USE OF A GENERAL PARTIAL DIFFERENTIAL EQUATION SOLVER FOR SOLUTION OF HEAT AND MASS TRANSFER PROBLEMS IN SOILS

A Thesis Submitted to College of Graduate Studies and Research in Partial Fulfillment of the Requirements for the Degree of Master of Science in the Department of Civil Engineering University of Saskatchewan Saskatoon, Canada

by

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ABSTRACT

The application of geotechnical principles to linear infrastructure developments, such as pipelines, has often been neglected due to the high cost of analysis. The requirements of producing geotechnical analyses inexpensively demand that new techniques be developed. Development of general partial differential equation solvers represents a tool by which these analyses can be performed. The objective of this research is to apply general partial differential equations solvers to the problem of heat and mass transfer in soils. Solutions using the general partial differential equation solver called FlexPDE (PDE Solutions, 1999) are compared with analytical and accepted numerical solutions of the problems.

The FlexPDE program was first verified against seepage problems analyzed using the program Seep/W. The results obtained showed that FlexPDE correctly solves seepage problems. The descriptor files of Nguyen (1999) for the PDEase2D program used in this stage showed that FlexPDE and PDEase2D produce similar results. The three-dimensional capabilities of FlexPDE demonstrated in a simple steady state example show an increased versatility of the FlexPDE program over PDEase2D.

Solution of conductive heat flow using FlexPDE showed that realistic functions of the soil-freezing curve are needed to ensure convergence. The FlexPDE solutions to the Neumann problem for conductive heat flow in a material undergoing phase change were compared to the Temp/W model. The Temp/W results were similar to the FlexPDE results provided the same interpretation of the slope of the soil-freezing curve, $m_s^f$, was used in both programs.

Solution of coupled heat and mass transfer in the present study attempted to use the theory developed by Wilson (1990) as modified by Joshi (1993). Successful modelling
of coupled heat and mass transfer was achieved in FlexPDE for cases where the gradients acting in the soil were relatively small. Large gradients, such as those occurring during evaporation from the soil surface, were not modelled satisfactorily in FlexPDE.

A methodology for using FlexPDE for practical engineering problems is included in this study. The methodology shows how use of a general partial differential equation solver allows the engineer flexibility in inputting the phenomena studied, material properties, problem geometry, and boundary conditions. This example specifically deals with the pipeline industry. The example shows how FlexPDE and similar programs are applicable for solving problems in practical geotechnical engineering. The example relates the theory and application presented in the thesis to the original objectives.
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# LIST OF SYMBOLS

- \( c \) - mass specific heat capacity (J/kg\(^\circ\)C)
- \( c_a \) - mass specific heat of dry air (J/kg\(^\circ\)C)
- \( c_i \) - mass specific heat of ice (J/kg\(^\circ\)C)
- \( c_p \) - heat capacity of fluid (J/kg\(^\circ\)C)
- \( c_s \) - mass specific heat capacity of soil solids (J/kg\(^\circ\)C)
- \( c_v \) - mass specific heat capacity of water vapor (J/kg\(^\circ\)C)
- \( c_w \) - mass specific heat capacity of liquid water (J/kg\(^\circ\)C)
- \( D_v \) - diffusion coefficient of water vapor through soil (kg-m/kN-s)
- \( h \) - specific enthalpy (kJ/kg)
- \( h_w \) - hydraulic head (m)
- \( i \) - hydraulic gradient (dimensionless)
- \( k_w \) - coefficient of permeability (m/s)
- \( L_f \) - latent heat of fusion (J/m\(^3\))
- \( m'_s \) - slope of the soil-freezing curve (1/\(^\circ\)C)
- \( m^{\infty}_s \) - storage coefficient (1/kPa)
- \( P_v \) - vapor pressure (kPa)
- \( q_c \) - rate of heat flow by conduction (J/m\(^2\)-s)
- \( q_{\text{conv}} \) - rate of heat flow by convection (J/m\(^2\)-s)
- \( q_v \) - rate of vapor flux by diffusion (kg/s)
- \( S \) - specific surface area (m\(^2\)/kg)
- \( ST_{ij} \) - surface tension between phases \( i \) and \( j \)
- \( T \) - temperature (\(^\circ\)C or K)
- \( T' \) - freezing point depression (\(^\circ\)C or K)
- \( u_{\text{sa}} \) - pore-air pressure (kPa)
- \( u_t \) - pore-ice pressure (kPa)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( u_w )</td>
<td>pore-water pressure (kPa)</td>
</tr>
<tr>
<td>( v_w )</td>
<td>velocity of liquid water in soil pores (m/s)</td>
</tr>
<tr>
<td>( v_o )</td>
<td>velocity of fluid in soil pores (m/s)</td>
</tr>
<tr>
<td>( w_i )</td>
<td>gravimetric ice content</td>
</tr>
<tr>
<td>( w_u )</td>
<td>gravimetric unfrozen water content</td>
</tr>
<tr>
<td>( \gamma_w )</td>
<td>unit weight of water (kN/m³)</td>
</tr>
<tr>
<td>( \theta_a )</td>
<td>volumetric air content</td>
</tr>
<tr>
<td>( \theta_i )</td>
<td>volumetric ice content</td>
</tr>
<tr>
<td>( \theta_s )</td>
<td>volumetric solids content</td>
</tr>
<tr>
<td>( \theta_u )</td>
<td>unfrozen volumetric water content</td>
</tr>
<tr>
<td>( \theta_w )</td>
<td>volumetric water content</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>thermal conductivity (W/m°C)</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>specific heat capacity</td>
</tr>
<tr>
<td>( \pi )</td>
<td>osmotic suction (kPa)</td>
</tr>
<tr>
<td>( \rho )</td>
<td>density (kg/m³)</td>
</tr>
<tr>
<td>( \rho_a )</td>
<td>density of dry air (kg/m³)</td>
</tr>
<tr>
<td>( \rho_{dry} )</td>
<td>dry density of soil (kg/m³)</td>
</tr>
<tr>
<td>( \rho_i )</td>
<td>density of ice (kg/m³)</td>
</tr>
<tr>
<td>( \rho_o )</td>
<td>density of fluid (kg/m³)</td>
</tr>
<tr>
<td>( \rho_s )</td>
<td>density of soil solids (kg/m³)</td>
</tr>
<tr>
<td>( \rho_v )</td>
<td>density of water vapor (kg/m³)</td>
</tr>
<tr>
<td>( \rho_w )</td>
<td>density of liquid water (kg/m³)</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>total stress (kPa)</td>
</tr>
<tr>
<td>( \psi )</td>
<td>total suction (kPa)</td>
</tr>
</tbody>
</table>
1.1 General

The distribution of unsaturated soils is widespread across the world. It is now well understood that the behavior of unsaturated soils is a function of the water content in the soil. The impact of water movement on soil characteristics such as shear strength and compressibility is well established. The present study considers the movement of heat and mass in an unsaturated soil. The study is set in the context of the pipeline industry as discussed below.

1.2 Geotechnique and the Pipeline Industry

The pipeline industry is a major contributor to the economy of Western Canada. Pipelines are an economical and safe way of transporting fluids, such as water, coal slurry, oil or gas, from their source to the end consumer. The strength inherent in the material of which pipelines are constructed causes pipeline designers to only be concerned with extremely large stresses acting on the pipeline. In general, the stresses imparted by the soil to a pipeline are small with a few exceptions.

The exceptions include such things as slope instability, frost heave, and thaw subsidence (Williams, 1986). All three are phenomena where changes occur in the amount of water in the soil. The last two also add a component of heat transfer. Therefore, it is necessary to be able to quantify the movement of water and heat in the soil around a pipeline to develop designs that will mitigate adverse environmental effects. Large strains can also be imposed on pipelines due to seismic activity (Whitelaw and Reppond, 1988). Movements associated with seismic activity are slope
failures, liquefaction, ground shaking, and fault movements (Whitelaw and Reppond, 1988). Pipelines fall into a class of structures that also includes roads and railways in the sense that these structures consist of narrow right-of-ways, ten to a hundred meters wide, extending for tens or hundreds of kilometers. The area that needs consideration for geotechnical characterization along the route of these structures ranges from 10,000 to 100,000 m²/km. It is generally not economically feasible to study this area to the same extent as a geotechnical engineer would study the location of a proposed structure. As such, it is important to develop techniques to help streamline the investigation and analyses performed on these lineal structures in an effort to improve engineering design.

The present study attempts to develop numerical modelling techniques that will assist in the analysis of lineal structures, particularly pipelines, with respect to the behavior of soils in the unsaturated zone.

1.3 Unsaturated Soil Mechanics and the Finite Element Method

The development of unsaturated soil mechanics as a subject in geotechnical engineering has occurred in parallel with the development of computer technology. This is in due to the difficulty in solving analytically the equations governing the behavior of unsaturated soils. Finite element methods are generally required to bring the theory of unsaturated soil mechanics into practice.

Historically, researchers were forced to develop finite element codes for each individual phenomenon being studied. This resulted in the creation of numerous finite element programs covering such topics as seepage, stress, contaminant transport, and heat flow. However, recent work has shown that it is possible to use a general partial differential equation solver, developed by mathematicians, physicists, and computer scientists, to conduct research into the behavior of unsaturated soil mechanics without the necessity of producing new finite element code. The advantage of using general partial differential equation solvers is to allow researchers the flexibility of testing various
representations of soil behavior, material properties, and boundary conditions without the necessity of creating new subroutines for existing finite element programs.

The benefit of using a general partial differential equation solver in performing research has been recognized; however, the applicability and potential of these methods to geotechnical engineering practice has not been fully explored. Problems that have been studied using general partial differential equation solvers include seepage and stress (Nguyen, 1999; Vu, 1999). One important area of geotechnique that warrants attention is the area of thermal problems. Thermal problems are of particular interest in soils undergoing freezing and thawing, and soils at the soil-atmosphere boundary. Soils undergoing freezing or thawing have important but often overlooked impacts on the design of structures in northern climates. The coupled phenomenon of heat and mass transfer has been shown to be of particular interest in near surface geotechnical practice, such as design of waste containment covers, heave, and others.

1.4 Objectives of Thesis

In light of the background information provided above, the following objectives have been identified for this thesis:

1. Using general partial differential equation solvers in order to solve seepage problems in soils in the context of the pipeline industry
2. Using general partial differential equation solvers in order to solve problems of heat flow in soils in the context of the pipeline industry
3. Using general partial differential equation solvers in order to solve two dimensional coupled heat and mass transfer problems in soils without freezing
4. Using general partial differential equation solvers in order to solve two dimensional coupled heat and mass transfer problems in soils with freezing
5. Application of above analyses to practical problems
In carrying out these objectives in this thesis, the general partial differential equation solver known as FlexPDE\(^1\) (PDE Solutions. 1999) has been used. This program is similar in nature to the program called PDEase\(^2\) (Macsyma. 1996). FlexPDE uses the finite element method to solve two and three-dimensional problems for steady state and transient conditions.

1.5 Organization of Thesis

The organization of this thesis is somewhat different from the traditional theses prepared in engineering and science. The first four chapters follow the traditional methodology of presenting an introduction, preparing a literature review, stating the theory that is being used in the present study, and discussing the methodology of the research program.

The literature review in Chapter 2 first details the requirements for pipeline-soil modelling, then presents highlights on the historical development of uncoupled and coupled flow laws for heat and water in soils, particularly unsaturated soils. Definitions of the material properties of importance in the later analysis are presented. A brief review of the techniques that have been used in the past for solving problems in heat and mass transfer concludes the chapter.

The theory used in this thesis is developed in detail in Chapter 3. The equations that have been used in the numerical modelling are derived in brief and explained. Material property functions are listed using common forms, describing the material properties as functions of water content or soil suction.

Chapter 4 provides an overview of the modelling research program undertaken in this thesis. The research program has been divided into four sections. The first section verifies the FlexPDE solution with seepage modelling results presented by Nguyen

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\(^1\) FlexPDE is a proprietary software package developed and produced by PDE Solutions Inc. of Antioch, CA, USA.

\(^2\) PDEase is a proprietary software package developed and produced by Macsyma Inc. of Arlington, MA, USA.
(1999) and the Geo-Slope (1999) model Seep/W. The second section deals with conductive heat flow in soils in steady state and transient conditions. The third section of the research program considers coupled heat and mass transfer problems. Finally a practical example is considered to try to demonstrate the usefulness of the methodology to engineering practice.

The thesis then diverges from the traditional thesis model in Chapter 5. Traditionally, researchers present the results of their research in one chapter, followed in a separate chapter with discussion and analysis of that data. This model is appropriate for theses in which a single phenomenon or experiment is studied. In the present work, fourteen separate problems are considered and modelled numerically. Therefore, results from the analyses conducted and discussion of those results are presented simultaneously for the sake of clarity.

Chapter 6 briefly summarizes the results, analysis, and discussion of Chapter 5 with reference to the objectives stated above. Finally, Chapter 7 concludes the thesis, detailing the relevant insights gained throughout the course of the research program. Specific conclusions for the various phenomena studied are presented. Recommendations on the use of any partial differential equation solver, but particularly FlexPDE, in geotechnical practice are given. Finally, some recommendations are given for future research on solution of coupled heat and mass transfer problems, freezing and thawing in soils, and further development of general partial differential equation solvers for the benefit of the geotechnical community.

Three appendices are provided. Appendix A provides details on the program FlexPDE that was used in the research program. Also included is a detailed example from the seepage verification-modelling program to provide a detailed example of the development of descriptor files in FlexPDE. Appendix B expands on the seepage problems not considered in the main body of the thesis, but used in verification of FlexPDE. Appendix C provides FlexPDE descriptors from the problems discussed in Chapter 5, and Appendix B.
CHAPTER 2
LITERATURE REVIEW

2.1 General

This chapter provides a brief review of the literature relevant to the thesis objectives described in Chapter 1. Section 2.2 describes the need for incorporating unsaturated soil mechanics into the design of pipelines. Section 2.3 reviews the development of the theory of movement of heat and mass in unsaturated soils for both the uncoupled and coupled cases. Section 2.4 defines the material properties that are needed in solution of heat and mass transfer problems. Finally, Section 2.5 reviews the historical development of solution methods for heat and mass transfer in soils.

2.2 Role of Unsaturated Soil Mechanics in the Pipeline Industry

The modeling of the soil-pipeline system is a soil-structure interaction problem, similar to a footing embedded in a soil. The analysis must take into account four factors as given by Selvadurai (1988):

1. The modeling of the soil behavior around the pipeline.
2. The modeling of the pipeline’s mechanical response to soil movement.
3. The modeling of the behavior of the pipe-soil interface.
4. The modeling of the loading process.

Rajani and Morgenstern (1993) give similar modeling criteria for pipelines imbedded in freezing soils:

2. Modeling of mechanical properties of frozen ground (soil behavior).
The prediction of the behavior of the soil around a pipeline is important in conducting analysis of soil-pipeline problems.

Pipelines are generally built above the water table in the unsaturated zone. Fredlund and Morgenstern (1977) showed that the stress state in an unsaturated soil could be represented by any two of \((u_a-u_w)\) \((\sigma-u_a)\) \((\sigma-u_w)\) where \(u_a\) is the pore-air pressure, \(u_w\) is the pore-water pressure and \(\sigma\) is the total stress. Generally, the variables used are \((u_a-u_w)\) and \((\sigma-u_a)\). The changes in the total stress, \(\sigma\), are related to changes in the loads applied to the soil by such things as soil self-weight and surcharge loads. An extensive volume of research is available for determining the effects of total stress changes on buried pipelines (Spangler, 1948; Hoëg, 1968; Rajani et al., 1995).

Spangler (1948) provided details on the stresses that will develop in the soil around a buried conduit. The research of Spangler (1948) was originally intended for the design of highway culverts. In 1954, Spangler extended the analysis for the prediction of the deformation of pressure pipelines due to soil loads.

Hoëg (1968) described an analytical method in which the stresses at any point in the soil around a buried pipeline could be estimated. The work of Spangler (1948) and Hoëg (1968) describe the stresses acting transversely on the pipeline cross section. Additional research, such as that by Rajani et al. (1995), focused on the longitudinal stresses acting on the pipeline due to phenomena such as landslide, frost heave, and thaw subsidence.

The variable \((u_a-u_w)\) is referred to as the matric suction (Fredlund and Rahardjo, 1993). Changes in matric suction occur in response to the movement of water through the soil. Matric suction plus the osmotic suction, \(\pi\), resulting from presence of salts in the pore-water of a soil, equal the total suction given by the symbol \(\psi\). Geotechnical engineers are primarily concerned with the effect of changes in matric suction. It can be assumed for most applications that the osmotic suction component will be small and is therefore commonly neglected.
The flow of a fluid in a soil results from a gradient being applied. Four types of gradients can drive fluid flow. These are hydraulic head, temperature, electrical, and chemical gradients (Mitchell, 1976). Hydraulic head gradients cause movement of liquid water in the soil. Temperature gradients drive movement of water vapor in unsaturated soils. The present study focuses on uncoupled and coupled phenomena of heat and water flow in unsaturated soils. Determination of the heat flow in a soil is necessary for determining the temperature gradients in the soil.

2.3 Movement of Heat and Water in Unsaturated Soils

The movement of heat and water in soils occur as coupled phenomena. However, in the past most researchers have uncoupled the phenomena to ease solution. Uncoupled seepage and heat flow are first considered followed by a review of the development of coupled solutions.

2.3.1 Water Flow

The flow of water in a porous media, such as soil, can be described through the use of Darcy’s law (1856). Darcy’s law states that the flow of water $v_w$ is directly proportional to the gradient of hydraulic head, $i$, in the soil (Mitchell, 1976). The constant of proportionality, $k_w$, is the coefficient of permeability, also frequently referred to as hydraulic conductivity. Darcy’s law can be written as:

$$v_w = -k_w i \quad [2.1]$$

Darcy’s law was originally formulated and verified for saturated soil conditions. Research by Childs and Collis-George (1950) and Brooks and Corey (1964) showed that Darcy’s law is applicable for soils that are not fully saturated. However, for unsaturated soils, the permeability is not a constant, as in the case of saturated soils, but varies as a function of the water content of the soil (Childs and Collis-George, 1950; Gardner, 1958; Brooks and Corey, 1964). The water content in turn varies with the matric suction in the soil.
In an unsaturated soil, water can also flow in the vapor phase. Vapor flow occurs by diffusion under partial pressure gradients and advection in bulk air flow (Philip and de Vries, 1957; Wilson, 1990). Fick’s law governs flow of vapor due to diffusion. The mass flux of vapor, \( q_v \), is proportional to the gradient of concentration of the vapor or the vapor pressure, \( P_v \). A proportionality constant, \( D_v \), related to the molecular diffusivity of water vapor in air and the cross-sectional area of the soil pores available to flow, completes Fick’s law given as:

\[
q_v = -D_v \frac{\partial P_v}{\partial x}
\]  

[2.2]

A correction factor is applied to Equation 2.2 to account for the bulk air movement component when large pressure gradients act in the soil.

### 2.3.2 Heat Flow

Research performed in the geotechnical community on heat flow through soils has primarily focused on freeze-thaw problems. The design of heated structures on permafrost terrain requires an estimation of the amount of thaw expected. Conversely, the design of cooled structures (e.g., chilled pipeline, hockey rinks, refrigerated storage) in non-permafrost terrain requires an estimation of the depth of freezing anticipated.

The flow of heat in a medium can occur by three mechanisms: conduction, convection, and radiation (Carslaw and Jaeger, 1959). For most problems involving the flow of heat in soils, the radiation component is neglected. Apart from the soil surface, the amount of heat transfer by radiation is several orders of magnitude smaller than the other two components and is therefore neglected (Harlan and Nixon, 1978).

Heat flow due to conduction can be estimated by an equation similar to Darcy’s law. The rate of heat flow through an object by conduction, \( q_c \), is proportional to the gradient of temperature, \( dT/dx \). The constant of proportionality in this case is referred to as the thermal conductivity, \( \lambda \). The amount of heat flow by conduction is given as:

\[
q_c = -\lambda \frac{dT}{dx}
\]  

[2.3]
Solution of the equation of conservation of energy for conductive heat flow was given by Carslaw and Jaeger (1959).

Convective heat transport is transmission of heat by movement of heated particles (Harlan and Nixon, 1978). In an unsaturated soil, convection results from movement of the pore fluids, either in vapor form or in liquid form. The amount of heat flow by convection is given as:

\[ q_{\text{conv}} = c_o \rho_o v_o \frac{\partial T}{\partial x} \]  \hspace{1cm} [2.4]

In the above equation, \( q_{\text{conv}} \) is the convective heat flow, \( c_o \) is the heat capacity of the fluid under consideration, \( \rho_o \) is the density of the fluid, and \( v_o \) is the fluid velocity determined by Darcy’s law for a liquid or Fick’s law for a gas.

Nixon (1975) suggested that the convective heat transfer in a soil undergoing freezing or thawing was much smaller than the conductive heat transport in most soils. Only in coarse soils will the convective effects be significant relative to the conductive heat flow. Therefore, Nixon (1975) suggested that the convective effects could be neglected in freeze-thaw analysis.

The pore-water in soils undergoing freezing or thawing undergoes a phase change from liquid to solid or vice versa. In the process, large quantities of heat is released or absorbed (Farouki, 1986). Figure 2.1 shows schematically the changes in energy in a soil undergoing freezing and thawing. A similar latent heat effect occurs when water undergoes phase change from liquid to vapor.

The latent heat changes affect the rate at which heat movement will occur. Theoretical development of the effect in freezing-thawing soils is provided in Chapter 3.
2.3.3 Coupled Heat and Mass Transfer

Coupled solutions of heat and mass transfer problems in the geotechnical community, before about 1990, were dominated by concerns for large deformation of structures built on permafrost. Since 1990, as concerns over migration of pollutants into the environment and the need to rationally design cover systems increased, the focus has shifted to the solution of coupled heat and mass transfer problems without freezing/thawing effects. The present study considers both of these situations.

2.3.3.1 Coupled Heat and Mass Transfer in Soils without Freezing

The flow of water in liquid water and water vapor is of interest in near surface problems, and in problems where the soil is under a temperature gradient. Coupled heat and mass transfer formulations account for flows in both phases. The majority of research in coupled heat and mass transfer without freezing was conducted by soil scientists, until recently when geotechnical engineers realized benefits for design of waste containment facilities.
Philip and de Vries (1957) presented equations describing the coupled movement of heat and mass in soils. Several of the assumptions of Philip and de Vries (1957) make the model proposed unsuitable for geotechnical engineering purposes. Philip and de Vries (1957) formulate the mass transfer equation in terms of flow occurring in response to gradients of water content. As discussed by Fredlund and Rahardjo (1993) flow of water due to water content gradients is contrary to accepted geotechnical practice, which states that water flow occurs in response to gradients of hydraulic head. However, even with the limitations to geotechnical engineering, some researchers in the geotechnical field have formulated coupled models based on the Philip and de Vries model (Ewen and Thomas, 1989).


The basic theory of the geotechnical models of coupled heat and mass transfer is the same consisting of the following components:

1. Liquid flow occurs in response to hydraulic gradients.
2. Vapor flow occurs in response to partial pressure gradients.
3. Heat flow occurs by conduction.
4. Phase change occurs to satisfy thermodynamic equilibrium between liquid and vapor phases. releasing or adsorbing heat.

The system satisfies partial pressure equilibrium of the water vapor, thereby coupling the heat and mass equations. The equations are coupled with the atmosphere through the vapor pressure.
2.3.3.2 Coupled Heat and Mass Transfer in Soils with Freezing

Interest in coupled heat and mass transfer in soils undergoing freeze-thaw accelerated in the years after World War II, as development increased in the polar regions of the world. Proposed development of arctic oil and gas fields in the 1970’s continued the interest in heat and mass transfer in freezing-thawing soils. In particular, stresses imposed on pipelines by frost heaving or thaw subsidence attracted researchers attention (Williams, 1986).

