddenly applied to the cold end after the soil column had reached the uniform initial temperature. From the direct measurement, it was found that the expected one-step change of temperature did not occur at the cold end. Rather, the time-temperature curve of the cold end showed that upon freezing, the temperature decreased rapidly to a certain temperature below $0^\circ$C, and then all of a sudden, a jump-like temperature rise of about $1.5$ to $2^\circ$C was revealed. After the jump, the temperature became cooler again and gradually approached the sub-freezing temperature imposed on the cold-end. The jump-like temperature rise is not an uncommon phenomenon when freezing a small amount of water in a closed chamber. The reason for this is attributed to the factor that freezing is not nucleated when the water reaches the standard freezing temperature. A large amount of latent heat, released when the supercooled water changes phase at the temperature of the initial crystal-
lization, causes the sudden increase of temperature. Because of the erratic change of temperature at the cold end during freezing, simulation of the temperature condition at the boundary presented some difficulties.

In an effort to avoid the difficulty encountered in treating the thermal boundary condition at the cold end during the early stages of cooling, model analyses of Test No. 8 and Test No. 9 were run from \( t = 6.0 \) to \( t = 72 \) hr. by using the measured temperature and water content values along the soil column at \( t = 6.0 \) hr. as the initial condition for the computation so that comparability between numerical and experimental results could be ensured. The numerical results for these two simulation runs, together with the respective experimental data, are presented in Figures 45, 46, 47, and 48. In modeling these two cases, the soil column was dissected into 45 grid points with variable space increments. The smallest space increments used were 0.03 cm in the areas near the freezing front and the largest were 2.5 cm for regions close to the warm end. The size of time steps used in the simulation ranged from 0.04 to 0.5 hour. As can be seen from the results, the model has faithfully predicted temperature and moisture distributions as observed in the experimental tests for both cases. Only small differences between calculated and measured values were noted. These differences probably are caused by not properly simulating the porous media characteristics.

Figure 49 shows the simulation analysis of Test No. 8 for \( t = 0 \) to \( t = 6.0 \) hr. by using a gradual change of temperature at the cold end as the thermal boundary condition.
FIGURE 45 CALCULATED TEMPERATURE PROFILES (t = 6.0 HR. TO t = 72.0 HR.) FOR TEST NO. 8, COMPARED WITH EXPERIMENTAL RESULTS
FIGURE 46 CALCULATED MOISTURE CONTENT PROFILES (t = 6.0 HR TO t = 72.0 HR) FOR TEST NO. 8, COMPARED WITH EXPERIMENTAL RESULTS.
FIGURE 47 CALCULATED TEMPERATURE PROFILES (t = 6.0 HR TO 72.0 HR) FOR TEST NO. 9, COMPARED WITH EXPERIMENTAL RESULTS
FIGURE 48 CALCULATED MOISTURE CONTENT PROFILES (t = 6.0 HR TO t = 72.0 HR) FOR TEST NO. 9, COMPARED WITH EXPERIMENTAL RESULTS
FIGURE 49  CALCULATED TEMPERATURE PROFILES AND MOISTURE CONTENT DISTRIBUTIONS (t = 0 HR TO t = 6.0 HR) FOR TEST NO. 8, COMPARED WITH EXPERIMENTAL RESULTS.
The temperature history of the cold end used in the calculation is given in the inset shown in the Figure. Because of the initially rapid rates of freezing, the time steps as small as 0.004 hour had to be used during the early stages of freezing; otherwise the numerical method would not converge properly. As shown in the results, major difference exist between the calculated and measured temperature at $t = 1.0$ and $t = 6.0$ hr. These differences result from the inability to adequately simulate the thermal boundary condition at the cold end.

Numerical results of simulating Test No. 13, along with respective measured values, are shown in Figures 50 (for temperature) and 51 (for moisture content). The model was run from $t = 0$ to $t = 72$ hr. The temperature history of the cold end used as the thermal boundary condition in the calculation is given in the inset shown in Figure 50. For this case, the 30 cm long soil column was dissected into 50 grid points with variable space increments ranging from 0.01 to 2.5 cm. The time steps used in the calculation varied from 0.001 to 0.4 hour; Again, because of the inability to adequately simulate the thermal condition at the cold end, differences between calculated and measured values are obvious during the early stages of freezing as can be seen in temperature profiles at $t = 1.0$ hr and $t = 6.0$ hr, however, these differences diminish as time progresses.

From the simulation analysis, the following observations are noted:

1. In general, the numerical results obtained from the model agree very well with the experimental data for both
FIGURE 50 COMPARISON OF NUMERICAL AND EXPERIMENTAL RESULTS FOR TEST NO. 13 — TEMPERATURE PROFILES
FIGURE 51 COMPARISON OF NUMERICAL AND EXPERIMENTAL RESULTS FOR TEST NO. 13 — MOISTURE CONTENT PROFILES
temperature and moisture content profiles under different conditions imposed on the system. Hence, it may be concluded that Harlan's model as well as the numerical solution used in this study can be successfully applied to solve the problem of heat and mass transfer in soil during freezing.

2. The simulation results show that the moisture content of the soil close to the cold end increases substantially after freezing, whereas, this does not appear in the experimental results. This is probably because the first measurement was taken one centimeter from the cold end and the high ice content occurred at a distance of less than one centimeter from the cold end. As a matter of fact, the substantial increase of moisture content close to the cold end upon freezing is revealed in the experimental results obtained by Dirksen (1964) and Hoekstra (1966).

3. The calculated moisture content in the unfrozen soil decreases sharply toward the freezing face during the early stages of cooling. As time progresses, the moisture content profiles become relatively uniform in the frozen region. No experimental data are available for comparison at times in the early stages of freezing. However, the moisture content profiles in the unfrozen zone obtained by Hoekstra (1966) (see Figure 18) also show a sharply decreasing moisture content near the freezing front.

In order to illustrate the effect of moisture migration in soil during freezing on the temperature field as well as the depth of freezing, temperature distributions of Test No.
were also computed from the model in which only the heat transfer process was considered thus assuming that moisture migration did not occur during freezing. The results of the computation are given in Figure 52. Comparison of temperature profiles obtained from the model considering simultaneous heat and mass transfer processes with those from the model using heat transfer equation only are presented in Figure 53. The differences between the two sets of temperature profiles with and without considering moisture migration are obvious. The position of the 0°C isotherm at $t = 72$ hr is 14.9 cm from the cold end of the soil column as obtained from the model considering moisture migration, while it is only 9.8 cm from the model considering heat transfer only, about 30% less than the actual measured value. In view of this, it is clear that moisture migration should be considered to improve the accuracy of thermal analyses when dealing with freezing and thawing of soils.
FIGURE 52 CALCULATED TEMPERATURE PROFILES FOR TEST NO. 13 BY USING HEAT TRANSFER EQUATION ONLY UNDER THE ASSUMPTION THAT MOISTURE MOVEMENT DOES NOT OCCUR DURING FREEZING
FIGURE 53 COMPARISON OF TEMPERATURE PROFILES CALCULATED BY USING SIMULTANEOUS HEAT AND MASS TRANSFER EQUATIONS WITH THOSE OBTAINED BY USING HEAT TRANSFER EQUATION ONLY FOR TEST 13
CHAPTER V

SUMMARY AND CONCLUSIONS

The transfer of heat and the movement of moisture are interrelated during freezing of a soil-water system. Hence, any proposed model describing this system must deal with coupling of the heat and mass transfer processes. Because of the complex nature of the phenomenon, earlier studies of a soil-water system, in which temperature was below freezing, has been directed toward the heat transfer process only, neglecting mass transfer. Only recently several investigators have embarked on projects to develop a generalized theory defining coupled heat and mass transfer in soils undergoing freezing and thawing (Kennedy and Lielmezs, 1973; Harlan, 1971, 1973; Bresler and Miller, 1975).