Soils in which freezing occurs add phase change from liquid water to solid water and from water vapor to solid water. Generally, the effects of vapor transport and phase change are neglected in the analysis, as the phase change from liquid water to ice dominates.

Taber (1930), in one of the earliest attempts to describe frost heaving, showed that movement of water in soils undergoing freezing occurs in response to capillary forces developing in the soil. Williams (1964b), Koopmans and Miller (1966), and others related the soil-water characteristic curve to the soil-freezing curve. The effect of ice formation on the soil suction is analogous to the formation of occluded air voids. Both result in a decrease of the continuity of the water phase, increasing soil suction. The resulting soil suction gradients that form in freezing soils drives moisture movement from unfrozen soil to the freezing front.

Harlan (1973) formulated a coupled model for heat and mass transfer in soils undergoing freezing in a hydraulic head framework. Harlan (1973) included a term in the total head to account for capillary potential because of freezing. Guymon and Luthin (1974) use a similar form of equations.

Jame and Norum (1980) used a slightly modified version of the model proposed by Harlan (1973) to model the results of a freezing experiment of an unsaturated soil. Based on the findings of Nixon (1975) and others, Jame and Norum (1980) neglect the
convective term in Harlan's (1973) model. The results obtained by Jame and Norum (1980) show good agreement between the experimental data and numerically modelled results using the equations given by Harlan (1973). Numerical solutions using the equation of Harlan (1973) require an iterative approach, because three unknowns are present in two equations.

Newman (1996) developed an equation to describe the freezing of a soil that is compatible with the model of Joshi (1993). Newman (1996) related the soil-freezing curve and the soil-water characteristic curve to produce a single equation for the movement of water and heat in soils undergoing freezing. Soil suction is back calculated from the same relationship. Newman (1996) verified the model proposed against the results of Jame and Norum (1980).

2.4 Material Properties

An important aspect of analysis in geotechnical engineering is definition of material properties. Material properties in the present study divide into seepage properties (i.e., soil-water characteristic curve and permeability) and thermal properties (i.e., soil-freezing curve, thermal conductivity, and volumetric specific heat capacity). These properties are defined using functions relating the property to the soil suction or water content of the soil.

2.4.1 Soil-Water Characteristic Curve

The soil-water characteristic curve is the curve that describes the relationship between the soil suction and the volumetric water content, gravimetric water content or degree of saturation (Fredlund and Rahardjo, 1993). Figure 2.2 shows an example of the soil-water characteristic curve for a sand. Important features to note in the curve are:

- the hysteresis present depending on whether the change of water content is following a wetting path or a drying path,
- the air entry value is the soil suction at which the soil begins to desaturate, and
- the residual stage is the stage where the soil is essentially dry, and any further reduction in water content or degree of saturation requires a large amount of energy.

Figure 2.2 An example of a soil-water characteristic curve highlighting some of the important features (adapted from Fredlund et al., 1994)

Definition of the soil-water characteristic curve needs to be both qualitative and quantitative. Various researchers (Gardner, 1958; Brooks and Corey, 1964; van Genuchten, 1980; Fredlund and Xing, 1994) have proposed mathematical relationships for describing the soil-water characteristic curve. Several of these relationships are discussed in Chapter 3.

The slope of the soil-water characteristic curve \( \frac{\partial \theta_s}{\partial \psi} \), also referred to as \( m_s^* \), defines the storage capacity of the soil. The \( m_s^* \) term defines how the water content changes as the soil suction is increased or decreased. This parameter is important in the analysis of water flow in transient conditions, as discussed in Chapter 3.
2.4.2 Coefficient of Permeability

The coefficient of permeability is the velocity of water flowing through a soil under a hydraulic gradient of one. For an unsaturated soil, the coefficient of permeability is not a constant, but is a function of the water content and therefore the water pressure in the soil. The saturated coefficient of permeability is relatively inexpensive to determine and can be determined in field conditions (i.e., slug or falling head tests) or under laboratory conditions (i.e., falling head or constant head tests).

Various researchers (Childs and Collis-George, 1950; Burdine, 1953; Gardner, 1958; Brooks and Corey, 1964; Campbell, 1973; van Genuchten, 1980; Fredlund et al., 1994) have proposed functions for defining the coefficient of permeability as a function of the soil suction or water content. Functions for permeability have been divided into empirical and statistical types (Fredlund et al., 1994). The statistical functions (Childs and Collis-George, 1950; Burdine, 1953; van Genuchten, 1980; Fredlund et al., 1994) attempt to account for the variation of the permeability in terms of the distribution of pores in the soil (Fredlund et al., 1994). Further consideration of statistical functions is not provided in this thesis. The empirical functions (Gardner, 1958; Brooks and Corey, 1964; Campbell, 1973) approximate the unsaturated coefficient of permeability at any suction using the saturated coefficient of permeability. Further discussion of empirical functions for the coefficient of permeability is given in Chapter 3.

2.4.3 Specific Heat Capacity

The specific heat capacity of a soil can be defined as the amount of heat required to increase the temperature of a unit volume or unit mass by a specified temperature (Farouki, 1986). Differentiation is made between the mass specific heat capacity (i.e., the amount of heat required to increase the temperature of unit mass of soil) and the volumetric specific heat capacity (i.e., the amount of heat required to increase the temperature of a unit volume of soil). Generally, the volumetric specific heat capacity is used in solving problems in geotechnical engineering.
Methods used for estimating specific heat capacity of a soil sum the heat capacities of the constituent materials. De Vries (1963) summarizes a method for predicting the specific heat capacity of a soil. The specific heat capacity of a soil can be estimated as the sum of the parts (i.e., water, air, soil minerals, and ice). Newman (1996) provided a modified method using the dry density of the soil and the gravimetric water and ice contents to estimate the volumetric specific heat capacity.

Williams (1964a) showed that the specific heat capacity of a soil undergoing freezing or thawing needs to include the effects of the latent heat due to phase change of the pore-water. The specific heat capacity of a soil undergoing freezing or thawing is referred to the apparent specific heat capacity of the soil (Williams, 1964a). The apparent specific heat capacity of a soil includes latent heat effects and the specific heat capacity of the constituent material of the soil.

2.4.4 Thermal Conductivity

The definition of thermal conductivity of a soil is the amount of heat that can flow through a unit area under a temperature gradient of one (Farouki, 1986). It is analogous to the coefficient of permeability used in seepage analysis.

Kersten (1949) conducted thermal conductivity tests on 19 different soils compacted to various densities, at various water contents. Kersten (1949) concluded that the thermal conductivity is dependent on the dry density, water content, temperature, texture, and mineralogy of the soil. Kersten (1949) provides a set of empirical relationships for estimating the thermal conductivity of a variety of soil types.

De Vries (1963) provides a method for predicting the thermal conductivity of a soil based on the components present in the soil. The method requires an estimate of the particle shape in order to estimate the inter-particle contact area. Smith (1942), Mickly (1951), and Johansen (1975) give other methods for estimation of thermal conductivity. A variety of methods for estimating thermal conductivity is given in Chapter 3.
2.4.5 Soil-Freezing Curve

As early as 1915 Bouyoucos showed that the pore-water in a soil does not freeze at a uniform temperature and that some freezing point depression occurs.

The unfrozen water content curve is a representation of the amount of water that remains unfrozen in a soil as the temperature of the soil decrease below the normal freezing point of the pore fluid (i.e., for pure water 0 °C). It is generally accepted that this freezing point depression is due to suctions generated in the soil due to ice formation. The ice acts as air does in an unsaturated soil, reducing the cross sectional flow area, and inducing capillary forces. The suctions that develop reduce the freezing point of the water. The unfrozen water content of a soil has been shown to be independent of the initial water content (Tice et al., 1966). Figure 2.2 shows examples of a soil-freezing curve for five soils.

![Soil-freezing curves for typical soils (from Nersesova and Tsytovich, 1963)](image)

Anderson et al. (1973), Anderson and Morgenstern (1973), Tice et al. (1976), and Black and Tice (1989) suggested empirical relationships and provided empirical constants for describing the soil-freezing curve.
Williams (1964b) demonstrated a method for predicting the soil-freezing curve using the soil-water characteristic curve and a Clapeyron type relationship relating soil suction and temperature depression. Miller (1966) identified that there is a relationship between the terms \((u_d-u_a)\) and \((u_r-u_w)\) where \(u_i\) is the ice pressure acting in the soil, and says the relationship will be different depending on whether the soil particles are in contact (sand) or separated by a water film (clays). Black and Tice (1989) apply the Clapeyron equation to relate \((u_d-u_a)\) and \((u_r-u_w)\). Figure 2.4 summarizes the results of Black and Tice (1989) comparing the soil-freezing/thawing curves with the soil-water characteristic curve for the same soil. Figure 2.4 shows both experimental results for the curves, and predictions based on the Clapeyron equation.

![Figure 2.4](image)

Figure 2.4 Experimental and theoretical soil-freezing and soil-water characteristic curves for Windsor sandy loam (after Black and Tice, 1989)

Newman (1996) used the results of Black and Tice (1989) to relate the slopes of the soil-freezing curve and the soil-water characteristic curve in order to obtain a single equation for heat flow and mass transfer in soils. Newman (1996) also showed that the coefficient of permeability of a partially frozen soil could be predicted from the unsaturated permeability using the soil-freezing curve.
2.5 Solutions for Heat and Mass Transfer in Soils

2.5.1 Solution of Water Movement (Seepage)

Cassagrande (1937) presented complete discussion on the use of the flownet technique for predicting the seepage through earth structures, originally developed by Forchheimer. Cassagrande (1937) divided the soil into two parts, the soil below the water table and the soil above the water. The assumption was made that water only flowed below the water table. The flownet method for “modelling” groundwater flow was used extensively in geotechnical practice.


2.5.2 Solution of Heat Transfer

One of the first methods for predicting freeze-thaw phenomena in soils was adapted from Carslaw and Jaeger (1959) presentation of Neumann’s solution for phase change in a material, from solid to liquid or vice versa. Neumann’s solution provides the depth of freezing or thawing that will occur for a given temperature boundary condition. The solution assumes phase change is occurring in the entire volume of interest. In a soil, it is only the pore-water that is undergoing phase change. Harlan and Nixon (1978) showed that the Neumann solution over predicts the thaw depth (or conversely under predicts the freeze depth). Harlan and Nixon (1978) show how it is possible to use Neumann’s solution for practical design.
A large amount of research was conducted in the 1970’s for development of numerical models for predicting heat flow in soils. This occurred in response to several proposals for construction of oil and gas pipelines in Northern Canada and Alaska. The models needed to account for the latent heat effects as the pore-water changes phases.

Ho et al. (1970), Nakamo and Brown (1971), and others developed finite difference models for heat flow in soils with phase change. Hwang et al. (1972) provided details on a finite element model for transient analysis of conduction in soils undergoing freezing and thawing. Hwang (1976) provided details related to the modification of the original model to better model surface conditions. These models include instantaneous phase change of the pore-water from liquid to solid or vice versa.

Coutts and Konrad (1994) propose a model that makes use of the “node state” method, which is basically a finite element method, but the nodes are assigned states on the basis of whether the water at the node is liquid, solid, or transitional. The latent heat effects are applied only at the transitional nodes. The Temp/W finite element package (Geo-Slope, 1999) uses an average value for the latent heat between time steps. The time average solution is reasonable provided sufficient time steps are included in the model.

The numerical models developed for heat flow in soils undergoing freeze-thaw try to reconcile an instantaneous phase change of the water. Various schemes are implemented to allow convergence of solution using this assumption. As discussed, the pore-water does not freeze at a single temperature, but over a range of temperatures. Improved stability can be obtained in numerical solutions if latent heat effects are applied over a broader range of temperatures. Furthermore, the results obtained are more realistic.

\[^1\text{Temp/W is a proprietary software package developed and produced by Geo-Slope International Ltd.,} \]

Calgary, AB, Canada
2.5.3 Solution of Coupled Heat and Mass Transfer

Solution of coupled heat and mass transfer is not generally feasible by analytical means. Early models focused on the freeze-thaw problem (Harlan, 1973; Jame and Norum, 1980). The models iteratively solved for the ice content of the soil, because the equations proposed by Harlan are indeterminate.

Ewen and Thomas (1989) developed a finite difference code for solution of coupled heat and mass transfer using the equations proposed by Philip and de Vries (1957). Li et al. (1997) modelled the results of Ewen and Thomas (1989) using the finite element method. Both these models were for conditions in which evaporation was not occurring.


2.5.4 Summary of Solution Methods

Solutions of problems in engineering are classified as analytical or numerical. Proponents of analytical or closed-form solutions, seek to develop closed-form solutions to the various differential equations that are used to describe various physical phenomena. The problem is that it is difficult to develop a closed-form solution for all but the simplest cases of a differential equation. Furthermore, closed-form solutions are only valid for the boundary conditions for which the equations were developed.

Closed-form solutions are not necessary for most physical phenomena. Development of numerical techniques such as finite difference and finite element has enabled engineers to solve extremely complex physical phenomena for a variety of boundary conditions.
and material properties. In the past thirty years, various researchers have developed application specific finite element or finite difference codes. The process of developing new code is laborious.

In the 1990’s, there appeared a greater acceptance and use of various pre-packaged finite element and finite difference codes. These codes could range from discipline specific products such as the Geo-Slope software to general partial differential equation solvers such as PDEase and FlexPDE. The advantage of the latter programs is the flexibility offered to researchers.
CHAPTER 3
THEORY OF HEAT AND MASS TRANSFER IN UNSATURATED SOILS

3.1 General

This chapter provides an overview of the theory that has been implemented through FlexPDE during the research program of this thesis. Heat and mass transfer in unsaturated soils is a coupled phenomenon. The theory is first developed for the uncoupled situation, followed by a discussion of the coupled situation.

3.2 Liquid Water Flow

The flow of water in soil occurs in response to hydraulic head gradients as discussed in Chapter 2. Section 3.1.1 provides the partial differential equation for seepage for unsaturated soils. Discussion of the material properties required for seepage analysis follows in Section 3.1.2.

3.2.1 Partial Differential Equation for Seepage

Seepage problems are among the most commonly analyzed problems in geotechnical engineering. Papagianakis and Fredlund (1984), Lam et al. (1987) and Nguyen (1999) among others provide details on the derivation of the partial differential equation for unsaturated seepage. Equation 3.1 presents the standard form of the equation in two-dimensions for transient seepage.

\[
\frac{\partial}{\partial y} \left( k_y \frac{\partial h_u}{\partial y} \right) + \frac{\partial}{\partial x} \left( k_x \frac{\partial h_u}{\partial x} \right) = -m_u \gamma_u \frac{\partial h_u}{\partial t}
\]  

[3.1]

where \( k_x \) and \( k_y \) are the coefficient of permeability in the x and y direction.

\( h_u \) is the hydraulic head (i.e., \( h_u = \frac{\gamma_u}{\gamma} + y \)).
\( u_a \) is the pore-water pressure,
\( \gamma_w \) is the unit weight of water, and
\( m_2^* \) is the storage coefficient.

For three dimensions, Equation 3.1 becomes:

\[
\frac{\partial}{\partial y} \left( k_y \frac{\partial h_w}{\partial y} \right) + \frac{\partial}{\partial x} \left( k_x \frac{\partial h_w}{\partial x} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial h_w}{\partial z} \right) = -m_2^* \gamma_w \frac{\partial h_w}{\partial t} \tag{3.2}
\]

where \( k_z \) is the coefficient of permeability in the \( z \) direction.

A general form of Equation 3.2 for the condition of \( k_x = k_y = k_z \) is given in Equation 3.3. In general, the numerical models developed in this research program used the form given by Equation 3.3.

\[
\nabla (k_w \nabla h_w) = -m_2^* \gamma_w \frac{\partial h_w}{\partial t} \tag{3.3}
\]

For steady state conditions, the right hand side of Equation 3.3 equals zero, and Equation 3.3 is re-written as Equation 3.4.

\[
\nabla (k_w \nabla h_w) = 0 \tag{3.4}
\]

### 3.2.2 Seepage Material Properties

Two material properties, the storage coefficient, \( m_2^* \), and the coefficient of permeability, \( k_w \), require definition for solution of Equation 3.3.

#### 3.2.2.1 Soil-Water Characteristic Curve

A description of the soil-water characteristic curve (SWCC) is important to the analysis of unsaturated soil problems. The SWCC describes the volumetric water content, \( \theta_w \), or degree of saturation, \( S \), as a function of the soil suction, \( \psi \). Equations describing the relationship between the volumetric water content and suction have been proposed by various researchers. Table 3.1 summarizes four of the more common methods for describing the SWCC mathematically.
<table>
<thead>
<tr>
<th>Function</th>
<th>Definitions</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_n = \frac{1}{1 + a \psi^n} )</td>
<td>( a ) = parameter related to air entry value, ( n ) = parameter related to slope of function</td>
<td>Gardner (1958)</td>
</tr>
<tr>
<td>( \Theta = \left( \frac{\psi_n}{\psi} \right)^n )</td>
<td>( \Theta ) = normalized water content, ( \Theta = (\theta_n - \theta_r) / (\theta_s - \theta_r) )</td>
<td>Brooks and Corey (1964)</td>
</tr>
<tr>
<td>( \theta_n = \frac{\theta_r}{1 + (a \psi)^n} )</td>
<td>( a ) = parameter related to inverse of air entry value of the soil, ( n ) = parameter related to slope of curve past the air entry value, ( m ) = parameter related to residual water content of the soil</td>
<td>van Genuchten (1980)</td>
</tr>
<tr>
<td>( \psi_r = c'(\psi) \frac{\theta_r}{\ln[\exp(1) + (\psi / a)^\nu]} )</td>
<td>( c'(\psi) = \frac{\ln(1 + \psi / \psi_r)}{\ln(1 + (1000000 / \psi_r))} )</td>
<td>Fredlund and Xing (1994)</td>
</tr>
</tbody>
</table>
The derivative or slope of the SWCC is the water storage coefficient used in Equation 3.3, such that:

\[ m_z^w = \frac{\partial \theta^w}{\partial \psi} \]  

[3.5]

Table 3.2 gives the derivatives of three of the SWCC functions given in Table 3.1.

### 3.2.2.2 Coefficient of Permeability

The coefficient of permeability in an unsaturated soil is function of the soil water content. The coefficient of permeability can also be defined as function of soil suction, given that the SWCC relates water content to soil suction. Various researchers have proposed functions for the coefficient of permeability in an unsaturated soil. Fredlund et al. (1994) divide the functions into empirical and statistical methods.

The empirical functions fit experimental data of unsaturated permeability and apply the curve fits to other soils for which the saturated coefficient of permeability is known. The statistical methods describe unsaturated permeability functions by estimating the pore size distribution in the soil. The present study uses the empirical functions. Table 3.3 presents three common functions for the unsaturated coefficient of permeability.
<table>
<thead>
<tr>
<th>Function</th>
<th>Source</th>
</tr>
</thead>
</table>
| \[
\frac{\partial \theta_n}{\partial \psi} = \frac{-1}{\left(1 + a \psi^n\right)^2} \frac{a \psi^n}{\psi} \]  | Gardner (1958)          |
| \[
\frac{\partial \theta_n}{\partial \psi} = -\frac{\theta_n}{\left(1 + (a \psi)^n\right)^m} \frac{mn}{\psi(1 + (a \psi)^n)} \]  | van Genuchten (1980)    |
| \[
\frac{\partial \theta_n}{\partial \psi} = \frac{1}{\left[\psi \left(1 + \frac{\psi}{\psi_r}\right) \ln\left(1 + \frac{1000000}{\psi_r}\right) \ln\left[\exp(1) + \left(\frac{\psi}{a}\right)^n\right]^{-1}\right]} \psi \left[\exp(1) + \left(\frac{\psi}{a}\right)^n\right]^{-1} \psi \left[\ln\left[\exp(1) + \left(\frac{\psi}{a}\right)^n\right]\right]^{-1} \psi \left[\ln\left[\ln\left(1 + \frac{\psi}{\psi_r}\right)\right] \lnight.\]  | Fredlund and Xing (1994) |
Table 3.3 Functions for unsaturated soil permeability

<table>
<thead>
<tr>
<th>Function</th>
<th>Definition</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_w = \frac{k_s}{1 + a\psi^n} )</td>
<td>( k_w ) = coefficient of permeability at soil suction ( \psi ) ( k_s ) = saturated coefficient of permeability ( a ) = related to air entry value of soil ( n ) = related to slope of soil-water characteristic curve</td>
<td>Gardner (1958)</td>
</tr>
<tr>
<td>( k_w = k_s ) for ( \psi \leq \psi_b ) ( \psi_b ) = air entry value of soil</td>
<td>Brooks and Corey (1964)</td>
<td></td>
</tr>
<tr>
<td>( k_w = k_s \left( \frac{\psi}{\psi_b} \right) ) for ( \psi \geq \psi_b )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( k_w = k_s \left( \frac{\theta}{\theta_s} \right)^n ) ( n ) = factor to adjust the prediction</td>
<td>Campbell (1973)</td>
<td></td>
</tr>
</tbody>
</table>

3.3 Heat Flow

Heat moves in three ways, namely by radiation, by convection, and by conduction. The present study focuses on conductive heat flow. The quantity of heat flow by radiation and convection are two or more orders of magnitude less than the conductive heat flow in all but the coarsest soils. Considering only the conductive heat flow is common in geotechnical engineering. Section 3.3.1 derives the partial differential equation for heat flow. The material properties for heat flow are defined in Section 3.3.2.

3.3.1 Partial Differential Equation for Conductive Heat Flow

An equation similar to Darcy’s law for seepage governs the flow of heat by conduction as given in Equation 3.6.

\[
q_z = -\lambda \frac{\partial T}{\partial x}
\]  
[3.6]
where \( q_e \) is the conductive heat flow, J/s-m²,

\( \lambda \) is the thermal conductivity, J/s-m°C (or K), and

\( T \) is the temperature, °C or K.

Applying conservation of energy with reference to Figure 3.1, results in Equation 3.7, with \( Q \) representing the heat flow per unit area of the element.

\[
\Delta Q = \left( \frac{\partial Q}{\partial y} \right) dy + \left( \frac{\partial Q}{\partial x} \right) dx \quad [3.7]
\]

Replacing \( Q \) with \( q_e dx \) and \( Q \) with \( q_e dy \), Equation 3.7 is rewritten as:

\[
\Delta Q = \left[ \left( \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) \right) dy \cdot dx \right] + \left[ \left( \frac{\partial}{\partial x} \left( \lambda_x \frac{\partial T}{\partial x} \right) \right) dx \cdot dy \right] \quad [3.8]
\]

where \( \lambda_x \) and \( \lambda_y \) are the thermal conductivity in the x- and y-directions, respectively.
For steady state conditions, Equation 3.8 simplifies to:

$$\frac{\partial}{\partial x} \left( \lambda, \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda, \frac{\partial T}{\partial y} \right) = 0$$  \[3.9\]

For cases where the thermal conductivity is not a function of position, Equation 3.9 further reduces to the Laplace equation. Equation 3.10 gives the Laplace equation, for which several analytical solutions have been proposed.

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$  \[3.10\]

For transient problems, a definition for change of energy of the element must be provided, as shown in Equation 3.11.

$$\frac{\partial Q}{\partial t} = \xi \frac{\partial T}{\partial t}$$  \[3.11\]

where $\xi$ is the specific heat capacity.

The specific heat capacity represents the amount of heat necessary to raise the temperature of a unit of material by 1 °C. In geotechnical engineering, volumetric specific heat capacities are generally specified. The specification of volumetric specific heats implies that the thermal conductivity will be given in compatible units. The volumetric specific heat capacity of a soil can be written as $c\rho$ where $c$ is the mass specific heat of the soil and $\rho$ is the density of the soil. Combining Equations 3.11 and 3.9 results in Equation 3.12, which is the general partial differential equation for conductive heat.

$$\frac{\partial}{\partial x} \left( \lambda, \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda, \frac{\partial T}{\partial y} \right) = c\rho \frac{\partial T}{\partial t}$$  \[3.12\]

Equation 3.12 generally applies for heat flow in soils. However, a modification must be made to the differential equation for cases where a change of phase is occurring in the soil (i.e., freezing/thawing). Accompanying this phase change is a large absorption or release of energy as the water changes from solid to liquid form, or vice versa.
The simplest method for modifying Equation 3.12 uses an apparent specific heat term. The apparent specific heat, $\overline{c_p}$, includes the volumetric specific heat capacity plus includes a term that accounts for the heat released or absorbed by phase change. The apparent specific heat is given as:

$$\overline{c_p} = c_p + L_f \frac{\partial \theta_u}{\partial T}$$

[3.13]

where $L_f$ is the latent heat of fusion of water, 334 MJ/m³.

$\theta$ is the volumetric water content at the initiation of freezing, and

$\partial \theta_u / \partial T$ is the change in unfrozen water content of the soil with temperature.

The term $L_f \theta \partial \theta_u / \partial T$ represents the amount of heat released or absorbed as the temperature of the soil change by $\partial T$. $\partial \theta_u / \partial T$ represents the slope of the soil-freezing curve, which describes the amount of unfrozen water present in a soil as a function of the temperature.

Equation 3.12 can be rewritten with the apparent specific heat replacing the volumetric specific heat as shown in equation 3.14.

$$\frac{\partial}{\partial x} \left( \lambda_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda_y \frac{\partial T}{\partial y} \right) = \left( c_p + L_f \theta \frac{\partial \theta_u}{\partial T} \right) \frac{\partial T}{\partial t}$$

[3.14]

Equation 3.14 reduces to 3.12 for cases where freezing or thawing are not occurring. Further discussion of volumetric and apparent specific heat capacities is provided in Section 3.2.3. The term $\partial \theta_u / \partial T$ has been referred to as $m'_2$ by Newman (1996) in analogy to the $m''_2$ term used in seepage analysis in unsaturated soils. A general form of Equation 3.14 for any number of dimension is written as:

$$\nabla(\lambda \nabla(T)) = \left( c_p + L_f \theta m'_2 \right) \frac{\partial T}{\partial t}$$

[3.15]
3.3.2 Thermal Material Properties

Three material properties need definition to solve problems of conductive heat flow. For cases where soil freezing or thawing is not occurring, the thermal conductivity, λ, and the volumetric specific heat, \( c_\rho \) or \( \xi \), need to be defined. For cases where freezing or thawing is occurring, the slope of the soil freezing curve, \( m'_s \), needs to be defined to allow description of the amount of heat absorbed or released.

3.3.2.1 Volumetric Specific Heat Capacity

The volumetric specific heat capacity of a soil is a function of:
1. the mass specific heats of the constituent material.
2. the density of the components, and
3. the fraction of each constituent material.

Mathematically, the above comments are represented as:

\[
c_\rho = \sum c_i \rho_i \theta_i
\]

[3.16]

where \( c_\rho \) is the volumetric specific heat, sometimes given the symbol \( \xi \),
\( c_i \) is the mass specific heat of soil component \( i \),
\( \rho_i \) is the density of soil component \( i \), and
\( \theta_i \) is the volumetric fraction of soil component \( i \).

Soils can consist of up to six components or phases. These phases include solid, liquid water, water vapor, dry air, and ice. Fredlund and Rahardjo (1993) also suggest treatment of the air-water interface or contractile skin as a separate phase. Therefore, the general form of the equation for predicting the volumetric specific heat of a soil, neglecting the contractile skin is:

\[
c_\rho = c_s \rho_s \theta_s + c_w \rho_w \theta_w + c_o \rho_o \theta_o + c_v \rho_v \theta_v + c_i \rho_i \theta_i
\]

[3.17]

where \( c_s, c_w, c_o, c_v, \) and \( c_i \) are the mass specific heat capacity of the solid, liquid water, dry air, water vapor, and ice phases, respectively.
\( \rho_s, \rho_w, \rho_o, \rho_v, \) and \( \rho_i \) are the densities of the solid, liquid water, dry air, water vapor, and ice phases, respectively, and

33
\( \theta_s, \theta_a, \theta_s, \theta_w, \) and \( \theta_i \) are the volumetric fractions of the solid, liquid water, dry air, water vapor, and ice phases, respectively.

Newman (1996) gives an equation for the volumetric specific heat capacity of a soil that is practical for use by geotechnical engineers, using commonly measured parameters such as dry density and gravimetric water content. This function neglects the air phase specific heat capacity, which is several orders of magnitude smaller than solid, liquid and ice components:

\[
cp = \rho_{dry} \left( c_s + c_u w_u + c_i w_i \right) \tag{3.18}
\]

where \( \rho_{dry} \) is the dry density of the soil,
\( c_s \) is the mass specific heat of soil solids,
\( c_u \) is the mass specific heat of unfrozen water, 4184 J/kg-°C,
\( c_i \) is the mass specific heat of ice, 2100 J/kg-°C,
\( w_u \) is the gravimetric water content of the soil, and
\( w_i \) is the gravimetric ice content of the soil.

Table 3.4 shows typical densities and mass specific heats for common soil constituents.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (kg/m³)</th>
<th>Mass Specific Heat Capacity (J/kg-°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>2660</td>
<td>755</td>
</tr>
<tr>
<td>Clay Minerals</td>
<td>2650</td>
<td>755</td>
</tr>
<tr>
<td>Organic Matter</td>
<td>1300</td>
<td>1930</td>
</tr>
<tr>
<td>Water</td>
<td>1000</td>
<td>4184</td>
</tr>
<tr>
<td>Ice</td>
<td>920</td>
<td>2100</td>
</tr>
<tr>
<td>Air</td>
<td>1.25</td>
<td>1000</td>
</tr>
</tbody>
</table>
3.3.2.2 Thermal Conductivity

The thermal conductivity of a soil is a function of:

1. the thermal conductivity of constituent material, 
2. the fraction of the soil volume each material represents, and 
3. the “connectedness” of the each constituent material.

The “connectedness” refers to the completeness of paths that are available for movement of heat through a soil. For example, in the solid phase, the soil grains touch at discrete points. The larger the area of contact between grains, the greater the thermal conductivity will be. Therefore, the thermal conductivity of a soil will increase if the “connectedness” of the high thermal conductivity components increases. The thermal conductivity increases with increasing soil density, increasing degree of saturation, and increasing ice content.

A variety of functions for estimating the thermal conductivity of a soil have been developed and presented in the literature. Farouki (1986) summarized the wide variety of possible functions. Farouki (1986) concludes that the Johansen (1975) method gives the best results for a variety of soil types, although the de Vries and Kersten methods are suitable for some soils. Table 3.5 (following page) presents some of the more common methods that are used by various researchers.
<table>
<thead>
<tr>
<th>Function</th>
<th>Definitions</th>
<th>Method Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda = n\lambda_f + (1 - n)\lambda_s$</td>
<td>$\lambda = $ thermal conductivity</td>
<td>Parallel Flow</td>
</tr>
<tr>
<td>$n = $ porosity</td>
<td>$\lambda_f = $ thermal conductivity of fluid</td>
<td></td>
</tr>
<tr>
<td>$\lambda_s = $ thermal conductivity of solids</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\frac{1}{\lambda} = n\frac{1}{\lambda_f} + (1 - n)\frac{1}{\lambda_s}$</td>
<td></td>
<td>Series Flow</td>
</tr>
<tr>
<td>$\lambda = \left(\frac{\lambda_f}{\lambda_s}\right)^n\lambda_s$</td>
<td></td>
<td>Geometric Mean</td>
</tr>
<tr>
<td>$\lambda = \lambda_s(n - P_\Omega) + x_s(1 + \alpha')/\left([1 + \lambda_s] + \left(1/\lambda_s\right) - \left(1/\lambda_f\right)\right)\alpha'/(1 + \alpha')$</td>
<td>$\lambda_a = $ thermal conductivity of air</td>
<td>Smith (1942) Method for Dry Soils</td>
</tr>
<tr>
<td>$P_\Omega = $ ratio of air volume to solids volume</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$x_s = $ total unit volume</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha' = $ empirical factor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda = [0.91\log w - 0.2]0.017^{1.4}$</td>
<td>$\lambda$ in btu in./ft² hr °F</td>
<td>Kersten (1949)</td>
</tr>
<tr>
<td>- unfrozen silt-clay soils</td>
<td>$w = $ moisture content</td>
<td>Empirical Equations</td>
</tr>
<tr>
<td>$\lambda = 0.01(10)^{0.0427} + 0.085(10)^{0.0087} + 0.085(10)^{0.0087}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>- frozen silt-clay soils</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda = [0.7\log w + 0.4]0.017^{1.4}$</td>
<td>$\gamma_d = $ soil dry density</td>
<td></td>
</tr>
<tr>
<td>- unfrozen sandy soils</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda = 0.076(10)^{0.017} + 0.032(10)^{0.0146}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>- frozen sandy soils</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Table 3.5 (cont.) Functions for thermal conductivity

<table>
<thead>
<tr>
<th>Equation</th>
<th>Definitions</th>
<th>Method Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda_{\text{dry}} = \lambda_0 a^2 + \lambda_1 (1-a)^2 + \frac{\lambda_0 \lambda_1 (2a - 2a^2)}{\lambda_0 (a) + \lambda_1 (1-a)} ) - dry soils</td>
<td>( a ) is related to porosity of soil</td>
<td>Mickley (1951) Method</td>
</tr>
<tr>
<td>( \lambda_{\text{sat}} = \lambda_0 a^2 + \lambda_1 (1-a)^2 + \frac{\lambda_0 \lambda_1 (2a - 2a^2)}{\lambda_0 (a) + \lambda_1 (1-a)} ) - saturated soils</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \lambda = \sum_{i=0}^{n} F_i \theta_i \lambda_i )</td>
<td>( \theta_i ) = volumetric fraction of the ( i^{th} ) component</td>
<td>De Vries (1963) Method</td>
</tr>
<tr>
<td>( F_i = \frac{1}{\lambda^i} \sum_{x \neq i} \left[ 1 + \left( \frac{\lambda_i}{\lambda_x} - 1 \right) g_a \right]^{-1} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \lambda = (\lambda_{\text{sat}} - \lambda_{\text{dry}}) K_r + \lambda_{\text{dry}} )</td>
<td>( K_c = ) Kersten number</td>
<td>Johansen (1975) Method</td>
</tr>
<tr>
<td>( K_r \geq 0.7 \log S_r + 1.0 ) - coarse unfrozen soils</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( K_r \geq \log S_r + 1.0 ) - fine unfrozen soils</td>
<td>( S_r = ) degree of saturation</td>
<td></td>
</tr>
<tr>
<td>( K_r = S_r ) - all frozen soils</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 3.6 gives thermal conductivities for common soil constituents.

Table 3.6  
Thermal conductivities for common soil constituents at 0 °C  
(adapted from de Vries, 1963)

<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal Conductivity (W/m·°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>8.8</td>
</tr>
<tr>
<td>Clay Minerals</td>
<td>2.9</td>
</tr>
<tr>
<td>Organic Matter</td>
<td>0.25</td>
</tr>
<tr>
<td>Water</td>
<td>0.57</td>
</tr>
<tr>
<td>Ice</td>
<td>2.2</td>
</tr>
<tr>
<td>Air</td>
<td>0.025</td>
</tr>
</tbody>
</table>

3.3.2.3 Soil-Freezing Curve

Water in a soil undergoing freezing does not freeze at a uniform temperature. Instead, the unfrozen water content is a function of the temperature of the soil. In some fine-grained soils, some water remains unfrozen at temperatures as low as -20 °C. The mechanism by which this freezing point depression occurs has been extensively studied. This freezing point depression is attributed to development of capillary forces or suctions, acting to reduce the freezing point of the pore-water as discussed in Chapter 2.

Empirical relationships are available for describing the soil-freezing curve. A variety of researchers (Anderson et al., 1973; Anderson and Morgenstern, 1973; Tice et al., 1976; Black and Tice, 1989) propose using Equation 3.19 for estimating the unfrozen water content of soils at subzero temperatures.

\[
w_u = a \exp(-bT')
\]  

[3.19]

where \( w_u \) is the unfrozen gravimetric water content.

\( T' \) is the freezing point depression, and

\( a \) and \( b \) are empirical constants dependent on soil type, density, etc.
Anderson and Morgenstern (1973), and Anderson et al. (1973) give a curve fit relationship based on plots of unfrozen water content and specific surface area of the soil.

\[ \ln(w_u) = a + b \ln S + c S^d \ln T' \]  \hspace{1cm} [3.20]

where \(a, b, c, d\) are empirical constants,

\(S\) is the specific surface area of the soil particles, and

\(T'\) is the freezing point depression.

It is desirable to relate the soil-freezing curve directly to the soil-water characteristic curve. Freezing point depression in a soil occurs in response to suction developing in the soil as ice forms in the soil. The ice acts in a manner similar to the presence of air voids in an unsaturated soil. It is reasonable to expect to be able to predict the freezing characteristics of a soil based on the soil-water characteristic curve. Figure 3.2 shows schematically the stresses acting in a soil undergoing freezing. Menisci form in the liquid water at the interfaces of the ice-water and air-water.

![Figure 3.2 Schematic of partially frozen soil showing stress state variables (from Newman, 1996)](image)

The pressures acting at the three interfaces depicted in Figure 3.2 are given below:
Air-water interface:

\[(u_i - u_w) = \frac{2ST_{aw}}{R_{aw}}\]  \[3.21a\]

where \(ST_{aw}\) is the surface tension between air and water, and \(R_{aw}\) is the radius of curvature of the air-water interface.

Ice-water interface:

\[(u_i - u_w) = \frac{ST_{iw}}{R_{iw}}\]  \[3.21b\]

where \(u_i\) is the ice pressure, \(ST_{iw}\) is the surface tension between ice and water, and \(R_{iw}\) is the radius of curvature of the interface.

Ice-air interface:

\[(u_i - u_a) = \frac{2ST_{ai}}{R_{ai}}\]  \[3.21c\]

where \(ST_{ai}\) is the surface tension between air and ice, and \(R_{ai}\) is the radius of curvature of the interface.

The Clayperon equation describes the relationship between the pressure and temperature in the system. Equation 3.22 gives the Clayperon equation.

\[\frac{dP}{dT} = \frac{\Delta h}{T\Delta V}\]  \[3.22\]

where \(P\) is the equilibrium pressure (kPa), \(T\) is the temperature (K), \(h\) is the specific enthalpy difference between phases (kJ/kg), and \(V\) is the specific volume difference between phases (m³/kg).

Black and Tice (1989) rewrite the Clayperon equation for describing the relationship between \((u_i-u_w)\) and the temperature as:
\[ u_u - u_i = \frac{L}{SG_i} \frac{T'}{273.15} \]  

where \( SG_i \) is the specific gravity of ice (0.918), and 
\( T' \) is the freezing point depression (\(^\circ\)C).

Rearranging Equation 3.23 and simplifying, provides an expression relating \((u_u-u_i)\) to the freezing point depression, given as:
\[ (u_i - u_u) = 1110 T' \]  

Miller (1966) stated that \((u_u-u_i)\) and \((u_i-u_u)\) are directly related. Koopmans and Miller (1966) showed that for soils in which capillary forces dominate, a correction factor needs to be applied to relate \((u_u-u_i)\) and \((u_i-u_u)\). Equation 3.25 depicts a general form of the relationship between \((u_u-u_i)\) and \((u_i-u_u)\): 
\[ \psi_{aw} = C_f \psi_{nw} \]  

where \( \psi_{aw} \) is \((u_u-u_i)\), 
\( \psi_{nw} \) is \((u_i-u_u)\), and 
\( C_f \) is a correction factor given.

Koopmans and Miller (1966) suggest that the \( C_f \) for capillary soils is the ratio of \( ST_{aw} \): 
\( ST_{nw} \) equal to 2.2 to 1. Using Equations 3.24 and 3.25 and the values of the \( C_f \) given above, the following relationships have been proposed for relating the \((u_u-u_i)\) and \((u_i-u_u)\).

For pure adsorption forces in soil:
\[ (u_u - u_u) = (u_i - u_u) \]
\[ (u_i - u_u) = 1110 T' \]  

For pure capillary forces in soil:
\[ (u_u - u_u) = \frac{ST_{aw}}{ST_{nw}} (u_i - u_u) \]
\[ (u_u - u_u) = 2.2 (1110) T' \]
Real soil behavior will lie somewhere between the extremes given in Equations 3.26 and 3.27, however, no research is available on predicting $C_f$ values in soils that have a mix of adsorptive and capillary forces.

Using the above relationships, estimation of the soil-freezing curve using the soil-water characteristic curve functions given in Table 3.1 is possible. For example, using the Fredlund and Xing (1994) fit and the relationships above, a soil-freezing curve is generated as:

$$\theta_a = C(T') \left[ \frac{1}{\ln \left( \exp(1) + \left[ \frac{C_f \cdot 1110 \cdot T'}{a} \right]^n \right]^m} \right] \cdot \theta_{sat}$$  \hspace{1cm} [3.28]$$

where $n$, $m$, and $a$ are curve fit parameters,

$C(T')$ is a curve fit correction factor given by:

$$C(T') = \left[ \frac{\ln \left( 1 + \frac{C_f \cdot 1110 \cdot T'}{C_r} \right)}{\ln \left( 1 + \frac{C_f \cdot 1110 \cdot 273}{C_r} \right)} \right], \text{ and}$$

$C_r$ is an additional curve fit parameter.

The term $m'$ or the slope of the soil-freezing curve is needed for solution of problems in heat flow. This is accomplished by differentiating Equation 3.28 using MathCAD, with the result given in Equation 3.29.
\[ m' = \frac{\partial \theta_n}{\partial T'} = \left[ \frac{-1110 \cdot C_j \cdot \theta_{\text{sat}}}{C_r \cdot \left( 1 + 1110 \cdot C_j \cdot \frac{T'}{C_r} \right) \cdot \ln \left( 1 + 303030 \cdot \frac{C_{j0}}{C_r} \right) \cdot \ln \left[ \exp(1) + \left( 1110 \cdot C_j \cdot \frac{T'}{a} \right)^n \right]^m} \right] \]

\[
\left[ \ln \left( 1 + 1110 \cdot C_j \cdot \frac{T'}{C_r} \right) \right] \cdot \theta_{\text{sat}} \cdot m \cdot \left( 1110 \cdot C_j \cdot \frac{T'}{a} \right)^n \left( \ln \left[ \exp(1) + \left( 1110 \cdot C_j \cdot \frac{T'}{a} \right)^n \right]^m \right] 
\]

This equation is unwieldy, and although it can be implemented in FlexPDE as it is given, the increase in solution time is not justified. As such, this equation was implemented in an Excel\(^1\) spreadsheet, from which table files were created to produce approximate values of \( m'_2 \) for use in FlexPDE. Other approximations of the soil-freezing curve using the soil-water characteristic functions presented in Table 3.1 were not attempted in the present study.

Soil-freezing curves can also be generated by integration of the \( m'_2 \) function if it is known. This technique was used in the present study for back-calculating the soil-freezing curve from the \( m'_2 \) versus temperature relationships produced by Temp/W verification examples.

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\(^1\) Excel is a proprietary software package developed and produced by Microsoft Co. of Redmond, WA. USA.
3.4 Coupled Heat and Mass Transfer

The equations governing coupled heat and mass transfer are presented first for the case in which the soil is not freezing, followed by the equations for soil in which freeze-thaw is occurring.

3.4.1 Partial Differential Equations for Coupled Heat and Mass Transfer without Freezing/Thawing

The equations for heat and mass transfer under atmospheric forcing as proposed by Wilson (1990) in one dimension are given as Equations 3.30 to 3.34. Equation 3.30 is the mass transfer equation. Equation 3.30 accounts for the movement of liquid water by the hydraulic head gradient term, and for the movement of water in vapor form using the vapor pressure gradient term.

\[
\frac{\partial h}{\partial t} = c_1^* \frac{\partial}{\partial y} \left( k \frac{\partial h}{\partial y} \right) + c_2^* \frac{\partial}{\partial y} \left( D_v \frac{\partial P_v}{\partial y} \right) \tag{3.30}
\]

where \( c_1^* \) is given as \( \frac{1}{\rho_w g m^*_2} \).

\( c_2^* \) is given as \( \frac{1}{\rho_w^2 g m^*_2} \).

\( P_v \) is the partial vapor pressure in the soil given by Equation 3.31,

\[
P_v = P_{v_s} \cdot rh_{sodl}, \tag{3.31}
\]

\( P_{v_s} \) is the saturated vapor pressure of water, given as \((1.36075 \times 10^8)\exp(-5239.7/(T+273.16))\) (kPa).

\( rh_{sodl} \) is the relative humidity in the soil pores, calculated by the Lord Kelvin equation:

\[
rh_{sodl} = \exp \left( \frac{\psi W_s}{\rho_s RT} \right) \tag{3.32}
\]

\( \psi \) is the soil suction (i.e., \( (u_d-u_w) \)).

\( D_v \) is given by \( D_v = \alpha \beta D_{vap} W_v/RT \).

\( \beta \) is the cross sectional area of soil available for vapor flow.

\( \alpha \) is a tortuosity factor given as \( \beta^{0.3} \).

\( D_{vap} \) is the molecular diffusivity of water vapor in air given by
Equation 3.33 is the heat transfer equation. Equation 3.33 accounts for both conductive heat flow and the latent heat effect of conversion of water from liquid to vapor phases or vice versa. Equations 3.30 and 3.33 are coupled through the vapor pressure term that accounts for the change of phase of water in the soil from liquid to vapor.

\[
\frac{\xi}{\partial t} = \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) - L_v \frac{\partial}{\partial y} \left( D_v \frac{\partial P_v}{\partial y} \right) \tag{3.33}
\]

where \( L_v \) is the latent heat of vaporization of water.

Equation 3.34 is Dalton's equation for evaporation. This equation couples Equation 3.30 and 3.33 to the atmosphere describing the partial vapor pressure at the surface.

\[
E = f(u)(P_{v,soil} - P_{v,air}) \tag{3.34}
\]

where \( E \) is the evaporation rate,

\( f(u) \) is a mixing parameter,

\( P_{v,soil} \) is the partial vapor pressure in the soil at the surface, and

\( P_{v,air} \) is the partial vapor pressure in the air above the soil surface.

Joshi (1993) modifies the equations proposed by Wilson (1990) to eliminate the vapor pressure term in the partial differential equations, and restates the equations in terms of soil suction, \( \psi \), and temperature, \( T \), thereby obtaining two equations in two variables. The equations are limited in that they only apply for unsaturated soil conditions. Equations 3.35 and 3.36 are implemented in FlexPDE in the present study.

\[
m_s \frac{\partial \psi}{\partial t} = \nabla (k \nabla (\psi / \gamma_w + y)) \nabla (D_s \nabla \psi) + \nabla (D_s \nabla T) \tag{3.35}
\]

\[
\frac{\xi}{\partial t} = \nabla (L \nabla T) - L_v \frac{\partial}{\partial y} \left( D_s \nabla \psi + D_s \nabla T \right) \tag{3.36}
\]
where:

\[ D_1 = \left( \frac{1}{\rho_w} \right)(D_v d_1). \]  
\[ D_2 = \left( \frac{1}{\rho_w} \right)(D_v d_2). \]  
\[ D_3 = (D_v d_1). \]  
\[ D_4 = (D_v d_2). \]

\( dP_v/dT \) is equal to \((1.36075 \times 10^8) \times 5239.7/((T+273)^2) \exp(-5239.7/(T+273)). \)

\[ d_1 = (P_v) \left( \frac{\partial h_v}{\partial \psi} \right) = (P_v) (h_v W / \rho_w RT) = (P_v W / \rho_w RT), \] and \[ d_2 = \left( \frac{\partial P_v}{\partial T} \right) (h_v) - (P_v W / (\rho_w R T^2)). \]

3.4.2 Partial Differential Equations for Coupled Heat and Mass Transfer with Freezing/Thawing

The equations proposed by Harlan (1973) are given in Equations 3.43 and 3.44 for mass flow and heat flow respectively.

\[ \frac{\partial}{\partial y} \left( k_w \frac{\partial h_v}{\partial y} \right) = \frac{\partial \theta_v}{\partial t} + \frac{\rho_w}{\rho_u} \frac{\partial \theta_v}{\partial t} \]  
\[ \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) - \xi_v \frac{\partial (v_v T)}{\partial y} = \xi \frac{\partial T}{\partial t} - L_v \rho_v \frac{\partial \theta_v}{\partial T} \frac{\partial T}{\partial t} \]

where \( \theta_v \) is the unfrozen volumetric water content.