Among the models proposed for describing the coupled heat and mass transfer processes in soils subject to freezing and thawing but without ice lens formation, the model developed by Harlan (1971, 1973) is of particular interest because it is based on well accepted soil physics principles. The primary objective of this study was to test the validity of Harlan's model. This required both the obtaining of suitable experimental data and the development of a computer program for the numerical solution of the model equations.

In this thesis, a detailed discussion of a soil-water system under sub-freezing condition is presented in order to provide the background material necessary for understanding the development of a mathematical model. The existing
models as well as the relevant physical properties of the soil material required as input parameters to the model are reviewed.

The temperature and water-content profiles in unsaturated soil columns of different moisture contents which were subjected to temperature gradients with the cold-side temperature below freezing were measured. The moisture contents within the soil samples as a function of time were determined by the gamma-ray attenuation method. The results of these studies showed that:

1. The moisture distribution profiles, in both frozen and unfrozen regions, measured by the gamma-ray attenuation method were in close agreement with those determined by the gravimetric samples. This indicates that the gamma radiation technique can be used to measure the water (ice) content of the soil under sub-freezing conditions provided frost heaving does not occur.

2. Freezing of a soil induces considerable moisture redistribution. An extremely sharp discontinuity in the moisture profile exists at the freezing front. Behind the freezing front the water (ice) content is substantially higher than the initial moisture content, while, the moisture content in front of the freezing front is lower.

3. The rate of advance of the freezing front into the soil has a significant effect on the shape of the moisture distribution profile; the longer the freezing front remains stationary, the greater the amount of water that accumulates near the freezing front.
4. Under a given temperature gradient, the higher the initial soil moisture content, the deeper the freezing front penetrates the soil.

To test the model developed by Harlan, the data from three laboratory tests were compared with solutions of the coupled heat and mass transfer equations. The model was solved numerically by the finite difference method using the Crank-Nicholson scheme. In the numerical simulation, the space-time domain of the system was subdivided into a rectangular grid system with variable space and time increments. Very close space-increments were used in the region near the freezing front to account for the wide and large variation in soil properties in that region. The relevant physical properties of the soil material required as input parameters to the model were either measured directly or estimated. From the simulation analysis, it could be concluded that:

1. The temperature and moisture profiles predicted by the model were in close agreement with the experimental results. Harlan's model and the numerical solution presented can be applied successfully to solve the coupled heat and mass transfer in soils during freezing.

2. For the model to be used successfully in practice in study of frozen soils, it is necessary to develop measurement techniques to obtain accurate estimates of their thermal and hydraulic transmission properties.
3. The mass transfer of water exerts a pronounced influence on the temperature regime of a freezing soil and therefore must be accounted for in a model defining the temperature regime.
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THOMAS ALGORITHM --- SOLUTION OF
TRIDIAGONAL SYSTEMS

Tridiagonal matrices arise frequently in solving
differential equations by the finite difference method. Let
\[ A X = b \] .... (1)
is the system to be solved, where \( A \) is a tridiagonal matrix
with the form
\[
A = \begin{bmatrix}
B_1 & C & 0 & \cdots & 0 \\
A_2 & B_2 & C_2 & \cdots & 0 \\
0 & A_3 & B_3 & C & \cdots \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & A_{n-1} & B_{n-1} & C_{n-1} \\
0 & \cdots & 0 & A_n & B_n
\end{bmatrix}
\] .... (2)

\[ X = \begin{bmatrix}
x_1 \\
x_2 \\
\vdots \\
x_n
\end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix}
b_1 \\
b_2 \\
\vdots \\
b_n
\end{bmatrix}
\]