\( \rho_w \) is the density of liquid water.

\( \xi_v \) is the specific heat capacity of liquid water, and

\( v_v \) is the fluid velocity in the y-direction.

Equations 3.43 and 3.44 contain three unknowns, \( h_v, \theta_v, \) and \( T \). Therefore, assumptions must be made regarding the ice content of the soil and an iterative solution must be used for solution of these equations.
Newman (1996) developed a formulation to allow freezing and thawing to be implemented in the model given by Joshi (1993). The equation proposed by Newman (1996) describes both heat and mass transfer. The equation relates the soil-freezing curve and the soil-water characteristic curve to describe the movement of water to the freezing front. This equation is implemented in the SoilCover model by "switching" between this equation and the equation given by Joshi (1993), depending on whether the temperature at a given node is above or below freezing. Temperatures are solved for using Equation 3.45, and then suction back-calculated based on the unfrozen water content estimated at the node.

\[
\left( \rho c + L_f \frac{\rho_u^2}{\rho} m'_2 \right) \frac{\partial T}{\partial t} = \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) - \left( L_v - L_f \frac{\rho_u}{\rho} \right) \frac{\partial}{\partial y} \left( D_1 G \frac{\partial T}{\partial y} + D_2 \frac{\partial T}{\partial y} \right) \\
+ L_f \frac{\rho_u^2}{\rho} \frac{\partial}{\partial y} \left( k_u G \frac{\partial}{\partial y} \left( \frac{T}{\rho_u g} + y \right) \right)
\]

[3.45]

where \( G \) is \( m'_2/m'_2 \).

The equations as given for the coupled freeze-thaw problem were not implemented in the present study, as discussed in later chapters. However, the equations are included for completeness of the theory of coupled heat and mass transfer.
CHAPTER 4
RESEARCH PROGRAM

4.1 General Features of Research Program

The research program undertaken analyzed several types of geotechnical and geo-environmental engineering problems using numerical methods. Field and laboratory work was not included in the present study. The numerical modelling results were compared with published experimental results and previously verified numerical or analytical solutions.

The research program outlined below consisted of three major parts, corresponding to the types of problems solved. Uncoupled seepage and heat flow, and coupled heat-mass transfer problems were examined for numerical solution using a general partial differential equation (PDE) solver. Comparison was made of numerical modelling solutions with results obtained either from “off-the-shelf” geotechnical analysis software or from results published in geotechnical and soil science literature. A final brief section provides details on an example problem to demonstrate a practical application of the techniques described in the study.

Detailed descriptions of the problems considered, including such information as material properties, boundary conditions, etc., are presented in detail in Chapter 5. This chapter provides highlights and brief descriptions of the problems.

4.1.1 Software

Solution of differential equations numerically necessitates either development of finite element software, or use of existing software. The latter course, taken in the present research, demonstrates the versatility and flexibility of general partial differential
equation solution software. Previous researchers (Nguyen, 1999; Vu, 1999) have used a program called PDEase (Macsyma Inc., 1996) in conducting research into the behavior of unsaturated soils. Other software for solution of partial differential equations is available. Consideration was given to the use of PDEase in the present research, but a decision was made to utilize a new software package.

FlexPDE (PDESolutions Inc., 1999) was chosen after a review of existing software packages. FlexPDE is a program similar to PDEase, but with the advantage of three-dimensional capabilities. FlexPDE is a general partial differential equation solver that uses the finite element method for numerical solution of boundary value problems. Major features of FlexPDE include:

- Capable of solving non-linear partial differential equations of second order or less.
- Adaptive grid refinement eliminates need for creating mesh manually as in most finite element software.
- Adaptive time refinement ensures that for transient problems time steps are correct size to reach convergence of problem.
- Variety of input methods available for material properties, boundary conditions, problem domains such as fully defined functions, piece wise defined functions, tables of values, etc.
- Two and three-dimensional modelling capabilities.

Appendix A provides more details on FlexPDE including a systematic description of the creation of descriptor files used in FlexPDE. The FlexPDE descriptor files generated in this study are compiled in Appendix C for reference.

Verification of water flow and heat flow problems used the Geo-Slope (1999) software packages Seep/W and Temp/W respectively for comparison with FlexPDE results. Seep/W and Temp/W are finite element programs developed for solution of geotechnical problems. Seep/W is a saturated/unsaturated seepage package. Temp/W is a thermal modelling program for handling freezing and thawing of soils. The
discussion of coupled heat and mass transfer under evaporation uses the SoilCover (1997) model.

When material properties had to be assumed in the numerical models, they were obtained using the soil database SoilVision¹ (SoilVision Systems Ltd., 1997) to estimate properties. SoilVision is a database of over 5000 soils with textural information and soil-water characteristic curves. Additional parameters such as coefficient of permeability, compression curves, and thermal conductivity are included for some soils. A knowledge base incorporated in SoilVision allows estimation of unsaturated properties based on saturated properties or from grain size data. The present study used SoilVision version 1.20. This version of SoilVision was limited in usefulness for the present study, as only nine soils had thermal properties defined. As such, the primary use of SoilVision in the thermal study was for obtaining curve fits for hypothetical data using the knowledge base.

The modelling program was implemented on a Pentium III 450 MHz computer with 128 MB of RAM running under the Windows 98² operating system.

4.1.2 General Solution Technique

The solution technique for each modelling area considered (i.e., seepage, heat flow, and coupled heat-mass transfer) generally followed the steps outlined as follows.

1. A simple descriptor file was developed and tested with constant material properties and simple boundary conditions. This step ensured proper implementation of the partial differential equations FlexPDE format.


¹ SoilVision is a proprietary software package developed and produced by SoilVision Systems Ltd. of Saskatoon, SK, Canada
² Windows 98 is a proprietary operating system developed and produced by Microsoft Co. of Redmond, WA, USA
3. Complex examples were then prepared using realistic material properties and boundary conditions. Chapter 5 contains these examples.

4. Further parametric modelling was conducted where necessary. This step tested the material non-linearity that can be introduced into FlexPDE without compromising program stability. Chapter 5 presents the parameters studied.

5. Analysis and discussion of the problems verified was prepared as necessary.

4.2 Water Flow Modelling in FlexPDE

Previous research considered solution of seepage problems using a general partial differential solver program (Nguyen, 1999). Nguyen (1999) used the program PDEase in solving this class of problems. These solutions represented an opportunity to verify that FlexPDE produced results comparable to PDEase as claimed by the producer of the FlexPDE software.

The series of seepage problems verified using FlexPDE is less extensive than that of Nguyen (1999). Solution to six seepage problems in the present study used FlexPDE. Chapter 5 presents three of these problems. The other seepage problems considered are in Appendix B for reference.

Seep/W (Geo-Slope, 1999) analysis of these problems verified the solutions obtained in FlexPDE. Figure 4.1 provides an overview of the seepage problems considered in the main body of this thesis. Figure 4.2 depicts the problems considered in Appendix B. Brief descriptions of the problems discussed in Chapter 5 are given below. Appendix B provides descriptions of the remainder of the seepage problems.

4.2.1 Two-Dimensional Seepage Problems

Chapter 5 presents two two-dimensional seepage problems. The first is an example of transient seepage. The second demonstrates a technique for implementing a review boundary condition in FlexPDE.
Two-Dimensional Seepage Verification Example No. 1
This problem depicts the conditions associated with the filling of a reservoir resulting in a change in the pore-water pressure and head regimes in an earth fill dam. This problem is of interest for determining gradients produced in rapid filling or draining of the reservoir leading to catastrophic failures of the dam structure.

Figure 4.1 Seepage problems considered in Chapter 5

Two-Dimensional Seepage Verification Example No. 2
The second problem represents the class of problems in which there is a free boundary condition. The example considers a method for implementing a “review” boundary condition in FlexPDE. The problem consists of an earth fill dam without a toe drain.
implying that the phreatic line will exit at some point on the downstream face. The location of this point is unknown; as a result, specification of the boundary condition on the downstream face requires use of an iterative solution. The solution technique and results obtained using the solution technique are presented in Chapter 5.

Figure 4.2 Seepage problems considered in Appendix B

4.2.2 Three-Dimensional Seepage Problem

One three-dimensional seepage problem is presented in Chapter 5. This problem is included to demonstrate the three-dimensional capabilities of FlexPDE.
Three-Dimensional Seepage Verification Example

A simple three-dimensional earth fill dam was implemented in FlexPDE. Pore-water pressures and hydraulic heads in the dam at steady state seepage conditions are determined. Comparison of FlexPDE results is made against two-dimensional solutions for two sections obtained in Seep/W. Material property functions are the same as used in the two-dimensional seepage verification examples.

4.3 Thermal Modelling in FlexPDE

Classification of heat flow problems in soil is made according to whether or not the soil undergoes freeze-thaw conditions. The distinction is due to the latent heat effects that occur if phase change (i.e., freeze-thaw) is occurring, as discussed in Chapters 2 and 3. This research program focuses on the freeze-thaw problem. Freeze-thaw analysis is the type of problem that is of primary interest to geotechnical engineers. One problem is considered without freeze-thaw effects. The remaining six verification problems considered fall into the freeze-thaw category. Figure 4.3 outlines the problems in heat flow modelling considered in this study.

4.3.1 Steady State Thermal Verification

Solutions to problems of steady state heat flow are first considered. Assuming that the soil is isotropic, the solution of steady state heat flow is the solution of the Laplacian equation. The present study considers two examples of steady state heat flow.

Two-Dimensional Thermal Verification Example No. 1

The first example consists of two parts. The basic problem geometry is the same in both parts. Two “semi-infinite” surfaces at two different temperatures are adjacent to each other on top of an infinitely thick homogeneous soil layer. In the first part of the problem, no geothermal gradient acts in the soil. In the second part of the problem, a geothermal gradient of 1°C/30 m acts in the vertical direction. The results obtained using FlexPDE are compared to analytical solutions for the two cases provided by Harlan and Nixon (1978).
Figure 4.3a  Thermal problems considered in research program
Two-Dimensional Thermal Verification Example No. 6

Initially Frozen Soil

15.5 °C

3 °C

-2 °C

Three-Dimensional Thermal Verification Example

Figure 4.3b  Thermal problems considered in research program (continued)
Two-Dimensional Thermal Verification Example No. 2

The second example considers the calculation of the depth of thaw that would occur beneath a heated structure founded on permafrost. A 100 m wide, infinitely long, heated strip rests on an infinitely wide permafrost area. The geothermal gradient acts in the soil for this problem. Harlan and Nixon (1978) provide a solution for the location of the interface between frozen and unfrozen soil. The Harlan and Nixon (1978) solution along with the solution obtained in Temp/W for this problem are compared with the FlexPDE results.

4.3.2 Two-Dimensional Transient Thermal Verification

The transient heat flow verification examples considered in this research study are briefly discussed below.

Two-Dimensional Thermal Verification Example No. 3

The first transient problem used for verification comes from the field of soil science. The results of Nobel and Geller (1987) were modelled using FlexPDE. The problem is a simple example of heat flow in an unfrozen soil. Modelled is the diurnal flux of heat into a soil. Nobel and Geller (1987) described experimental and numerical model results for conditions of dry and wet soil. The problem is essentially one-dimensional although in FlexPDE the problem is modelled in two-dimensions. The material properties (thermal conductivity and volumetric specific heat capacity) are assumed to be constant for a given soil condition (e.g., for the wet case the thermal conductivity is a constant value). Results obtained in FlexPDE are compared with the experimental and modelled results given by Nobel and Geller (1987).

Two-Dimensional Thermal Verification Examples No. 4 and 5

The fourth and fifth thermal verification problems are opposite cases of the same problem. Example no. 4 considers thawing of a soil from the surface downwards. Example no. 5 considers freezing of the soil from the surface downwards. These two
problems are the first to include the effect of latent heat due to phase change as discussed in Chapter 3.

Researchers have used the problems in the past for verification of heat flow models because an analytical solution developed by Neumann, as given by Carslaw and Jaeger (1959), is available for comparison. The Neumann solution is for a pure substance undergoing phase change. The solution will over predict the rate of freezing or thawing in a real soil, because:

1. soil is a composite material in which only a portion (i.e., the water phase) will be undergoing phase change during freeze-thaw and
2. the water phase in a soil will not all change phase at a uniform temperature due to the freezing point depression effect as discussed in Chapter 3.

The example presented in Chapter 5 maintains the assumption that the entire volume of the soil is undergoing a phase change. However, it is necessary to include the freezing point depression in order to obtain a stable solution in FlexPDE. The results in Chapter 5 explore the effect of the freezing point depression, represented by the soil-freezing curve, and of the $m'_2$ term on the solution. Use of various soil-freezing curves in the solution attempts to approximate the Neumann solution. The $m'_2$ function is a continuous function of the temperature when implemented in FlexPDE. The results obtained using FlexPDE are compared with the analytical solution given by the Neumann solution and with the Temp/W solution to this problem.

Two-Dimensional Thermal Verification Example No. 6

The sixth example considered in two-dimensional heat flow considers the case of a heated foundation constructed on permafrost. The concern is that the warm foundation will melt the permafrost resulting in consolidation of the soil. Consolidation will occur as liquid water flows from the soil in response to the foundation loading. Hwang et al. (1972) presented a finite element model for solution of this problem. The results obtained in FlexPDE are compared with the solution for this problem obtained in Temp/W.
Two-Dimensional Thermal Verification Example No. 7

The final two-dimensional thermal verification example considers a chilled fluid pipeline constructed in a non-frozen soil. The Norman Wells Pipeline in Northern Alberta and the Northwest Territories constructed in the 1980's is a chilled fluid pipeline (Burgess, 1988). The chilled pipeline technique prevents thawing and subsequent settlement of permafrost terrain. However, in discontinuous permafrost zones the chilled pipeline will freeze previously unfrozen soil resulting in migration of moisture to frost front and expansion of the pore fluid as it converts from water to ice resulting in heave of the pipeline. Coutts and Konrad (1994) presented a solution to this problem using the node state model briefly discussed in Chapter 2. The results obtained in FlexPDE are compared with the solution of this problem obtained in Temp/W.

4.3.3 Three-Dimensional Steady State Thermal Problem

One three-dimensional steady state thermal problem was considered in the present study.

Three-Dimensional Thermal Verification Example

The three-dimensional thermal verification example considered in this study is a three-dimensional version of two-dimensional thermal verification example no. 6. The problem consists of a circular tank on initially frozen ground. The tank has a temperature of 15.5 °C. The analysis consists of a rectangular “block” of soil below the tank. The symmetry of the problem allows analysis of one quarter of the problem in FlexPDE, reducing computing requirements. Comparison of the results is made to the FlexPDE results for the steady state solution of thermal verification example no. 6 in two-dimensions.
4.4 Coupled Heat and Mass Transfer Modelling in FlexPDE

Solution of problems in coupled heat and mass transfer are categorized depending on whether the soil is undergoing freezing or not. Originally, the research program was to consider the components listed in Figure 4.4. However, difficulties, discussed in Chapter 5, prevented completion of all the proposed study as outlined.

Figure 4.4 Originally proposed verification examples studied in coupled heat and mass transfer using FlexPDE
4.4.1 Closed System Verification

The research program first considers closed system verification of the coupled heat and mass transfer equations. The FlexPDE formulation uses the equations given by Joshi (1993) for coupled heat and mass transfer.

Coupled Heat and Mass Transfer Verification Example No. 1

The first coupled verification problem is one described by Ewen and Thomas (1989) involving redistribution of water content within a closed cylinder filled with soil. A heater placed in the center of the cylinder of soil provides heat to the system, resulting in a movement of water in response to thermal gradients. No flow is occurring external to the system considered. The material properties given by Ewen and Thomas (1989) were determined experimentally. Ewen and Thomas (1989), and Li et al. (1997) modelled the problem numerically. These numerical results are compared with the FlexPDE results for this problem.

4.4.2 Coupled Heat and Mass Transfer Under Large Gradients

The original research program proposed was to consider problems in which evaporation or soil freeze-thaw was occurring. Brief descriptions of the problems originally considered are given below.

Coupled Heat and Mass Transfer Verification Example No. 2

The second verification example considered in this research is the work of Wilson (1990). Wilson (1990) studied the movement of water from a soil undergoing evaporation. The experimental data of Wilson (1990) used a sand column undergoing evaporation in an arid environment over a period of 42 days. SoilCover models of Wilson’s (1990) experiment are available.

Coupled Heat and Mass Transfer Verification Example No. 3

The third verification example considered in coupled heat and mass transfer, is the freezing experiment Jame and Norum (1980) described and Newman (1996) re-
analyzed. The experiment described by Jame and Norum (1980) consisted of a horizontal “column” of silica flour, prepared to a specified moisture content. Initiation of progressive freezing of the soil from one end, resulting in a redistribution of moisture from the warm soil to the freezing front, followed.

4.5 Comprehensive Verification Example

The comprehensive verification example highlights various aspects of the flexibility of using a general PDE solver in geotechnical engineering. The comprehensive verification example solved for the following conditions:

1. Steady state seepage.
2. Non-freezing steady state heat flow using results from no. 1 above as input for determination of material properties.
3. Freeze-thaw analysis.
4. Parametric study on the effect of the soil-freezing curve on freeze-thaw analysis.

Various abilities of FlexPDE tested include:

1. Ability to handle various input functions for material properties.
2. Ability to use variable boundary conditions.
3. Ability to model various phenomena.
4. Ability to perform parametric studies.

Figure 4.5 presents an overview of the solution method used in the practical problem.

Two different soils are represented in the problem. The two soils were chosen to represent two methods of inputting material properties, i.e., table of values and fully defined functions. Boundary conditions as implemented were intended to mimic natural climatic conditions using suitable constant values or sinusoidal functions. This example solves seepage and heat flow separately.

Initially grain size curves, saturated volumetric water content, specific gravity, density, and saturated permeability were input into SoilVision. Using this information and
suitable assumptions, soil-water characteristic curves, soil-freezing curves, derivatives of the two curves (i.e., $m'_s$ and $m'_t$), and unsaturated permeability functions were generated using SoilVision. Representation of soil properties predicted by SoilVision in FlexPDE was by fully defined function or table of values.

![Diagram](image)

Figure 4.5 Overview of practical example solution method

The methods for predicting thermal conductivity and volumetric specific heat capacity in SoilVision are not appropriate for soils undergoing phase change. SoilVision
predicts thermal conductivity and volumetric specific heat capacity solely as functions of water content. These two material properties are functions of both water content and ice content in soils undergoing freeze-thaw. As a result, implementation of equations for thermal conductivity and volumetric specific heat capacity in FlexPDE is by the methods outlined by de Vries (1963) and Newman (1996) respectively, and discussed in Chapter 3. These methods include solid, liquid and ice phases in the determination of thermal properties.

Seepage Analysis
The first step was determination of the initial water content distribution before initiation of freezing. A steady state analysis, using an average surface flux and average ground water depth as boundary conditions, provides an approximation of the water content distribution in the soil. This approximate water content distribution is input into the thermal analysis for determination of thermal properties.

Thermal Analysis
A steady state non-freezing thermal analysis, using the water content distribution obtained in the seepage analysis, provides input into the transient analysis. The transient analysis includes freeze-thaw effects caused by the chilled pipeline. Boundary conditions are applied to the problem in two manners. First, a constant surface temperature acts on the soil surface. In the second case, the surface temperature is a sinusoidal function of time, representing changes in surface temperature over a year of pipeline operation.

Parametric Study
A brief parametric study analyzed the effect of the soil-freezing curve on the freezing process. Thermal analyses simplified to consist of one material, with constant boundary conditions tested the effect of the soil-freezing curve on analysis. In addition, the material non-linearity FlexPDE is capable of handling was determined.
4.6 Representation of Material Properties in FlexPDE

FlexPDE allows input of material properties in a variety of ways. The techniques used in this study include:

- **Fully defined functions:**
  
  Fully defined functions provide values of the variable over all possible variation in the independent variable. For example, the SWCC for the Beaver Creek sand obtained from SoilVision (1997) in the form proposed by Gardner (1958) is given in Equation 4.1.

  \[
  \theta_s = \frac{0.36}{1 + \frac{1}{778 \psi^{3.24}}} \quad [4.1]
  \]

  Equation 4.2 is the FlexPDE format of Equation 4.1.

  \[
  \text{thetaw} = 0.36/(1 + 1/778 * \text{suct}^{3.24}) \quad [4.2]
  \]

  Figure 4.6 plots the function described by Equation 4.2.

  ![Figure 4.6](image)

  **Figure 4.6** Curve obtained from a fully defined function for the soil-water characteristic curve for Beaver Creek sand
• **Piece-wise defined functions:**

Piece-wise defined functions are formed using *if...then...else* statements defining sections of the curve. For example, SWCC's have three distinct zones, as discussed in Chapter 2. It is possible to assign one value of volumetric water content for suctions less than the air-entry value. The volumetric water content through the de-saturation zone is assigned a straight-line approximation. Finally, the volumetric water content past the residual value of soil suction is assigned a second straight-line approximation. The piece-wise representation of the soil-water characteristic curve for Beaver Creek sand becomes Equation 4.3.

\[
\text{thetaw} = \begin{cases} 
0.36 & \text{if } suct < 2 \\
0.36 - (0.0238 \times (suct - 2)) & \text{if } suct < 15 \\
0.05 - (0.0005 \times (suct - 15)) & \text{else}
\end{cases}
\]  

[4.3]

Figure 4.7 plots the function obtained using Equation 4.3.

![Figure 4.7 Curve obtained from a piece-wise defined function for the soil-water characteristic curve for Beaver Creek sand](image-url)
Table of values:
The *table* function in FlexPDE allows users to create a table of values using a program such as Microsoft Excel or SoilVision. The table is then imported into FlexPDE and the program linearly interpolates values as needed. For example, consider a table created in Excel defining the soil-water characteristic curve for a sand given in Table 4.1.

Table 4.1 Table defined for soil-water characteristic curve in FlexPDE

<table>
<thead>
<tr>
<th>Soil Suction (kPa)</th>
<th>Volumetric Water Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.36</td>
</tr>
<tr>
<td>1</td>
<td>0.36</td>
</tr>
<tr>
<td>2</td>
<td>0.36</td>
</tr>
<tr>
<td>5</td>
<td>0.29</td>
</tr>
<tr>
<td>10</td>
<td>0.1</td>
</tr>
<tr>
<td>14</td>
<td>0.05</td>
</tr>
<tr>
<td>20</td>
<td>0.016</td>
</tr>
<tr>
<td>40</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Figure 4.6 displays the points specified by the table, and plots the linear interpolation based on these points.

Figure 4.8 Curve obtained from a table of values function for the soil-water characteristic curve for Beaver Creek sand
CHAPTER 5
NUMERICAL MODELLING
RESULTS AND DISCUSSION

5.1 General

This chapter provides details of the results of the modelling program undertaken in this thesis. All FlexPDE descriptor files for problems described in this chapter are presented in Appendix C for reference. Section 5.2 provides the relevant results of the seepage verification program. Similarly, Section 5.3 discusses the thermal verification program. Section 5.4 discusses the successes and difficulties encountered in attempting coupled heat and mass transfer verification in FlexPDE. Finally, Section 5.5 pulls together the results from the other sections in considering a comprehensive example problem set in the context of the pipeline industry.

5.2 Seepage Verification

The verification of seepage problems presented is divided into two sections based on the number of dimensions of the problem. Section 5.2.1 provides results from two two-dimensional problems, followed by Section 5.2.2 presenting results from one three-dimensional problem.

5.2.1 Two Dimensional Seepage

The verification of FlexPDE for seepage results in two dimensions is mostly a reanalysis of the research study conducted by Nguyen (1999). The purpose of this study is to ensure that FlexPDE performs in a manner that is consistent with PDEase and Seep/W. Therefore, only two problems in two dimensions are presented in the main text below. The first problem describes transient seepage through an earth-fill
dam. The second problem describes a method for approximating the “review” elevation boundary condition used in Seep/W for locating the exit point on an unconfined surface in FlexPDE. Additional results can be found in Appendix B for more problems in twodimensional seepage.

5.2.1.1 Two-Dimensional Seepage Verification Example No. 1 – Transient Seepage

The seepage verification example presented is for the case of transient seepage through an earth fill dam, as the reservoir level is raised. Figure 5.1 depicts the problem geometry, initial conditions, and boundary conditions. The permeability functions used are given in Figure 5.2. A constant coefficient of volume change with respect to the water phase, \( m'_v \), of 0.003 \( 1/\text{kPa} \) was assumed for both materials.

Figure 5.1  Problem geometry and boundary and initial conditions for two-dimensional seepage verification example no.1
The transient analysis of this problem follows two stages: establishing initial conditions and solving for transient conditions. The initial conditions are determined using a steady state analysis with the water level at 4 m above datum, resulting in a constant head boundary condition to an elevation of 4 m, with a "no flow" boundary condition on the upstream face above 4 m elevation. Figure 5.3 shows the computation grid that FlexPDE generates when solving for the steady state conditions. Figure 5.4 and 5.5 present comparisons of the computed heads and pressure, respectively, computed by FlexPDE and Seep/W for the initial conditions. Figure 5.6 and 5.7 depict the velocity vectors produced by FlexPDE and Seep/W for the initial conditions. The results in all three cases are similar.

Figure 5.2 Coefficient of permeability functions used in seepage verification examples

Figure 5.3 Computation grid used by FlexPDE for two-dimensional seepage verification example no. 1 initial conditions
Figure 5.4  Comparison of computed head (m) contours for two-dimensional seepage verification example no. 1 initial conditions (Seep/W results in black, FlexPDE results in color)

Figure 5.5  Comparison of computed pore-water pressures (kPa) for two-dimensional seepage verification example no. 1 initial conditions (FlexPDE results in color, Seep/W in black)

Figure 5.6  Velocity vectors for two-dimensional seepage verification example no. 1 initial conditions generated by FlexPDE
Figure 5.7  Velocity vectors for two-dimensional seepage verification example no. 1 initial conditions generated by Seep/W

The initial conditions established are used as input into the transient model. Figure 5.8 presents one of the computation grids generated by FlexPDE during the transient analysis. As FlexPDE uses adaptive grid refinement, multiple computation grids can be developed over the course of the solution as the solution error dictates. In order to obtain an accurate solution in FlexPDE, it was necessary to place a line feature below the upstream surface, in order to force a denser computation grid at the upstream face where the head is changing rapidly at early time steps. The addition of a feature below boundaries where large changes are occurring in the dependent variable often helps improve the reliability of the FlexPDE results.

Figures 5.9 through 5.18 present the heads and pressures computed by FlexPDE and Seep/W at time steps 15, 255, 1023, 4095, 16383 hr. Generally, good agreement is obtained between the two models at most time steps. Some differences appear, likely due to differences in temporal and spatial discretization between the two programs.
Figure 5.8  Computation grid generated by FlexPDE for two-dimensional seepage verification example no. 1 at time step 16383 hr

Figure 5.9  Comparison of computed heads (m) for two-dimensional seepage verification example no. 1 time step 15 hr (Seep/W results in black, FlexPDE results in color)

Figure 5.10  Comparison of computed pore-water pressures (kPa) for two-dimensional seepage verification example no. 1 time step 15 hr
Figure 5.11  Comparison of computed heads (m) for two-dimensional seepage verification example no. 1 time step 255 hr (Seep/W results in black, FlexPDE results in color)

Figure 5.12  Comparison of computed pore-water pressures (kPa) for two-dimensional seepage verification example no. 1 time step 255 hr

Figure 5.13  Comparison of computed heads (m) for two-dimensional seepage verification example no. 1 time step 1023 hr (Seep/W results in black, FlexPDE results in color)
Figure 5.14  Comparison of computed pore-water pressures (kPa) for two-dimensional seepage verification example no. 1 time step 1023 hr

Figure 5.15  Comparison of computed heads (m) for two-dimensional seepage verification example no. 1 time step 4095 hr (Seep/W results in black, FlexPDE results in color)

Figure 5.16  Comparison of computed pore-water pressures (kPa) for two-dimensional seepage verification example no. 1 time step 4095 hr
5.2.1.2 Two Dimensional Seepage Verification Example No. 2 – Review Boundary Conditions

The second verification example included in this section highlights a method for approximating a “review” boundary condition in FlexPDE. A “review” boundary condition is necessary when there is a requirement for determining the location of the seepage exit point in a problem. This class of problem has been traditionally referred to as unconfined flow. Two review boundary conditions are implemented in Seep/W, review by elevation and review by pressure. Only the review by elevation boundary condition is considered here.
The case considered is seepage through an earth fill dam without a toe drain such that the zero pressure isobar intersects a free surface. Figure 5.19 shows the problem geometry and boundary conditions for the problem considered. The permeability is assumed to be constant of $1 \times 10^{-7} \text{ m/s}$. Figure 5.20 shows the solution grid generated in FlexPDE for this problem. Again a *feature* is used along the downstream boundary to increase the density of the solution grid along the free surface.

Seep/W (Geo-Slope, 1999) uses the method described below for determining the exit point. First, all nodes on the boundary are assigned a zero flux boundary condition on the first iteration. After calculating the heads based on this assumption, Seep/W modifies the boundary condition at any boundary node where the head is calculated to
be greater than the elevation (implying the pressure is greater than zero, since \( h = y + u\gamma \)). If this is the case, Seep/W changes the boundary condition at the lowest node to be a \( \text{value}(h)=y \) condition. Iterations continue, with the boundary conditions changing up the face of the free surface as necessary.

Implementation of the review boundary condition is not directly possible in FlexPDE. FlexPDE does not allow boundary conditions to be switched from one type to another in a given problem run. This option may be included in future versions of FlexPDE (Nelson, 2000). Presently, it is possible to approximate a solution with a minimum of human intervention.

The method proposed to expedite the solution of a free seepage face uses a staged approach in solving the problem, which produces a set of results that can then be checked to find an approximate exit point. After an approximate point has been found, the descriptor can be refined to allow a more precise solution to be found if desired.

The manner in which the boundary condition can be imposed is as follows. In FlexPDE, it is possible to force the value of a dependent variable to a specific value by specifying a very large flux or natural boundary condition that is proportional to the value required. Therefore, by setting the natural boundary condition to a big \( \text{value} \times (h-y) \), the value of \( h \) is forced equal to \( y \). Therefore, two natural boundary conditions can be written:

Boundary Condition #1: \( \text{natural}(h)=0 \)

Boundary Condition #2: \( \text{natural}(h)=\text{big}(h-y) \)

Under boundary condition #1, a zero flux is imposed along the boundary (i.e., the condition above the phreatic surface). In the region (i.e., below the phreatic surface) where boundary condition #2 applies, the value of the variable \( h \) is forced to be equal to \( y \) through use of the natural boundary condition shown. An if..then..else statement can
then be used to define the boundary condition continuously along the downstream face of the problem.

Combined Boundary Condition: \( \text{natural}(h) = \text{if } y < \text{exit} \text{ then } \text{big} \times (h-y) \text{ else } 0 \)

The problem still remains to identify where the exit point occurs. In doing this, a staged problem descriptor is used wherein the value of the exit elevation is changed between problem stages. For each stage, a plot is produced of the water pressure versus the distance along the downstream face. For cases where the assumed exit elevation is too low, a positive pressure will be solved for at points between the assumed exit elevation and the calculated exit. At the correct exit point, the profile will be zero up to the assumed exit point, and negative above. When the assumed exit elevation is too high, the same profile will exist, except the assumed and calculated exit points will not correspond. Only at the correct exit point will the assumed and calculated exit points correspond. Therefore, by increasing the elevation of the exit point, curves with positive pressures will be produced until the elevation is approximately correct, at which point the curves produced will not have positive pressures. The solution technique for locating the seepage exit point is summarized in Figure 5.21.

The descriptor file for the present problem considered uses 15 stages to move up the side of the dam face. Figure 5.22 shows a plot of the pressure at the surface versus the length for stages \( y = 3 \) to \( y = 6.5 \) along the downstream face of the dam. The length along the face can be related to the elevation by the relationship \( y = l/2/1.118 \) for the present problem geometry.
Define problem geometry; select an assumed exit point near the bottom of the surface of interest

Solve problem and plot pressure along the surface of interest

If pressure at any point along surface > 0

Else

If calculated exit point = assumed exit point

Then

Else

Decrease elevation of exit point

Else

Increase elevation of exit point

Then

End

Figure 5.21  Flow chart for solution of review by elevation boundary conditions

From Figure 5.22, it can be seen that the exit points that produce the correct pressure profiles are those greater than approximately 6 m elevation. The pressure profile for the assumed exit point of 6 m shows both the correct behavior and the switch from zero pressure to negative pressure occurs at approximately 6 m elevation. Using the results for the assumed exit point at elevation 6 m, comparison is made with Seep/W’s solution to this problem. Seep/W also identified the exit point at approximately 6 m. Head contours are compared in Figure 5.23 and pressure contours are compared in Figure 5.24. Comparison between the two programs shows identical results, suggesting that the method used in FlexPDE is correct. Finally, Figures 5.25 and 5.26 compare the velocity vectors generated by the two programs for this solution.
Correct exit point from Seep/W and as determined in FlexPDE

Figure 5.22 Pressure profiles along downstream dam face as calculated by FlexPDE
Figure 5.23  Comparison of computed head contours for two-dimensional seepage verification example no. 2 (Seep/W results in black, FlexPDE results in color)

Figure 5.24  Comparison of computed pore-water pressure contours for two-dimensional verification example no. 2

Figure 5.25  Velocity vectors for two-dimensional seepage verification example no. 2 generated by FlexPDE
The method described above is only valid for steady state seepage problems as the stage command in FlexPDE is only valid in steady state problems. In FlexPDE for transient problems it will be necessary to run the problem several times, stopping the program and manually entering a new exit point. It is possible in PDEase to implement a staged problem in transient problems. Implementing the review boundary condition in PDEase was not attempted in the present study.

5.2.2 Three Dimensional Seepage

The capability of FlexPDE for solving three-dimensional problems was investigated in the course of this study. One three-dimensional seepage verification example was considered in FlexPDE. This example is discussed below.

5.2.2.1 Three-Dimensional Seepage Verification Example

The three-dimensional seepage verification example considered in this section is steady state seepage through an earth fill dam. The material properties are the same as was used in the two-dimensional seepage problem discussed in Section 5.2.1. The permeability functions can be found in Figure 5.2. The basic problem geometry is similar to what has been considered in the two-dimensional seepage verification problem no. 1. The dam is 12 m high, with a crest 4 m wide, and 2:1 side slopes, resulting in a total width of 52 m. The abutment is assumed to also be at a 2:1 slope as
well. Figure 5.27 provides plan and profile views of the structure along with the sections for which detailed analysis is presented later. Coordinates shown correspond to the FlexPDE definitions. Boundary conditions applied to this problem are 10 m head on the upstream face, and 0 m head at the toe filter. All other boundaries have no flow boundary conditions imposed. Figure 5.28 illustrates 3 three-dimensional views of the dam taken from the FlexPDE grid used to solve the problem.

![Diagram](image)

Figure 5.27 Plan and profiles of dam analyzed in the three-dimensional seepage verification example

Three sections of the dam were considered in detail, and the results compared with two-dimensional analysis done in Seep/W. The location of the sections analyzed is shown on Figure 5.27. Section A-A' was expected to produce results that are essentially the same as the two-dimensional case. Section B-B' is in a location where it was expected the three-dimensional effects of the problem would be important. Section C-C' running along the centerline of the crest of the dam shows the variation in the variables along the length of the dam, demonstrating the effect of the third dimension on problem solution. of course this section was not analyzed in Seep/W.
Figures 5.28 and 5.30 show the heads and pressures, respectively, computed by FlexPDE and Seep/W at section A-A'. The results compare quite favorably with only small discrepancies noticed. This is expected; because near the center of the dam, end effects are expected to be minimal and the flow regime is expect to be essentially two-dimensional. Differences between the two sets of results are likely due to lack of
discretization in FlexPDE in the three-dimensional problem; fewer nodes are used in any one y-plane than would be in a two-dimensional analysis.

Figures 5.31 and 5.32 show the heads and pressures, respectively, computed by FlexPDE and Seep/W at section B-B’. As expected, the results differ quite substantially showing that three-dimensional effects are being modelled in FlexPDE. Figures 5.33 and 5.34 show the heads and pressures computed by FlexPDE at section C-C’. Section C-C’ represents the centerline of the dam. As can be seen the pressure and heads along the length of the dam are not constant, and it appears that there is some flow occurring from the abutments of the dam towards the center.

![Comparison of computed heads (m) for the three-dimensional seepage verification example at section A-A’ (Seep/W results in black, FlexPDE results in color)](image1)

![Comparison of computed pore-water pressures (kPa) for the three-dimensional seepage verification example at section A-A’ (Seep/W results in black, FlexPDE results in color)](image2)
Figure 5.31  Comparison of computed heads (m) at section B-B', a) FlexPDE three-dimensional, b) Seep/W
Figure 5.32  Comparison of computed pore-water pressures (kPa) at section B-B', a) FlexPDE three-dimensional results, b) Seep/W

Figure 5.33  Head (m) contours along section C-C' as determined in the FlexPDE three-dimensional seepage verification example
Figure 5.34 Pore-water pressure (kPa) contours along section C-C’ as determined in the FlexPDE three-dimensional seepage verification example
5.3 Thermal Verification

The thermal problems undertaken as part of this focus on the aspect of freeze/thaw, with some emphasis on uncoupled heat flow in soils where the temperature is above the freezing point of the soil.

5.3.1 Two-Dimensional Verification of FlexPDE for Steady State Heat Flow

The solution of steady state heat flow in isotropic soils is governed by the Laplacian equation as shown in Chapter 3.

5.3.1.1 Two-Dimensional Thermal Verification Example No. 1

The first verification example involves the determination of steady state conditions in the soil below two adjacent semi-infinite areas with a surface temperatures of +4 °C and -5 °C as depicted in Figure 5.35. This problem is solved for two conditions, with the first case involving no geothermal gradient acting in the soil. The second case includes a geothermal gradient of 1 °C/30m acting in the soil. The geothermal gradient is due to heat generated deep within the earth (Burdick et al., 1978). It is possible to solve both cases through the use of a single descriptor file in FlexPDE.

![Figure 5.35](image)

Figure 5.35 Problem setup for two-dimensional thermal verification no. 1
The analytical solution given by Harlan and Nixon (1978) has the form of:

\[ T - T_g = \frac{T_s - T_g}{\pi} \tan^{-1} \frac{z}{x} \]  

[5.1]

where \( T \) is the temperature at any point given by \( x \) and \( z \),

\( T_g \) is the cool ground temperature, and

\( T_s \) is the hot ground temperature.

For the case where the geothermal gradient is present the equation is modified as follows:

\[ T - T_g = \frac{T_s - T_g}{\pi} \tan^{-1} \frac{z}{x} + Gz \]  

[5.2]

where \( G \) is the geothermal gradient in °C/m.

The grid used by FlexPDE for solving the problem is shown in Figure 5.36. Figure 5.37 compares the solution obtained from FlexPDE for the first case (no geothermal gradient) with the analytical solution that was provided by Harlan and Nixon (1978). The solution given by FlexPDE agrees quite well with the analytical solution. This result should be anticipated, given that it is the solution of the common Laplace equation.

![Solution grid generated by FlexPDE for steady state heat flow verification example no. 1](image-url)
Figure 5.37  Comparison of a) FlexPDE and b) analytical solution for steady state heat flow verification example no. 1, the case of two semi-infinite adjacent surfaces at temperatures of +4 °C and -5 °C
For the second case where a geothermal gradient is present, Figure 5.38 provides a comparison between FlexPDE’s results and the analytical solution given in Harlan and Nixon (1978). Again, good agreement is obtained between FlexPDE and the analytical solution.

Figure 5.38 Comparison of a) FlexPDE and b) analytical solution for steady state heat flow verification example no. 1 the case of two semi-infinite adjacent surfaces at temperatures of +4 °C and -5 °C with a geothermal gradient of 1 °C/30m
5.3.1.2 Two-dimensional Thermal Verification Example No. 2

The second verification example is for the case of a heated strip on a permafrost type of terrain at initial temperatures of -5 °C at the surface, increasing at a rate of 1 °C/30m with depth. A 100 m wide heated strip is placed on the ground surface at a temperature of +4 °C. Figure 5.39 presents the problem geometry and boundary conditions. Figure 5.40 provides the solution grid generated in FlexPDE.

![Problem geometry and boundary conditions](image1)

![Solution grid](image2)
Figure 5.41 gives the results obtained in FlexPDE. The problem was also modelled using Temp/W. Results from FlexPDE and Temp/W are compared with the analytical solution provided by Harlan and Nixon (1978). Harlan and Nixon's (1978) solution only identifies the location of the freezing front and provides no information on the isotherms in the soil mass. Good agreement is obtained for the location of the freezing front using FlexPDE. The FlexPDE results also agree with the Temp/W results.

a) FlexPDE result (color) and Temp/W result (black)

b) Analytical result (from Harlan and Nixon, 1978)

Figure 5.41 Comparison of a) FlexPDE and Temp/W with b) analytical solution for steady state heat flow verification example no. 2, heated strip on initially frozen ground with geothermal gradient of 1 °C/30 m
5.3.2 Two-Dimensional Verification of FlexPDE for Transient Heat Flow

Verification of FlexPDE for transient heat flow is done through several examples. Transient heat flow without freezing is verified in the first example considered. The next four examples consider the case of a soil undergoing freezing or thawing, in which case latent heat effects need to be considered.

5.3.2.1 Two-Dimensional Thermal Verification Example No. 3

The first example is an example of heat flow in a soil in which no freezing is taking place. The problem modelled is taken from Nobel and Geller (1987). The problem is a column of soil 0.44 m deep. Figure 5.42 gives the material properties for the soil as given by Nobel and Geller (1987). Two cases are modelled, one for the soil in a dry condition, the second for the same soil in a moist condition. The dry soil had a volumetric water content of 3%. The wet soil had a volumetric water content of 29%. Based on the given volumetric water contents, constant material properties were selected from Figure 5.42 for use in the FlexPDE modelling.

Figure 5.43 shows the temperature profiles that were observed on the top and bottom of the soil for the wet and dry conditions. These are used as boundary conditions for the FlexPDE modelling that was performed. Temperature profiles were determined at a point 0.09 m below the soil surface. Figure 5.44 shows the results for the dry soil case produced by FlexPDE compared with the results obtained by Nobel and Geller (1987) in their model and with the experimental results that were obtained in a field study. Figure 5.45 shows the same data for the wet soil case. In both cases, it can be seen that the results are very close. The similarity of the results are expected for the case where the material properties are constant.
Figure 5.42  a) Soil water characteristic curve and b) thermal properties as a function of water content for thermal verification example no. 3 (from Nobel and Geller, 1987)
Figure 5.43  Temperature boundary conditions as a function of time for a) dry soil case, b) wet soil case thermal verification example no. 3 (from Nobel and Geller, 1987)
Figure 5.44  Comparison of temperature calculated by FlexPDE and the model from Nobel and Geller (1978) model with experimental results for thermal verification example no. 3 dry soil case at 0.09 m below surface

Figure 5.45  Comparison of temperature calculated by FlexPDE and the model from Nobel and Geller (1987) with experimental results for thermal verification example no. 3 wet soil case at 0.09 m below surface
5.3.2.2 Two-Dimensional Thermal Verification Example No. 4 and 5

The fourth and fifth heat flow verification examples considered add freeze-thaw effects to the basic transient analysis considered in example no. 3. This solution is the Neumann solution given by Carslaw and Jaeger (1959). The analytical solution is described in detail by Harlan and Nixon (1978) and is also presented in the Temp/W User's Manual (Geo-Slope, 1999).

Verification example no. 4 considers the case of a thaw front developing and progressing downwards through a column of soil. Figure 5.46 shows the basic setup of this problem with the material properties that are used in the problem. \( C_u \) and \( K_u \) are the unfrozen volumetric specific heat capacity and thermal conductivity, respectively. \( C_f \) and \( K_f \) are the corresponding values for the soil in the frozen condition.

Verifikation example no. 5 is essentially identical to verification example no. 4, except that the situation is reversed, and the soil is undergoing freezing from the surface downwards. Figure 5.47 shows the problem setup for verification example no. 5. For
both verification examples the assumption is that the entire volume of the column undergoes a phase change from solid to liquid or vice versa. This is not realistic for a soil, but is necessary for comparison with the analytical solution.

The analytical solution of this problem assumes that the latent heat is released instantaneously at a temperature of exactly 0°C. This implies that the term $\partial \theta_s / \partial T$, referred to as $m_1'$ in the present study, becomes infinitely large at a temperature of 0°C. If the phase change is considered in terms of the soil-freezing curve described earlier, the curve implemented in the analytical solution is as shown by the curve as shown in Figure 5.48. The value of $m_1'$ corresponding to this curve is shown in Figure 5.49. FlexPDE cannot handle the discontinuity that would be applied if this model of unfrozen water content of the soil was followed. This curve is only valid for pure substances and is therefore not realistic for actual soils encountered in geotechnical engineering. The soil-freezing curve for real soils will extend over some range of temperatures.
For verification example no. 4, various curves were attempted. Figure 5.48 depicts the range of curves that were attempted. The curve used in the analysis was the steepest curve that maintained numerical stability in FlexPDE. The \( m'_2 \) curve that corresponds to this soil-freezing curve is shown in Figure 5.49. As discussed in Chapter 3, in the present research a function for \( m'_2 \) was first selected and then the corresponding soil-freezing curve was generated.

![Figure 5.48 Volumetric unfrozen water content curves used for initial analysis of verification example no. 4 Neumann thaw analysis](image)

The results that were obtained using the curve for \( m'_2 \) shown in Figure 5.48 are compared with Temp/W and the analytical solution in Figure 5.50, which shows the depth of thaw versus time. Figure 5.51 presents a history of the temperature versus time for three points beneath the soil surface, comparing results from Temp/W and FlexPDE. The results between the two programs are comparable, but not identical. This can be attributed to the differences in interpretation of the soil-freezing curve as implemented by the two programs.
Figure 5.49 Slope of unfrozen water content curve ($m_z$) used for initial analysis of verification example no. 4 Neumann thaw analysis

Figure 5.50 Comparison of thaw depths computed using analytical solution, Temp/W and FlexPDE for verification example no. 4 with initial unfrozen water content functions
The FlexPDE model incorporates a function describing $m'_z$ as a continuous function of temperature. Temp/W interpolates the value of $m'_z$ from the soil-freezing curve in an approximate fashion. A second analysis was performed of this problem to attempt to show these differences. Figure 5.52 shows the soil-freezing curve that was used in the second analysis. Figure 5.53 gives the $m'_z$ curve corresponding to the soil-freezing curve shown in Figure 5.52. Also shown in Figure 5.53 is the curve that can be obtained from Temp/W for the soil-freezing curve given in Figure 5.52.
Figure 5.53  Comparison of slopes of unfrozen water content curve \( (m'_2) \) as determined from a point wise differentiation and as calculated by Temp/W for unfrozen water content curve given in figure 5.52

As can be seen in Figure 5.53 the \( m'_2 \) function used in the two programs is different, even though the same soil-freezing curve is assumed. Figures 5.54 and 5.55 show the results for the analysis using these \( m'_2 \) functions are presented. As can be seen there are substantial differences between the two solutions.