The matrix \( A \) can be factored into the product
\[ A = L U \] .... (3)
where \( L \) is lower triangular matrix in the form
and \( \bar{U} \) is upper triangular matrix in the form

\[
\bar{U} = \begin{bmatrix}
1 & r_1 & 0 & \cdots & \cdots & 0 \\
0 & 1 & r_2 & 0 & \cdots & 0 \\
0 & 0 & 1 & r_3 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\
0 & \cdots & \cdots & 0 & 1 & \gamma_{n-1} \\
0 & \cdots & \cdots & \cdots & 0 & 1
\end{bmatrix}
\]

With these forms for \( \bar{L} \) and \( \bar{U} \) the product \( \bar{L} \bar{U} \) is itself tri-diagonal and by direct multiplication yields

\[
\bar{L} \bar{U} = \begin{bmatrix}
\beta_1 & \beta_1 y_1 & 0 & \cdots & \cdots & 0 \\
\alpha_2 & (\alpha_2 y_1 + \beta_2) & \beta_2 y_2 & 0 & \cdots & 0 \\
0 & \alpha_3 & (\alpha_3 y_2 + \beta_3) & \beta_3 y_3 & 0 & \cdots \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\
0 & \cdots & \cdots & 0 & \alpha_n & (\alpha_n y_{n-1} + \beta_n) \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots
\end{bmatrix}
\]

On equating the nonzero elements of \( \bar{L} \bar{U} \) with those of \( \bar{A} \), the following recursive formulas for the \( \alpha_i \), \( \beta_i \), \( \gamma_i \) can be obtained:

\[
\beta_1 = B_1 \quad \gamma_1 = \frac{C_1}{\beta_1}
\]
\[ a_i = A_i \quad \beta_i = B_i - a_i \gamma_{i-1} \quad \gamma_i = \frac{C_i}{\beta_i} \quad i = 2, 3, \ldots, n-1 \]

\[ a_n = A_n \quad \beta_n = B_n - a_n \gamma_{n-1} \]  

provided that \( \beta_i \neq 0 \) for \( i = 1, 2, \ldots, n \).

So all \( \beta_i \) and \( \gamma_i \) (\( i = 1, 2, \ldots, n \)) are solved. Since \( a_i = A_i \), no computation is required to form \( a_i \).

Now

\[ A X = LUX = b \]

Let

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\[ U X = Y \]

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hence, \( \mathbf{X} \) can be solved by back-substitution, beginning with \( \mathbf{X}_n \). Thus,

\[ \mathbf{X}_n = \mathbf{Y}_n \]
\[ \mathbf{X}_j = \mathbf{Y}_j - \mathbf{X}_{j+1} \mathbf{Y}_j \quad j = n-1, n-2, \ldots, 1 \]

... (11)

To summarize, the complete algorithm for the solution of the tridiagonal system is

1. to generate \( \beta_1, \beta_2, \ldots, \mathbf{Y}_1, \mathbf{Y}_2, \ldots, \mathbf{Y}_{n-1} \) from equation (7), that is,

\[ \beta_1 = \mathbf{B}_1 \]
\[ \mathbf{Y}_i = \frac{\mathbf{C}_i}{\beta_i} \quad i = 1, 2, \ldots, n-1 \]
\[ \beta_i = \mathbf{B}_i - \mathbf{A}_i \mathbf{Y}_{i-1} \quad i = 2, 3, \ldots, n \]

2. to generate \( \mathbf{Y} \) recursively from equation (10), that is,

\[ \mathbf{Y}_1 = \frac{\mathbf{b}_1}{\beta_1} \]
\[ \mathbf{Y}_j = \frac{\mathbf{b}_j - \mathbf{A}_j \mathbf{Y}_{j-1}}{\beta_j} \quad j = 2, 3, \ldots, n \]
(3) to obtain \( x \) with

\[
x_n = y_n
\]

\[
x_k = y_k - x_{k+1} y_k \quad k = n-1, n-2, \ldots 1
\]