Figure 5.54  Comparison of thaw depths computed using Temp/W and FlexPDE, where FlexPDE used point wise differentiation of unfrozen water content curve, Temp/W used its method of determining \( m'_2 \).
A third model run was conducted in FlexPDE in which the $m'_2$ function as obtained from the Temp/W results was used (i.e., the $m'_2$ curve as given in Figure 5.53). The results from this analysis are presented in Figures 5.56 and 5.57, showing excellent agreement between the two solution methods. Therefore, it can be concluded that if the same interpretation of the soil-freezing curve is used in the two programs the results will be comparable.

Figure 5.55  Comparison of temperature histories at three points below ground surface for case described in Figure 5.54 for thermal verification example no. 4

Figure 5.56  Comparison of thaw depths calculated by Temp/W and FlexPDE, using Temp/W interpretation of $m'_2$ in FlexPDE for thermal verification example no. 4
Figure 5.57 Comparison of temperature histories calculated by Temp/W and FlexPDE using Temp/W interpretation of $m'_2$.

Thermal verification example no. 5 as discussed above is the opposite condition to example no. 4, i.e., freezing of the soil from surface down as opposed to thawing of the soil. Figure 5.58 shows the steepest soil-freezing curve that was successfully implemented in FlexPDE. The steep soil-freezing function best approximated the analytical solution. Figure 5.59 shows the corresponding $m'_2$ curve implemented in FlexPDE. Also shown in Figures 5.58 and 5.59 are the curves that are assumed in the analytical and initial Temp/W solution.

Figure 5.60 shows the depth of freezing calculated using FlexPDE, Temp/W and by the analytical solution. The FlexPDE results are significantly different than the results obtained using Temp/W and the analytical solution. Figure 5.61 plots the temperature versus time at three points below the soil surface as obtained in FlexPDE and Temp/W. The results show that the two programs provide similar behavior; however, the actual computed values are somewhat different.
Figure 5.58  Volumetric unfrozen water content curves used for initial analysis of verification example no. 5 Neumann freeze analysis

Figure 5.59  Slope of unfrozen water content curves ($m'_2$) used for initial analysis of thermal verification example no. 5 Neumann freeze analysis
Figure 5.60  Comparison of freeze depths computed using analytical solution, Temp/W and FlexPDE for thermal verification example no. 5 with initial unfrozen water content functions

Figure 5.61  Comparison of temperature histories at three points below ground surface as computed by FlexPDE and Temp/W for verification example no. 5 with initial unfrozen water content functions
Similar to the procedure used in verification example no. 4, a new function for the soil-freezing curve and thus $m_2'$ was used in FlexPDE and Temp/W. Figure 5.62 shows the soil-freezing curve that was used for the simulations. Figure 5.63 shows the $m_2'$ curve that should have been generated by Temp/W based on the soil-freezing curve given in Figure 5.62. Also shown is the curve that was generated by the Temp/W solution for this problem. This second curve was implemented in FlexPDE and the results are presented in Figures 5.64 and 5.65. The results obtained are similar, suggesting the importance of having a consistent definition of $m_2'$ in order to obtain a correct solution.

Figure 5.62  Volumetric unfrozen water content curve used in second analysis of thermal verification example no. 5 Neumann freeze analysis

Figure 5.63  Slope of unfrozen water content curve used in second analysis of thermal verification example no. 5 Neumann freeze analysis
Figure 5.64  Comparison of depths of freezing calculated using Temp/W and FlexPDE using the Temp/W generated \( m_1 \) curve in FlexPDE for second analysis of thermal verification example no. 5

Figure 5.65  Comparison of temperature histories at three points below ground surface as computed by Temp/W and FlexPDE for second analysis of thermal verification example no. 5
5.3.2.3 Discussion on Determination of Slope of Soil-Freezing Curve

The above discussion shows that there are differences between the way Temp/W calculates $m'_f$ and the way it is being implemented in FlexPDE. Temp/W solves for $m'_f$ in an approximate fashion. At time step 1, Temp/W assumes $m'_f$ is equal to 0. For the next time step, in the first iteration the program determines new temperatures through the solution domain using this assumption. Using the temperature calculated in the first iteration of time step 2, and the temperature given in the initial conditions, the program accesses the user inputted soil-freezing curve and calculates a constant $m'_f$ from time step 1 to time step 2 by the equation:

$$m'_f = \frac{(\theta_{a1} - \theta_{a2})}{(T_1 - T_2)}$$  \[5.3\]

where $\theta_{a1}$ and $\theta_{a2}$ are the unfrozen water content at times 1 and 2 respectively, and $T_1$ and $T_2$ are the temperatures at times 1 and 2. After the program calculates this value, Temp/W then performs another iteration using this value of $m'_f$ in place of 0. If the convergence criteria are met, the program stops the iteration and produces a temperature profile at time 2. If not, the program repeats the process with the new temperatures calculated using the new value of $m'_f$.

The major problem with the scheme described above is that if the time steps are not sufficiently small, the change in temperature between any two time steps can be significant, with the consequence being an extremely poor estimation of the value of $m'_f$ (i.e. if the temperature is changing by 1 or 2 °C in a time step, and the entire range of the soil-freezing curve is only 0.5 °C, the value of $m'_f$ will be significantly in error). The solution to this potential error is to increase the number of time steps in a problem run, especially at times when it is anticipated that major changes in the temperature regime of the soil are expected.

In FlexPDE, $m'_f$ has been implemented as the derivative of the soil-freezing curve. As such, for any value of the temperature there is a value for $m'_f$, which is used in the
calculation. Approaches for implementing the \( m'_i \) function in FlexPDE can include a fully defined function or an approximate function. Nguyen (1999) showed that approximate functions for \( m'_i \) give reasonably similar results to fully defined functions. It is anticipated that a similar situation is true for \( m'_i \). An added advantage is the increase in speed of computation. If the fully defined equation as given in the theory section is considered, it can be seen that the implementation in any program will result in significant computational requirements. In the remainder of the problems considered in this research program, a table function has been implemented in FlexPDE for definition of the \( m'_i \). Provided sufficient points are included the function will be close to what would be obtained with a fully specified equation, with the advantage of shorter computation times.

5.3.2.4 Two-Dimensional Thermal Verification Example No. 6

The next thermal verification example considered is the case of particular interest for construction of a heated foundation on permafrost terrain. Geotechnical engineers are concerned with determining the depth of thaw that should be anticipated to avoid unacceptable settlement of the foundation.

The first numerical solution to this problem was given by Hwang et al (1972). GeoSlope (1999) uses this problem as a verification example in Temp/W. In the present case, an 80 m wide foundation that is heated to 15.5 °C is placed on permafrost soil that has a pre-construction temperature profile ranging from −2 °C at the surface to 0°C at a depth of 60 m. Figure 5.66 shows the problem geometry and initial conditions.

The material properties of the soil that have been used in this analysis are shown in Figure 5.67. The soil-freezing curve is given as the unfrozen fraction, which is given as \( \theta_u / \theta \), where \( \theta \) is the volumetric water content of the soil at the initiation of freezing. It is assumed that \( \theta \) is equal to 0.18 for this problem. The thermal conductivity and volumetric specific heat capacity of the soil are functions of temperature to the extent
that one value exists above the freezing point, and another below the freezing point. Ideally, these should be functions of the ice and unfrozen water contents of the soil, but for the present analysis a simplified model of these soil properties is used.

Figure 5.66 shows the initial conditions used in this analysis. Only half of the problem is analyzed due to the symmetry of the problem setup. It was found necessary to include several "feature" statements in FlexPDE for this solution. For this problem, three lines are added just below the surface to improve the accuracy of the solution. Figure 5.68 shows the solution grid that was generated by the FlexPDE solution of this problem.

Figures 5.69 through 5.73 show isotherms that were produced using FlexPDE and these values compared with the Temp/W solution. The solutions obtained by the two programs agree quite well. The slight differences that can be seen in the two solution methods can be attributed to the differences in the interpretation of $m'$ as discussed above, although attempts were made to minimize this effect by increasing the number of time steps taken in the Temp/W solution.

Figure 5.74 presents the temperature profiles determined in the solution beneath the centerline of the foundation. The results from FlexPDE agree well with the results of Temp/W. As the solution approaches steady state conditions, the FlexPDE results approach the Temp/W results as the effect of $m'$ on the solution lessens.
Figure 5.66  Problem geometry and initial conditions for thermal verification example no. 6 heated foundation on permafrost

Figure 5.67  Material properties specified for thermal verification example no. 6 heated foundation on permafrost
Figure 5.68  Computation grid used by FlexPDE for thermal verification example no. 6 heated foundation on permafrost

Figure 5.69  Comparison of computed temperatures between FlexPDE and Temp/W for thermal verification example no. 6 time step 10000 hr
Figure 5.70 Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black, for thermal verification example no. 6 time step 100,000 hr

Figure 5.71 Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black, for thermal verification example no. 6 time step 220,000 hr
Figure 5.72 Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black for thermal verification example no. 6 time step 250,000 hr

Figure 5.73 Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black for thermal verification example no. 6 time step 400,000 hr
Figure 5.74 Temperature profiles at centerline (i.e., x=0) of thermal verification example no. 6 heated foundation on permafrost for various times, comparing Temp/W and FlexPDE computed temperatures
5.3.2.5 Two-Dimensional Thermal Verification Example No. 7

The final two-dimensional thermal verification example considers a classic problem that is of interest to the pipeline industry. One option for shipping oil and gas from northern fields to the south is to chill the product and thus avoid thawing of permafrost terrain. The problem arises, though, in discontinuous permafrost, when the pipeline traverses non-frozen terrain. It would be expected that freezing of the soil would be initiated. This example was considered by Coutts and Konrad (1994) and is also used in the verification of Temp/W.

A pipeline with an outside temperature of -2 °C is embedded in a soil initially at a temperature of 3 °C. The soil has the soil-freezing curve, and thermal properties as shown in Figure 5.75. As in example no. 6, the soil-freezing curve is given as the unfrozen fraction versus temperature. \( \theta \) is assumed equal to 0.377 for this problem. A constant surface temperature of 3 °C is assumed. Figure 5.76 shows the geometry of the problem, boundary and initial conditions. Figure 5.77 displays the computation grid that was generated by FlexPDE for this problem.

Figures 5.78 through 5.82 show the isotherms around the pipeline for various time steps. As expected, the results between the two programs differ significantly at early time steps due to the differences in interpretation of the \( m'_2 \) function. At larger time steps the differences become smaller, as the effect of differing \( m'_2 \) decreases. At steady state conditions (i.e. time step 730 days), the results are identical. This is to be expected, as at steady state, \( \partial T / \partial t \) goes to 0 and \( m'_2 \) has no effect on the solution.

Figure 5.83 shows a temperature history at four points around the pipe, comparing the temperatures calculated by FlexPDE and Temp/W. The figure shows that the results between the two programs are essentially the same, provided sufficient time steps are included in the Temp/W analysis. If fewer time steps are used in Temp/W the two solutions begin to diverge significantly during the transient analysis, although steady state conditions are identical.
Figure 5.75  Material properties specified for thermal verification example no. 7 chilled pipeline in unfrozen ground

Figure 5.76  Problem geometry, initial conditions and boundary conditions for thermal verification example no. 7
Figure 5.77  Computation grid used by FlexPDE for verification example no. 7 chilled pipeline in unfrozen ground

Figure 5.78  Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black for verification example no. 7 time step 7 days
Figure 5.79  Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black for verification example no. 7 time step 15 days

Figure 5.80  Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black for verification example no. 7 time step 31 days
Figure 5.81  Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black for verification example no. 7 time steps 127 days

Figure 5.82  Comparison of computed temperatures (°C), FlexPDE in color, Temp/W in black for verification example no. 7 time steps 730 days
Figure 5.83  Temperature (°C) history at four points around the chilled pipeline for verification example no. 7 chilled pipeline in unfrozen ground
5.3.3 *Three-Dimensional Verification of FlexPDE for Heat Flow*

Solution of three-dimensional problems in FlexPDE for heat flow was limited to one problem in steady state heat flow. Solution of the steady state condition eliminates the need to consider $m'_2$ in the solution. The $m'_2$ term can cause computational difficulties in two dimensions, so the effect in three-dimensions is anticipated to be significant.

5.2.3.1 *Three-Dimensional Thermal Verification Example*

The problem considered for the three-dimensional analysis is analogous to the foundation on permafrost example considered in the two-dimensional verification example no. 6. Instead of a square or rectangular foundation however, a circular foundation is considered, which may correspond to a storage tank. Only one quarter of the problem needs to be analyzed assuming homogenous soil beneath the foundation.

Figure 5.84 shows the plan and profile of the problem considered. A temperature of 15.5 °C is assumed under the foundation. Ambient air temperature is assumed to be equal to -2 °C. A soil volume of 50 x 50 x 60 m is considered in the FlexPDE analysis. Three vertical sections and two horizontal sections in the soil mass beneath the tank are considered. Results at the $y = 50$ m section are compared with steady state results from the FlexPDE analysis of two-dimensional thermal verification example no. 6. Figure 5.85 shows a view of the three-dimensional grid generated by FlexPDE for solution of this problem.

Figure 5.86 presents the isotherms generated by FlexPDE for section A-A'. In traditional geotechnical analysis of this problem, it would be assumed that section A-A' can be accurately represented by a two-dimensional analysis. Figure 5.87 represents the FlexPDE two-dimensional solution to this problem. Comparing the two figures, it can be seen that the two-dimensional analysis appears to over-predict the increase in temperature in the soil beneath the structure as compared to the three-dimensional solution. It can therefore be anticipated that the two-dimensional solution will over predict depths of thaw for cases where determination of thaw progression is important.
Figure 5.84  Plan and profile of three-dimensional thermal verification example

Figures 5.88 and 5.89 show the isotherms for sections B-B' and C-C' for the three-dimensional solution. Figures 5.90 and 5.91 show surface plots of temperature in horizontal planes at section D-D' and E-E'. It is possible to visualize a heated "bulb" of soil beneath the warm foundation from these plots. This "bulb" is of interest for producing settlement calculations for structures that are built on permafrost terrain.
Figure 5.85  Three-dimensional mesh generated by FlexPDE for steady state solution of heated foundation on permafrost
Figure 5.86  FlexPDE isotherms (°C) for section A-A’ (y = 50m) for three-dimensional thermal verification example

Figure 5.87  FlexPDE isotherms (°C) for two-dimensional steady state solution for heated foundation on permafrost
Figure 5.88  FlexPDE isotherms (°C) for section B-B' (y = 25m) for three-dimensional thermal verification example

Figure 5.89  FlexPDE isotherms (°C) for section C-C' (y = 10 m) for three-dimensional thermal verification example
Figure 5.90  Plot of temperature (°C) on plane D-D' showing the thaw "bulb" beneath the heated foundation

Figure 5.91  Plot of temperature (°C) on plane E-E' beneath the heated foundation
5.4 Coupled Heat and Mass Transfer Verification

This section describes the attempts made in the present study to implement coupled heat and mass transfer using FlexPDE. The solution of coupled heat and mass transfer problems using FlexPDE was only partially successful.

5.4.1 Coupled Heat and Mass Transfer with Small Gradients

Problems involving moisture transfer due to thermal gradients were considered first. The system analyzed was a closed system, implying no water flow occurs external to the system. The effect of the closed system is that changes in the dependent variable $\psi$ are not expected to be significant.

5.4.1.1 Coupled Heat and Mass Transfer Verification Example No. 1

The example considered is an experiment reported by Ewen and Thomas (1989) involving the heating of a cylinder of soil and monitoring of the effects of heat flow on the water content distribution in the soil. Ewen and Thomas (1989) provide modelling results using a finite difference model. Li et al. (1997) re-analyzed the results of Ewen and Thomas (1989) using a finite element model.

Figure 5.92 shows schematically the set up used by Ewen and Thomas (1989). The experiment consisted of a circular drum filled with sand and a heater placed in the center of the drum. Ewen and Thomas (1989) give material properties as a function of volumetric water content. Figure 5.93 gives the soil-water characteristic curve provided by Ewen and Thomas (1989). The defined curve is only valid for soil suctions greater than approximately 2.4 kPa. Therefore, it was necessary to estimate a complete soil-water characteristic curve from the available curve and the porosity of the soil, as shown in Figure 5.93. Figure 5.94 shows the thermal conductivity and volumetric specific heat capacity functions given by Ewen and Thomas (1989) and used in the present analysis. These functions were defined in FlexPDE as continuous functions of
volumetric water content. Figure 5.95 shows the permeability function used in the FlexPDE solution of this problem.

Figure 5.92 Problem geometry, boundary, and initial conditions for coupled verification example

Figure 5.93 Soil-water characteristic curve for the coupled verification example
Figure 5.94  Thermal properties for the coupled verification example

Figure 5.95  Permeability as a function of volumetric water content for the coupled verification example
The boundary and initial conditions used in the problem are shown in Figure 5.92 along with the problem geometry. Only half the problem needs to be analyzed using FlexPDE due to the symmetry of the problem. The boundary conditions shown are those used in the Li et al. (1997) analysis of this problem.

Figure 5.96 shows the contours of temperature and volumetric water content that were generated in FlexPDE. The FlexPDE results can be compared with the results given by Ewen and Thomas (1989) as shown in Figure 5.97 and the results of Li et al. (1997) as shown in Figure 5.98. The Ewen and Thomas (1989) plot temperature in °C and volumetric water content in percent, whereas the FlexPDE and Li et al. (1997) results are plotted in °C and in decimal form, respectively. The three sets of results all show the same type of behavior occurring, but the value of the temperatures and volumetric water contents calculated are different. The differences are likely due to the slight differences in the material properties and boundary conditions for the three analyses. The FlexPDE results show behavior that is comparable to the other two analyses, indicating that a coupled solution is being found in FlexPDE.

Figure 5.99 presents histories of temperature and volumetric water content at eight points along section A-B shown in Figure 5.93. The distances correspond to the distance from the heater. Figure 5.100 presents the same plot taken from the results of Li et al. (1997). Similar behavior is observed with respect to time, but the absolute values of temperature and volumetric water content are significantly different. The differences are likely due to differences in the material properties used in the two models.
Figure 5.96  FlexPDE computed results for a) temperature (K) and b) volumetric water content (decimal) at time = 300 hr
Figure 5.97  Ewen and Thomas (1989) results for a) temperature (°C) and b) volumetric water content (%) at steady state conditions

Figure 5.98  Li et al. (1997) results for a) temperature (K) and b) volumetric water content (decimal) at steady state conditions
Figure 5.99  History of a) temperature (K) and b) volumetric water content as determined in FlexPDE analysis
Based on the above analysis the form of coupled heat and mass transfer equation as proposed by Joshi (1993) appears to be working correctly in FlexPDE for cases of relatively small gradients in the dependent variable, \( \psi \), which is the soil suction. The fact that the results do not match exactly is primarily due to ambiguities in the published data to which comparisons are being made.
5.4.2 Observed Problems in Handling Large Imposed Gradients

Two types of coupled phenomena in geotechnical engineering that were considered in this thesis result in large gradients being either imposed on the system or generated within the system. Imposed gradients are due to atmospheric forcing. Gradients are generated within the system in the case of moisture redistribution due to freezing in the soil. It was found in the course of the present study that both of the above cases are presently unsolvable in FlexPDE. These two cases are considered separately below.

5.4.2.1 Coupled Heat and Mass Transfer with Atmospheric Forcing

Coupled heat and mass transfer due to atmospheric forcing is a highly non-linear process involving large gradients that are imposed on the soil. The gradients must be dissipated over small depths. Evaporation moves water from the soil to the air, resulting in a decrease in the water content of the soil surface, with a corresponding increase in soil suction.

The suction at the soil surface will come to equalize with the moisture in the air, such that the relative humidity in the soil pores at the surface, \( r_{h_{\text{soil}}} \), will be the same as the relative humidity in the air, \( r_{h_{\text{air}}} \). At equilibrium:

\[ r_{h_{\text{air}}} = r_{h_{\text{soil}}} \]  \[5.4\]

Replacing \( r_{h_{\text{soil}}} \) with Equation 3.32 and solving for soil suction gives

\[ \psi = \frac{R T \rho_w}{W_v} \ln(r_{h_{\text{air}}}) \]  \[5.5\]

where \( R \) is the universal gas constant.

\( T \) is the temperature in K.

\( \rho_w \) is the density of water. and

\( W_v \) is the molecular weight of water

Table 5.1 tabulates the equilibrium surface soil suction with various atmospheric relative humidity for a constant temperature of 30 °C.
Table 5.1  Soil suction at the surface for various values of atmospheric relative humidity at equilibrium (assumed temperature = 30 °C)

<table>
<thead>
<tr>
<th>Air Relative Humidity (%)</th>
<th>Equilibrium Surface Soil Suction (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>99</td>
<td>1430</td>
</tr>
<tr>
<td>90</td>
<td>15,000</td>
</tr>
<tr>
<td>75</td>
<td>41,000</td>
</tr>
<tr>
<td>50</td>
<td>99,000</td>
</tr>
<tr>
<td>25</td>
<td>198,000</td>
</tr>
</tbody>
</table>

During the transient evaporation process, the Dalton equation given in Equation 3.34 can be rearranged to solve for the relative humidity in the soil as given in Equation 5.6.

\[
rh_{\text{soil}} = \left( \frac{E}{f(u)} + P_{\text{v}_{\text{air}}} \right) / P_v, \tag{5.6}\]

where \( E \) is the evaporation rate in units of m/day,

\( f(u) \) is the mixing parameter in units of m/kPa-day, and

\( P_{\text{v}_{\text{air}}} \) is the partial vapor pressure in the air above the soil and is equal to the

\[ rh_{\text{air}} \times P_v, \quad P_v \]

and \( rh_{\text{air}} \) is the air relative humidity.

The soil suction is solved for using Equation 5.6 as shown in Equation 5.7.

\[
\psi = \frac{RT\rho_{\text{w}}}{W_v} \ln \left( \left( \frac{E}{f(u)} + P_{\text{v}_{\text{air}}} \right) / P_v \right) \tag{5.7}\]

Wilson (1990) measured the evaporation rate and temperature at the soil surface for a sand column. Using this data and Equation 5.7, a plot of soil suction versus time at the soil surface is plotted in Figure 5.101. Also plotted on Figure 5.101 is the measured evaporation rate. The soil suction at the surface is initially relatively constant, since the soil is able to provide sufficient moisture from below the soil surface to satisfy evaporative demand. However, at some point, the evaporation rate starts decreasing, because the soil is no longer able to provide sufficient moisture fast enough to the surface. At this point, the surficial soil dries out with a corresponding increase in soil suction.
The movement of water is restricted to the vapor phase, as the permeability in the liquid phase essentially goes to zero, resulting in the first term of the right hand side of Equation 3.30 also going to zero. The vapor phase is not as efficient in distributing moisture to the evaporating front as the liquid phase. At this point, a large soil suction gradient exists between the soil at the surface and soil some distance below the surface.

Figure 5.102 shows a plot of suction versus elevation for various times as generated by SoilCover for Wilson’s (1990) experimental data. Initially, the soil is close to saturation, with low soil suction. As evaporation proceeds, suction in the soil increases as water content decreases. The effect is greatest at the surface, decreasing with depth. The suctions can be seen to vary several orders of magnitude over only a few centimeters of soil depth. The gradients of soil suction head acting in this case are in the order of magnitude of 200,000.

The above discussion shows that difficulties with large gradients of soil suction can be expected in any modelling attempt of evaporation from a soil surface. The SoilCover model is specifically designed for modelling the evaporation process. The SoilCover model uses a dense grid at the soil surface, solves in one-dimension only, and has various checks and balances to aid in modelling the highly non-linear process described above.

Attempts to model evaporation in FlexPDE used the grid shown in Figure 5.103. The discretization near the evaporating surface was fine in an attempt to model the high gradients imposed by evaporation on the soil suction. Boundary conditions at the surface were implemented both as flux boundary conditions and as a value type boundary condition using the soil suctions computed in the above analysis. Furthermore, a variety of values for air relative humidity was used in an attempt to obtain a solution in FlexPDE. In all cases, as soon as the soil surface began to dry, the FlexPDE solution became unstable.
Figure 5.101 Soil suction at surface and evaporation rate with time for the experiment of Wilson (1990)

Figure 5.102 Soil suction versus elevation for various times from the SoilCover model of the experiment of Wilson (1990)
The FlexPDE program then tried to obtain a solution by increasing the number of elements at the surface, or by decreasing the size of the time steps. The efforts ultimately failed to achieve a satisfactory solution. A FlexPDE descriptor file that was attempted is presented in Appendix C as “Two-Dimensional Coupled Heat and Mass Verification Example No. 2”.

Solution of this problem in FlexPDE will require additional efforts. The development of a new formulation of the theory of coupled heat and mass transfer may allow solution of this problem in FlexPDE. These studies were considered to be beyond the scope of this study. This study was intended to implement solution of existing partial differential equations, not to develop new solutions. The involvement of PDE Solutions will also likely be required.

![Figure 5.103 Mesh used in attempted solution of Wilson (1990) evaporation experiment in FlexPDE](image-url)
5.4.2.2 Coupled Heat and Mass Transfer with Freezing

The modelling of coupled heat and mass transfer in soils undergoing freezing was not successfully implemented in the present study. Mathematical descriptions of the coupled heat and mass transfer equation for the freeze-thaw case are not determinant in FlexPDE. The equations used by Harlan (1973) and Jame and Norum (1980) presented in Chapter 3 have three variables, \( T \), \( h \) (sometimes \( \theta_h \)), and \( \theta_i \), but only two equations. The solution method used by Jame and Norum (1980) solved the equations first with the assumption that no moisture redistribution occurred, thereby obtaining a first estimate of the ice content. The equations were then solved again allowing for moisture redistribution using the estimate of ice content obtained.

The equation proposed by Newman (1996) has one variable, \( T \), and one equation. However, Newman (1996) implements this mathematical model in SoilCover by “switching on or off” the equation to be used depending on whether the soil is undergoing freezing or not. This is not possible in FlexPDE. Therefore, new equations must be developed for the implementation of coupled heat and mass transfer undergoing freezing in FlexPDE. This was considered beyond the scope of the present study.

An additional difficulty that is expected to appear is that large gradients will develop in a soil undergoing freezing. As discussed in Chapter 3, if a pressure based (or head based) system of equations is used, the soil suction that will develop in freezing soils will range from 1110 to 2442 kPa/°C. For a soil in which a rapid temperature change is occurring, significant gradients can be expected to be developed, on par with those expected in a soil undergoing atmospheric forcing.
5.5 Comprehensive Pipeline Example Problem

This section shows how the analysis techniques that have been described in this study can be used in practical engineering design and analysis. The problem considered is one of interest as development of oil and gas resources in the Canadian north continues. A hypothetical gas pipeline is to be constructed over discontinuous permafrost. The gas to be transported will be chilled to -2 °C in the pipeline to prevent thawing of permafrost in the continuous permafrost zone. The problem is that in the discontinuous permafrost zone the pipeline will freeze unfrozen soil, potentially resulting in frost heave and damage to the pipeline. The concept behind this problem is similar to the problem analyzed by Coutts and Konrad (1994) as discussed in Section 5.3. The analysis predicts the expected development of a frozen zone of soil around the pipeline using the heat flow equation given in Chapter 3 and used in Section 5.3.

The geometry of the problem considered is given in Figure 5.104. A 0.3 m diameter pipeline is installed in a 0.5 m wide trench with the pipe invert at 0.6 m below ground surface. It is assumed that the trench is cut 0.1 m below the pipe invert. The soil is assumed to be a frost susceptible sandy silt. Material in the trench is assumed to have been disturbed, with a corresponding decrease in the density of the soil.

![Disturbed Soil Diagram](https://example.com/disturbed-soil-diagram.png)

**Figure 5.104** Basic geometry of practical example problem showing pipeline installation and soil zones

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The analysis completed is given in the following steps:

1. Steady state seepage modelling to approximate soil volumetric water content in the soil prior to the initiation of freezing.
2. Steady state heat flow modelling to establish initial conditions prior to operation of the chilled pipeline.
3. Transient heat flow modelling assuming a constant surface temperature.
4. Transient heat flow modelling assuming a variable surface temperature.
5. Parametric study of effects of different soil-freezing curves on the formation of a frozen soil zone.

5.5.1 Seepage Modelling

Steady state modelling of seepage around the pipeline assumes that a constant ground water table is present 1.4 m below the pipe invert or 1.3 m below the bottom of the trench. An upward flux of $5 \times 10^{-9}$ m/s acts at the soil surface, corresponding to a net long-term evaporation rate of 0.8 mm/day. Left and right boundaries and the pipe itself, act as no flow boundaries.

Figure 5.105 shows the soil-water characteristic curves for the soil in the disturbed and undisturbed state. The curves were generated using SoilVision, with estimated soil grain size analyses and other required soil properties (i.e., dry density and porosity). Fredlund and Xing (1994) fits of the soil-water characteristic curves were implemented in FlexPDE in two ways; for the disturbed soil, a fully defined function is used, for the undisturbed soil, a table of values was generated and then imported into FlexPDE using the table function. The permeability functions for the soil in the two states are given in Figure 5.106. The Campbell (1973) function for permeability is assumed to provide a reasonable fit. For the disturbed soil, the Campbell (1973) equation is defined in FlexPDE, and for the undisturbed soil, a table of values generated using the Campbell (1973) equation is imported into FlexPDE.
Figure 5.105  Soil-water characteristic curves used in the seepage portion of the pipeline example problem

Figure 5.106  Permeability functions used in the seepage portion of the pipeline example problem

The analysis was run and the volumetric water contents corresponding to steady state were exported for input into a heat flow analysis. Figure 5.107 shows the volumetric water contents that were determined for the example problem.
5.5.2 **Heat Flow Modelling**

The initial temperature profile in the soil was determined using a steady state analysis assuming a surface temperature of 5 °C and a constant temperature of 2 °C at a depth of 2 m. Volumetric water contents computed in the seepage analysis were used to determine the thermal conductivity, and the volumetric ice content was assumed to be equal to zero.

The determination of the thermal conductivity was obtained through use of the de Vries (1963) formulation. The air phase is neglected. Volumetric specific heat capacity of the soil was determined by the method described by Newman (1996) and discussed in Chapter 3. The soil dry density was assumed to be 1550 kg/m³ for the undisturbed soil and 1450 kg/m³ for the disturbed soil. The soil-freezing curve for the soils were developed using the Fredlund and Xing (1994) fit curve and assuming the shape of the
curve based on similar soils. Figure 5.108 presents the soil-freezing curves used in the analysis for the disturbed and undisturbed soil.

![Soil-freezing curves](image)

Figure 5.108  Soil-freezing curves used in thermal analysis of the pipeline example problem

Figure 5.109 shows the steady state temperatures calculated using this analysis. The temperatures calculated were then input into the transient analysis that was run to simulate conditions after pipeline operation began.

For the first set of transient analyses, a constant surface temperature of 3 °C was assumed, representing an average surface temperature on the pipeline right-of-way through the year. The problem was run for a six month time period. The isotherms produced at time, t, equal to 11.5 days and 6 months are presented in Figures 5.110 and 5.111, respectively. Figure 5.112 plots a history of temperature versus time at six points around the pipeline.

The analysis shows that steady state conditions are reached before 50 days. The resulting frost “bulb” extends well below the pipe. Using this analysis, the amount of ice formation that can be estimated and a corresponding estimate of frost heaving can be calculated.
Figure 10: Initial temperature profile (°C) used as initial condition in transient heat flow analysis of the pipeline example problem.

Figure 11: Temperature profile (°C) for first transient heat flow analysis at time equal to 11.5 days for the pipeline example problem.
Figure 5.111 Isotherms (°C) for first transient heat flow analysis at time equal to 6 months for the pipeline example problem

Figure 5.112 Temperature history at six points for first transient heat flow analysis for the pipeline example problem
For the second transient analysis, a variable surface temperature was used. A sinusoidal function with an amplitude of 5, a period 365 days, with the average surface temperature of 3 °C was used. The problem was run for one year. The analysis considers frost penetration that will occur naturally on a seasonal basis in the soil and more accurately reflects the cumulative effect of frost heaving due to the pipeline and due to normal winter conditions.

Figures 5.113, 5.114, and 5.115 present the isotherms for time, \( t \), equal to 1 month, 6 month and 1 year. Figure 5.116 presents a history plot at six points around the pipeline.
Figure 5.114 Isotherms (°C) for second transient problem, using a variable surface temperature function, at time equal to 6 month for the pipeline example problem.

Figure 5.115 Isotherms (°C) for second transient problem, using a variable surface temperature function, at time equal to 1 year for the pipeline example problem.
Figure 5.116  Temperature histories at six points for second transient heat flow analysis for pipeline example problem

This analysis shows that an assumption of a constant boundary condition will not accurately reflect the condition of the soil in a real environment. Repetitive freeze-thaw cycles in the soil around the pipeline over the course of several years will occur in the soil. However, the soil directly below the pipeline after one year is likely to remain frozen year round as indicated by Figure 5.114. As a result, predictions can be made that the majority of movement of the pipeline will occur in the first year of operation.

5.5.3  Parametric Study for Pipeline Example Problem

For the present study, a brief parametric study of the effect of the soil-freezing curve on the freezing of soil is considered. In FlexPDE it is possible to study every variable, material property, equation, boundary condition, etc., for the effect of changes on the problem solution. This can lead to potentially an infinite number of parametric studies. The soil-freezing curve has been discussed in some detail in previous sections, and a brief study of its effect in the pipeline-freezing problem is considered here.
The problem described in Sections 5.5.1 and 5.5.2 is simplified in the parametric study to assume only one material. The soil-freezing curves and $m'$ functions are fully defined using the Fredlund and Xing (1994) fit function. Furthermore, the initial water content is assumed uniform in the soil. Table 5.2 presents the parameters used in the Fredlund and Xing (1994) fit to the soil-freezing curve for the various curves shown in Figure 5.117. The value of the $a$, $n$, $m$, and $cf$ parameters are given corresponding to the curves in Figure 5.117.

Table 5.2 Curve fit parameters used in parametric study of pipeline example problem

<table>
<thead>
<tr>
<th>Curve No.</th>
<th>a</th>
<th>n</th>
<th>m</th>
<th>cf</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>400</td>
<td>3</td>
<td>1</td>
<td>2.2</td>
</tr>
<tr>
<td>2</td>
<td>400</td>
<td>2</td>
<td>1</td>
<td>2.2</td>
</tr>
<tr>
<td>3</td>
<td>400</td>
<td>4</td>
<td>1</td>
<td>2.2</td>
</tr>
<tr>
<td>4</td>
<td>400</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>1000</td>
<td>3</td>
<td>1</td>
<td>2.2</td>
</tr>
</tbody>
</table>

Figure 5.117 Soil-freezing curves used in parametric study of pipeline example problem
In all cases, the analysis was conducted and the temperature history at a point located horizontally 0.5 m from the pipeline springline (i.e., the point midway between the crown and the invert along the outside of the pipe). The location of this point is slightly outside of the maximum frost “bulb” that develops. Figure 5.118 presents the history at this point for the various curves given in Figure 5.117. The results shown are similar at the point considered, except for the results from curve no. 2. Curve no. 2 was slightly unstable in the solution resulting in a history curve that is significantly different from the others. The reason for the instability can be seen in Figure 5.119, which re-plots Figure 5.117 on a logarithmic scale of temperature in degrees below zero. Curve no. 2 actually has the steepest function at higher temperatures, resulting in higher values of \( m'_2 \). Figure 5.120 plots the \( m'_2 \) function versus temperature for the five curves considered. When freezing starts, FlexPDE is unable to handle the discontinuity of \( m'_2 \) going from 0 to 0.69 that is present in curve no. 2 without some instability. In the case of the other curves, the discontinuity is not as great, allowing FlexPDE to solve the problem with less instability.

![Temperature history graph](Figure 5.118)

Figure 5.118 Temperature history for parametric study of pipeline example problem
Figure 5.119 Logarithmic plot of soil-freezing curves used in parametric study of pipeline example problem

Figure 5.120 $m'_2$ functions for curves used in parametric study of pipeline example problem
Overall, the actual results appear to be insensitive to the soil-freezing curve that is used. It is important to note that the soil-freezing curves that were used in this portion of the study are similar overall (i.e., the range of temperatures covered by the curves is constant). If the curves were extended over a broader range of temperatures, the results would be expected to differ.

Figure 5.121 shows the zone of frozen soil resulting using the different soil-freezing curves at steady state conditions. The result shows that the frozen zones predicted by the different curves are relatively uniform. Curves no. 4 and 5 are similar in shape and produce a similar thaw zone as shown in Figure 5.120. It would be expected that curves 1 and 3 would also produce similar results, but curve 1 produces a larger frozen zone. However, when the results for the FlexPDE model with curve no. 3 were reviewed, instability in the area below the advancing frost front was noted, indicating the results shown are questionable. Curve no.2 is not presented in Figure 5.120 due to the instability discussed above.

Figure 5.121 Location of frozen zone corresponding to soil-freezing curves 1, 3, 4 and 5 calculated by FlexPDE for curves used in parametric study.
CHAPTER 6
SUMMARY OF RESULTS

6.1 General

The objectives originally outlined in Chapter 1 of this thesis involved:

1. Using general partial differential equation solvers in order to solve problems related to seepage in soils in the context of the pipeline industry
2. Using general partial differential equation solvers in order to solve problems related heat flow in soils in the context of the pipeline industry
3. Using general partial differential equation solvers in order to solve problems related two dimensional coupled heat and mass transfer in soils without freezing
4. Using general partial differential equation solvers in order to solve problems related two dimensional coupled heat and mass transfer in soils with freezing
5. Application of above analyses to practical problems

Objectives 1, 2, and 5 have been successful met in the course of the numerical modelling undertaken in this thesis. Objective 3 was partially successful. Objective 4 was not met in the present study.

6.2 Summary of Results with Respect to Thesis Objectives

This section provides a summary of some of the results relevant to the objectives outlined above.

6.2.1 Analysis of Seepage Problems

The seepage modelling performed in this study verified that solutions of partial differential equations obtained using the FlexPDE program are comparable to
established solutions. The results presented in Section 5.1 and Appendix B provide sufficient confidence in the solution accuracy of FlexPDE for seepage problems.

The similarity of the FlexPDE results to the Seep/W results shows that FlexPDE solves the differential equations in a suitable manner. The program Seep/W is widely used in geotechnical practice and has been verified against many known solutions. The results also show that FlexPDE works in fundamentally the same manner as PDEase2D, which Nguyen (1999) used for modelling two-dimensional seepage problems. These results provided confidence to proceed with FlexPDE modelling of other geotechnical phenomena.

A methodology provided in Chapter 5 allows seepage problems with free boundary conditions to be solved with a minimum of user intervention in FlexPDE. The method makes use of the mathematical representation of flux or natural type boundary conditions in FlexPDE to force the specified natural boundary condition to behave as a value boundary condition.

Three-dimensional modelling of steady state seepage through an earth fill dam showed that for problems demanding three-dimensional modelling FlexPDE is a suitable modelling package. Although FlexPDE appears to have promise for use in performing three-dimensional analysis of geotechnical problems, solution times and memory requirements for three-dimensional problems are quite excessive. The three-dimensional seepage problem that was considered was a simple steady state problem with simple boundaries, and isotropic material properties. Increasing the complexity of the problems considered will lead to a corresponding increase in solution time and computer resources.

The seepage problems that were considered in the verification of FlexPDE were not directly related to the pipeline industry. However, as will be discussed in the practical applications below, using FlexPDE is appropriate for problems involving the pipeline industry.
6.2.2 *Analysis of Heat Flow Problems*

Conductive heat flow modelling was successfully implemented in FlexPDE. Steady state and time dependent problems were considered. A three-dimensional steady state problem was also analyzed. The equation solved in FlexPDE for steady state heat flow was the Laplacian equation. The FlexPDE solution compared well with the analytical solutions given by Harlan and Nixon (1978) for the three cases considered in this thesis.

FlexPDE was unable to handle the material non-linearity associated with the solution of the Neumann problem for freeze-thaw analysis. The Neumann solution assumes all phase change occurs at one temperature, implying the \( m'_1 \) term becomes infinitely large. It is necessary in FlexPDE to apply the phase change over a range of temperatures, reducing the value of \( m'_1 \). Solution was achieved in FlexPDE only when the slope of the soil-freezing curve, \( m'_1 \), was decreased to values that realistically reflect the behavior of soil pore-water.

FlexPDE uses a continuously defined function of \( m'_1 \) that is the slope or derivative of the soil-freezing curve. This representation of the soil-freezing curve represents a mathematically correct interpretation of the theory outlined in Chapter 3. Comparison between Temp/W and FlexPDE solutions showed that by defining \( m'_1 \) as a continuous function of temperature accurate results can be obtained without considering effects of temporal discretization on the solution.

The effect of the differences between solutions decreases as the problems approach steady state conditions. The sixth and seventh thermal verification examples show this effect clearly. The Temp/W and FlexPDE results compare better at later time steps, as the effect of \( m'_1 \) on the solution decreases.

Modelling of heat flow processes involving phase change showed that the ability to use a variety of functions for describing material properties can be advantageous over traditional finite element solution for problems which rigidly enforce the definition of
material properties. FlexPDE allows definition of thermal conductivity and volumetric specific heat capacity for any soil water content, ice content, or air content. Temp/W only allows definition of these properties as functions of temperature, resulting in the exclusion of the effects of partial saturation on thermal properties in analyses.

The three-dimensional problem considered showed that a two-dimensional approximation of a tank produced significantly different results. This indicates that two-dimensional solutions are incorrectly predicting the amount of thawing or freezing beneath structures. An axisymmetric solution to this problem was not considered.

The FlexPDE model that was developed for heat flow with freezing-thawing is applicable to analysis of pipelines constructed in temperature sensitive soils. The utility of this model was further demonstrated in the practical problem considered in this thesis.

6.2.3 Analysis of Coupled Heat and Mass Transfer

Coupled heat and mass transfer problems were divided in Chapter 5 into those with small gradients of soil suction, and those with large gradients of soil suction. A solution was obtained to problems with small gradients acting, but solution of problems with large gradients acting was not successful.

In this study, the theory developed by Wilson (1990) was implemented. It is desirable to use the equations proposed by Wilson (1990) directly in the FlexPDE analysis. However, it is necessary to use the form of the equations given by Joshi (1993) to achieve a coupled solution in FlexPDE. The results of the FlexPDE model of a closed system (i.e., small gradients of soil suction are acting) when compared to published results displayed similar behavior. The FlexPDE results were significantly different from the results of Li et al. (1997) to which comparison was made. The reason for this is due to differences in material properties or boundary conditions between the FlexPDE model and the model used by Li et al. (1997).
In the case of large changes in the soil suction resulting from evaporation, solutions failed to converge. The results obtained by Wilson (1990) were used for verification of the model. Attempts were made to force discretization on the system, but no acceptable solution was obtained from this portion of the modelling program.

Coupled heat and mass transfer with freezing or thawing occurring was similarly unsuccessful. No mathematical model is available that could be implemented in FlexPDE directly. In addition, the suctions that develop in a freezing soil are large. It is unknown if the FlexPDE program would be stable under the gradients that would be imposed by the freezing soil.

6.2.4 Practical Applications

The practical problem considered in this thesis is a simple example of how a partial differential equation solver can be used in geotechnical practice. The flexibility of the software makes it attractive for solving problem for which commercial software is not available. The same software package was used in this example to solve seepage and heat flow.

Definition of material properties in two ways was demonstrated in the practical problem. The use of a table of values for definition of material properties was used extensively in all the problems considered in this thesis. Curves can be developed in SoilVision or Excel, and then imported in text file format into FlexPDE. The results using the table function were indistinguishable from results obtained using a fully defined function. The computational savings of using the table function are significant relative to a fully defined function.

Using FlexPDE to first predict the water content of a soil and then to estimate the heat flow properties can be used in practice. Other analyses could be added, such as stress-strain to allow prediction of heave.
CHAPTER 7
CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

Conclusions presented in this chapter are divided into four sections: verification of FlexPDE, thermal modelling in FlexPDE, coupled heat and mass transfer solution using FlexPDE, and application of FlexPDE to problems in geotechnical practice.

7.1.1 Verification of FlexPDE

1. The partial differential equation solver FlexPDE has been verified against well-established numerical solutions for problems of seepage. Comparison against Seep/W results shows close agreement between the solutions. The descriptor files used were those used by Nguyen (1999). These results show that FlexPDE behaves functionally the same as PDEase2D.

2. Three-dimensional models run in FlexPDE appear to provide correct results. Comparison was made with two-dimensional sections. For the two-dimensional sections, the results were similar. Three-dimensional behavior was observed in the three-dimensional structure considered, but no comparison was made with other three-dimensional models. Three-dimensional solution in this thesis was limited to steady state problems with relatively constant material properties.

7.1.2 Heat Flow Modelling in FlexPDE

1. Steady state solutions of heat flow in soils obtained with FlexPDE compare well with the analytical solutions available in the geotechnical literature.
2. The FlexPDE solutions were compared with the analytical solution of the Laplacian equation given by Harlan and Nixon (1978).
4. The FlexPDE solution of transient heat flow in a soil undergoing freezing-thawing correctly modelled the Temp/W results, provided the interpretation of the soil-freezing curve was the same in the two models. The soil-freezing curves used in FlexPDE had to be modified to accurately reflect the Temp/W interpretation of the curve.
5. Continuous definition of the $m'_i$ function in FlexPDE was successful. Defining $m'_i$ as a continuous function is desirable as it accurately represents the behavior of real soils undergoing freezing and thawing.
6. Fit of the soil-freezing curve to the soil-water characteristic curve using the form of the Clayperon equation suggested by Black and Tice (1989) provides suitable estimations of the soil-freezing curve.
7. FlexPDE is unstable if the $m'_i$ curve used is too steep (i.e., $m'_i$ becomes very large). FlexPDE is stable for $m'_i$ curves that reflect real soil behavior. FlexPDE was unable to model the effects of instantaneous phase change, as used in the Neumann solution for freeze-thaw.
8. Three-dimensional solution of a thermal problem of a tank on permafrost showed that the two-dimensional solution over predicts the corresponding depth of thaw.

7.1.3 Using General Partial Differential Equation Solvers for Coupled Heat and Mass Transfer Modelling

1. Solution of coupled heat and mass transfer problems in which the gradients acting in the system are small is feasible in FlexPDE. The work by Ewen and Thomas (1989) modelled in this study displayed coupling of the solution. The FlexPDE model of the system exhibited the same behavior as
the results of Li et al. (1997), but the FlexPDE results were significantly different in the values of temperature and water content calculated.

2. Solution of coupled heat and mass transfer problem in which large gradients are acting was not successful in this study. The current version of FlexPDE is unable to handle the problem. Attempts to model evaporation from a soil column as in Wilson (1990) resulted in program errors as the surface gradient of soil suction became very large. Increased discretization of the system is needed temporally and spatially, but increased solution times made solution attempts impractical.

3. Solution of the equations proposed by Harlan (1973) and Newman (1995) is not possible in FlexPDE. The equations of Harlan (1973) are in terms of three unknowns in two equations, requiring an iterative solution technique. Newman (1995) uses a technique whereby the equation solved for is switched on or off depending on whether the node being solved is undergoing freezing. Neither of these methods can be implemented directly in FlexPDE.

7.1.4 Applying FlexPDE to Practical Problems

1. An example was presented in which a hypothetical soil-freezing problem was considered. The method used showed the flexibility of using a program like FlexPDE for solving a variety of geotechnical phenomena.

2. The ability of FlexPDE to handle a variety of input methods for material properties allows for easy parametric studies. In the present study the effects of the Fredlund and Xing curve fit to the soil-freezing curve were briefly investigated.
7.2 Recommendations

General partial differential equation solvers have been used with some success in research in the geotechnical field.

7.2.1 Recommendations on Use of General Partial Differential Equation Solution Software in Geotechnical Engineering

The following recommendations are made based on the results of the present study:

1. FlexPDE should be adopted as a tool in geotechnical research. The flexibility in implementing material properties, boundary conditions, and equations make it possible to model most geotechnical phenomena with one piece of software.

2. A “front end” should be developed for FlexPDE to simplify creation of descriptor files. The front end would allow inexperienced users of the FlexPDE software to create and run models. The “front end” could involve either the use of computer aided drafting (CAD) software or spreadsheet software that would automate creation of the FlexPDE descriptors. A truly universal front end could be created that when coupled with FlexPDE would allow solution of seepage, heat flow, stress, and contaminant transport problems. Creation of a “front end” would allow adoption of FlexPDE by various engineering agencies.

3. The basic descriptor files for FlexPDE solution of geotechnical problems should be made available in the public domain to increase the use of general partial differential equation solvers in practice. The examples would demonstrate to practicing engineers the utility of this method for solution of geotechnical problems.
7.2.2  Recommendations for Further Study

The following recommendations for further study have developed as a result of the present study:

1. Further study into coupled heat and mass transfer under evaporation conditions should be attempted using FlexPDE. The extremely high gradients that occur at the soil surface during evaporation cause numerical instability when gradients exceed 1,000. Converting the equations of Joshi (1993) into logarithmic forms will reduce the size of the gradients acting, perhaps allowing solution in FlexPDE. Other mathematical fixes may allow the solution of the problem in FlexPDE.

2. Further study should be made into coupled heat and mass transfer with freezing and thawing occurring. Mathematical formulation of determinate equations for the phenomena should be developed.

3. Further examination of the results for the coupled heat and mass transfer presented in this thesis to determine if the results presented are reasonable. It may be necessary to perform a laboratory study of a setup similar to the one described by Ewen and Thomas (1989), with boundary conditions and material properties more precisely defined.

4. Collection of a three-dimensional data set for a problem of seepage should be undertaken to be able to verify the three-dimensional capabilities of FlexPDE.

5. Further study should be undertaken into the relationship between the soil-freezing curve and the soil-water characteristic curve. Very little experimental data is available for comparison of soil-freezing curve prediction based on the soil-water characteristic curve.

6. Research should be conducted into using FlexPDE for frost heave analysis. Suitable equations need definition for the processes of heat and mass flow, and heave of soil due to formation of ice in the soil pores.
LIST OF REFERENCES


Kersten, M.S., 1949. Laboratory research for the determination of the thermal properties of soils. Engineering Experiment Station, University of Minnesota. St. Paul, USA.


SoilCover, 1997. SoilCover User’s Manual Version 4.01. Unsaturated Soils Group, Department of Civil Engineering, University of Saskatchewan, Saskatoon, Canada.


APPENDIX A
INFORMATION ON FLEXPDE VERSION 2.15

A.1 Introduction

This Appendix presents a brief introduction to the computer program, called FlexPDE. The major features of the program are summarized from information presented in the FlexPDE reference manual and from the author’s experience in using the program. This discussion has been adapted from Nguyen (1999) and Vu (1999) who used the program PDEase2D, a similar program, in earlier research conducted at the University of Saskatchewan. Input files are presented to show the main sections and the most common commands used to describe the input for a problem run when using the FlexPDE software. An explanation of each section of the input file is given. Some commands are selected from each section of the input file for more detailed consideration. A comprehensive, hypothetical seepage problem is used to demonstrate the capability of the FlexPDE software.

A.2 Overview of FlexPDE

FlexPDE is a general-purpose computer program that can be used to obtain numerical solutions of many classes of steady-state boundary value problems, time dependent boundary value problems, initial value problems, and eigenvalue problems. FlexPDE can be used to solve two and three-dimensional, steady state problems and two and three-dimensional, time-dependent problems involving heat transfer, solid mechanics, reaction/diffusion, fluid mechanics, electromagnetics, groundwater flow, quantum mechanics and field problem from other fields of science and engineering.

FlexPDE is a highly automated finite element analysis solver. The user specifies the equations to be solved, the region to be considered, the boundary conditions, and the
material properties. The software automatically generates the element grid, then refines the mesh to meet error tolerances, uses non-linear solution methods as needed, and adaptively selects time steps in transient problems.

Version 2.15 of FlexPDE was released in December 1999. FlexPDE is a continually evolving product, additional releases with added features, bug fixes, and modifications are released approximately every 3-6 months.

A.3 About the Developer

PDE Solutions Inc. was founded in 1992. PDE Solutions Inc. develops and markets FlexPDE finite element analysis software. The company was formed by the former staff of SPDE Inc., the developers of the PDEase software.

    PDE Solution Inc.
    2120 Spruce Way
    Antioch, CA 94509
    Voice: (925) 776-2407
    Fax: (925) 776-2406
    URL: http://www.pdesolutions.com

A.4 Principal Features of FlexPDE

The principal features of FlexPDE are listed below:

- **Language-based problem specification**: FlexPDE command script can be prepared with any standard ASCII text editor.

- **Powerful finite element spatial dependence solver**: FlexPDE uses the finite element method. FlexPDE divides the domain into triangles, or prisms of triangular cross-section. The variables are represented by simple polynomials over the domain. The program solves partial differential equations by
determining the values of the dependent variables at discrete nodes. (i.e., at the corners of the triangles and at the midpoints between corners). If a sufficiently fine grid and a high order of polynomial are used, a solution can be found within specified error limit. This method ensures highly accurate results and rapid convergence.

• **Fully automated adaptive grid refinement:** One of the difficult tasks in implementing the finite element method is the design of the mesh. FlexPDE solves this problem by starting with a coarse grid of triangular elements. FlexPDE then uses an interactive process to refine the grid to suit the problem. When each iteration is completed, FlexPDE determines the error in each element and subdivides only those elements, where the error exceeds the default or user specified error limit. After subdividing, recalculation is fast because of the reasonable starting estimate provided by the previous iteration.

• **Powerful evolution time dependence solver:** Evolution solvers are used to break continuous time dependent boundary/initial value problems into discrete time intervals that can be solved using the finite element method.

• **Fully automatic time step refinement:** The FlexPDE evolution solver automatically and continuously adjusts its time step interval. When FlexPDE encounters a region of rapid change, it reduces the time interval and it increases the time step interval when it encounters a region of slow change. This automatic refining of the time step interval provides maximum accuracy for a minimum number of time steps.

• **Support for both value and natural boundary conditions:** FlexPDE supports both value and natural boundary conditions. It correctly interprets the natural boundary condition for equations written as the divergence of a vector, (i.e., \( \text{Div}(D) + s = 0 \)), as the dot product of the outward directed normal, and the vector D. FlexPDE correctly interprets the natural boundary condition for
equations written as the curl of a vector, i.e., $\text{Curl}(h) - j = 0$, as the cross product of the outward directed normal and the vector.

- **Automatic handling of internal boundary conditions in multi-region problems**: When solving multi region problem, FlexPDE guarantees that problems expressed in divergence form or curl form are continuous at the region interfaces of both the normal component of flux density and the tangential component of the field intensity.

- **Eigenvalue “modal” analysis**: Using the “subspace interaction” method to reduce the number of degrees of freedom, FlexPDE can calculate and list a user-selected number of the smallest eigenvalues of specified linear systems.

- **Non-analytic data import and export**: FlexPDE’s table function allows the software to import and export numerical data in ASCII format. This feature can be used to import numerical data from programs that gather experimental data or to export data for special post processing.

- **Automatic or user-controlled solution flow**: FlexPDE solves most linear and non-linear problems automatically using built-in default selectors to control the internal flow of the solution. For particularly difficult problems, over twenty built-in selectors may be used to improve problem convergence.

- **Graphic output viewing and recall**: FlexPDE produces a series of output graphics, in a variety of forms, such as contours, histories, and elevation plots. Export of data in ASCII and netCDF format are included.

- **Hardcopy using Windows**: Windows printers can be used as its hardcopy device.
• **Data import of region geometry and boundary conditions in DXF format:**
DXF (AutoCAD) formatted files can be imported to describe boundary geometry.

• **Three-dimensional modelling:** FlexPDE allows specification of three-dimensional geometries based on the concept of layered extrusion. The object is first projected on the x-y plane with all dividing boundaries of the three dimensional figure. The object is extruded in the z dimension and the extrusion divided into layers.

### A.5 Skeleton of a Descriptor

Each problem descriptor file is divided into sections. Each one describes a different type of information that is needed to specify the problem. Each section is composed of a series of statements. The order of various sections and their most common commands are illustrated in Figure A.1.

Except the `BOUNDARIES` and `END` sections, the use of any particular section in a problem descriptor file is optional. All the problem descriptor files must contain at least a `BOUNDARIES` section and an `END` section.

```
TITLE
  '..........'  (User's comments)

SELECT
  errlim =    gridlimit =
  converge =  subconverge =
  contours =  surfacegrid =
  vectorgrid =

COORDINATES
  cartesian
  cartesian3

VARIABLES
  temp  (range = . )

DEFINITIONS
  lamb =    vshc =
  heater=0.001*t-0.002*t^2
```
Figure A.1   Skeleton of a FlexPDE descriptor file

A.6   Input Language of FlexPDE

A skeleton of the problem descriptor file is presented above. The demonstration or explanation of each section and their command is presented in the FlexPDE Reference Manual. However, some of the commands are considered in detail here.

TITLE
This section contains text title to identify the problem in output files and plots.

SELECT
This section can be used for setting certain parameters, which control the detailed operation of FlexPDE.
The statement, \( errlim = 1e-4 \) means that we desire that the average relative error of the solution to be less than 1 part in 10,000. FlexPDE solves a system of algebraic equations by successive approximation. The above command specifies the accuracy that must be reached in this process before any refinement of the grid is allowed. The command \( nodelimit = 1000 \) limits the number of nodes at approximately 1000, which is helpful to avoid overflow.

There are several commands that can be used to control plotting options. The statement \( contours = 5 \) means that 5 contour curves are requested over the problem domain. FlexPDE offer a similar command for vector plots. The number of arrows can be controlled by \( vectorgrid = 20 \), which yields 20x20 arrows in total over the domain.

**COORDINATES**
This section allows the user to select the coordinate system used to define the problem. FlexPDE accepts two and three-dimensional Cartesian coordinate systems as well as cylindrical coordinate systems.

**VARIABLES**
The names given to the dependent variables are listed in this section. For instance, temperature \( temp \) in thermal analysis or total head \( h \) in seepage analysis, are dependent variables. In the case of transient problems, a range of variations for the dependent variable can be declared (e.g., \( temp \ (range = -10, 10) \)).

**DEFINITIONS**
Geometrical dimensions and material properties are declared in this section. For example, \( lamb = 0.2e-6 \) and \( vshc = 3e-6 \) specify the value of thermal conductivity and volumetric specific heat capacity respectively. If the descriptor file contains more than one region, the material properties could be specified for each one of these regions in the **BOUNDARIES** section. This can be done if the parameter is declared in the **DEFINITIONS** section (e.g., \( lamb \) and \( vshc \), without a value or expression following).
Various functions of the parameters, of the independent variables \( x, y \) and \( t \), as well as the dependent variables, can be defined in this section.

The arithmetic rules are close to those of FORTRAN, and the internal functions are also similar, for example, \( SQRT() \), \( EXP() \), \( SIN() \), \( COS() \)...

**INITIAL VALUES**

For steady state problems, initial values are not always required. The time needed to execute an analysis can be significantly reduced if the order of magnitude of the solution variable is specified. If a problem is highly non-linear, it might even be necessary to supply a function that is approximate to the solution. If no initial value is specified, FlexPDE uses zero as the first approximation of the dependent variables.

For transient problem, the initial value (or function) is part of the problem definition and must always be specified as exact values.

**EQUATIONS**

FlexPDE has a unique feature that allows the user to enter a partial differential equation (PDE), or a system of partial differential equations (PDE's), using ordinary characters. The software then interprets the partial differential equations and adapts the algorithm to the problem.

A PDE consists of functions and derivatives, expressing some relationships pertinent to the physical problem. For example, the following equation expresses the conservation of energy for a soil mass in one dimension:

\[
dx[lamb*(dx(temp))] + s = vshe*dt(temp)\]

There must be as many equations as there are the dependent variables. The equations must appear in a certain order, related to the nature of the problem and the list of dependent variables.
CONSTRAINTS
This section allows expression of the conservation of mass or energy in an integral form over the domain. Use of this heading has not been required in development of solutions to geotechnical engineering problems.

EXTRUSION
The EXTRUSION section is used in three-dimensional problem for defining layers in the third or z-dimension. The extrusion into the z-dimension is accomplished by defining surface and layers that exist between the surfaces. The bottom surface is specified using the surface “surface1” z=0 statement. A boundary condition can be applied to this statement if required. Between two surfaces is a layer defined by the command layer “layer1”. Material properties can be specified after the layer command for the material between surface 1 and surface 2. Figure A.2 shows diagrammatically the differences between layers and surfaces.

Figure A.2 Conceptual extrusion in three dimensions

BOUNDARIES
This section specifies the geometry of the object and the conditions on its boundaries. It may also contain expressions for material properties. The declaration of the main boundary begins with region 1, which has a different status than any following regions of higher number. This first region defines the total extent of the object, and the following regions (if any) are sub-domains of the first region.
Region 1 covers the entire space interior to the object under study. The outside world imposes various conditions on the boundary of the subject. Therefore, region 1 not only specifies the geometry but also specifies the boundary conditions of the problem. A typical clause for the main region can be written as follows:

\begin{verbatim}
Region 1   lamb=vshc=
  start(0,0)
  value(temp) = 5    line to (0,-10)
  value(temp) = 0    line to (40,-10)
  value(temp) = 0    line to (40,0)
  natural(temp) = 0  line to (30,0)
  natural(temp)=heater line to finish
\end{verbatim}

The first line in the above table contains the values for thermal conductivity and volumetric specific heat capacity defined for region 1. These values can also be specified in the DEFINITIONS section. After giving the start coordinates \((x,y)\), the statements \(\text{value}(\text{temp}) = 5\) specifies a constant temperature along the boundary. The \(\text{natural}(\text{temp}) = 0\) specified on the segment \((40,0)\) to \((30,0)\) means that there is no change in the dependent variable \text{temp} across the boundary (i.e., no heat flow across the boundary). The boundary \(\text{natural}(\text{temp}) = \text{heater}\) means that the heat flux across the boundary is equal the variable \text{heater} which is defined in the DEFINITIONS section. The keyword \text{finish} is necessary to indicate that the polygon is finished. The term \text{finish} is equivalent to the coordinate pair of the start point.

The boundary must be specified around the object in the positive sense (i.e., counterclockwise). If a hole in the object need to be cut out, the boundary must be specify in the positive sense.

There are three different statements for the boundary conditions; namely, \(\text{value()}\), \(\text{natural()}\) (or \text{load()} and \text{point value()}). The last statement is useful for anchoring the solution at a single point.

For region 2 and higher, which are sub-domains of the main region, the same rule can be used to draw the boundaries. The essential purpose of these secondary regions is to
specify new material properties. Material property values usually already exist for the main region, but new properties specified for a sub-region will over-write the global ones. In this way, the material property data is entered for all the parts of the object under study.

In specification of three-dimensional problems, an additional instruction must be provided such that the program knows to which extruded layer a region belongs to, such that the above statement will become:

```
Region 1
Layer "layer1"
lamb = vshc =
start(0,0)
value(temp) = 5...
```

Regions can be specified to contain multiple layers, with different material properties for each layer.

**MONITORS**

This section may contain various plot commands. These commands are identical to those described in the PLOTS section. The difference is that these plots are not stored but only appear on the screen. The main purpose of the monitors is to let the user observe how the calculations are proceeding. In particular, the monitors monitor how much change there is from one gridding to the next. This is particularly useful when solving non-linear problems. Monitors can also be used to control the time increments used by FlexPDE. The program is forced to solve the systems of equations for the time specified.

**PLOTS**

There are five different types of graphical display implemented in FlexPDE. The graphical displays are grid (x,y), contour (), surface (), vector () and elevation (). The statement grid (x,y) shows the latest grid. The two arguments need not simply be x and y, but can by any function of the variables declared. The statement grid (x+10*u,
\( y + 10^3 y \) displays the deformation of a strained object, exaggerated by a factor of 10. The statement \( \text{grid}(x,y,z) \) produces a three-dimensional plot of the computation grid that can be manipulated in three dimensions to produce the desired view. The \( \text{contour}(u) \) and \( \text{surface}(u) \) types of plots allow the visualization of a three-dimensional surface. A \( \text{contour}(u) \) statement shows the curves of intersection between the surface \( u(x,y) \) and a number of planes of constant \( u \). A \( \text{surface} \) plot displays the surface in perspective. Both the \( \text{contour} \) and \( \text{surface} \) plots also supply the integral of the surface, i.e., the volume between the surface and the \( x, y \) plane.

The command \( \text{vector}(j_x, j_y) \) displays a set of arrows indicating the direction of a field, the length of the arrows being related to (but not proportional to) the magnitude.

After any of the four above plots, a \( \text{zoom} \) command can be added to enlarge part of it (e.g., \( \text{contour}(u) \) \( \text{zoom}(20,-5,10,5) \)) positioning the lower left corner of the viewing window by the first two coordinates and giving the window size by the width and the height.

The last statement, the \( \text{elevation} \) plot shows only a curve along the surface, taken vertically above a specified, straight line in the \( x, y \) plane. An example of this type of plot is \( \text{elevation}(v) \text{from}(0,0) \text{to}(30,0) \). The second coordinate pair should have larger coordinate values. The value of the integral of the curve (i.e., the area between the curve and the line defined in the command) is also obtained from the \( \text{elevation} \) statement.

In transient problems, several fields at given values of the time may be plotted. For example, the statement \( \text{for } t = 1, 10, 100 \text{ contour(temp) surface(temp)} \) yields three snapshots, each in the form of two plots.

**HISTORIES**

As an alternative to plots at specific times, the evolution of a variable with time at given points in space can be followed. This give rise to number of curves, and a statement, for instance, could be written as, \( \text{history(temp) at}(5,0) \text{ at}(5,-5) \text{ at}(5,-10) \). This statement
will produce a plot of temp versus time at the specified points. The display is updated at the same time that specified monitors or plots are produced.

A.7 Comprehensive Example

The following example goes through in detail how a problem can be developed in FlexPDE. It attempts to show the steps that need to be taken to solve problems in FlexPDE. The basic steps are analogous to the steps used in solving any problem in engineering:

1. Define the problem boundaries
2. Define the equation to be solved
3. Define the known values (material properties)
4. Define the outputs required
5. Solve the problem

Problem Definition

The problem considered is another of the examples that was verified by Nguyen (1999). Steady state modelling of seepage through an earth fill dam with a low permeability core is to be analyzed.

Definition of Problem Boundaries

The problem geometry is shown in Figure A.3

Figure A.3 Problem geometry and boundary conditions for comprehensive example
Using the FlexPDE convention for describing problem geometry, region 1 is first defined, consisting of the outer boundaries of the earth fill dam. Starting at the left most lowest point in the problem and moving in a counter clockwise direction, the boundary is specified as shown below.

| BOUNDARIES |
| region 1 |
| start (-26,0) |
| line to (14,0) |
| line to (26,0) |
| line to (2,12) |
| line to (-2,12) |
| line to (-6,10) |
| line to finish |

Figure A.4 Definition of outer boundary of system for comprehensive example

Next, boundary conditions need to be applied to the outer boundary of the system. Referring to Figure A.3, from (-26,0) to (14,0) a no flow boundary exists, i.e., \( natural(h) = 0 \). From (14,0) to (26,0) is the toe drain, which can be represented as a \( value(h) = 0 \) boundary, meaning the head is constant and equal to zero. The segments (26,0) to (2,12), (2,12) to (-2,12), and (-2,12) to (-6,10) all have zero flux boundary conditions. Finally, the segment form (-6,10) to (-26,0) represents the lagoon acting on the dam with a constant head of 10 m. Modifying the Figure A.4 to account for these boundary conditions, results in the description given in Figure A.5.

| BOUNDARIES |
| region 1 |
| start (-26,0) | \( natural(h) = 0 \) |
| line to (14,0) | \( value(h) = 0 \) |
| line to (26,0) | \( natural(h) = 0 \) |
| line to (2,12) | \( natural(h) = 0 \) |
| line to (-2,12) | \( natural(h) = 0 \) |
| line to (-6,10) | \( value(h) = 10 \) |
| line to finish |
After the outer boundaries of the system have been defined, the boundaries of the low permeability cutoff are entered. Note that no boundary conditions need to be specified as the cutoff is entirely internal to the area defined by region 1 above.

![Figure A.5](image)

The system boundaries have been completely defined, with the appropriate boundary conditions applied.

**Definition of Equations to be Solved**

The governing equation for seepage in two-dimensions can be stated as:

$$
\frac{\partial}{\partial x}\left(k_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial h}{\partial y}\right) = m^2 \gamma_w \frac{\partial h}{\partial t} 
$$

where $x, y$ are coordinates in Cartesian format,

- $k_x, k_y$ are the coefficients of permeability in $x, y$ and $z$ directions respectively,
- $h$ is the hydraulic head, i.e. $h = u/\gamma_w + y$,
- $u$ is the pore water pressure,
- $\gamma_w$ is the unit weight of water,
- $m^2$ is the slope of the soil water characteristic curve, and
- $t$ is time.

Equation A.1 can be rewritten in FlexPDE format as:

$$
\frac{dx(k_x * dx(h)) + dy(k_y * dy(h)) + dz(k_z * dz(h)) + s = m^2 w * u * w * w * dt(h)}
$$

where $s$ is a source/sink term that may or may not be required depending on the problem analyzed.
For the case where \( k_x = k_y \), Equation A.2 can be rewritten as:

\[
\text{div}(k \cdot \text{grad}(h)) + s = m2w \cdot uww \cdot dt(h)
\]  \[\text{[A.3]}\]

If the problem is to be analyzed using steady state conditions, the right hand side of Equation A.3 can be set equal to zero, such that:

\[
\text{div}(k \cdot \text{grad}(h)) + s = 0
\]  \[\text{[A.4]}\]

Equation A.4 is entered in the problem descriptor as shown below. The variable that is being solved for, \( h \), is entered in the variables section as shown.

**VARIABLES**

\[
\begin{align*}
  h & \quad \{\text{definition of dependent variable}\} \\
\end{align*}
\]

**EQUATIONS**

\[
\text{div}(k \cdot \text{grad}(h)) + s = 0
\]

Figure A.7  Equation for comprehensive example problem

**Definition of Known Values**

It is now necessary to define the required material properties for solution of this problem. As can be seen from Equation A.4, only the permeability function needs to be defined. The Brooks and Corey (1964) permeability function is used to define the permeability in the present problem. The Brooks and Corey (1964) function can be defined in FlexPDE terms as:

\[
k = \text{if } u > = \text{ub then } ksat \text{ else } ksat \cdot (u/\text{ub})^{(-n)}
\]  \[\text{[A.5]}\]

where

- \( k \) is the permeability at any water pressure,
- \( u \) is the pore water pressure, \( u = (h-v) \cdot uww \),
- \( uww \) is the unit weight of water,
- \( \text{ub} \) is the air entry value,
- \( ksat \) is the saturated permeability, and
- \( n \) is an empirical coefficient.
The common fill for the earth fill dam is assumed to be a silty sand, with a saturated coefficient of permeability of 1e-6 m/s and a air entry suction value of 10 kPa. The low permeability core is assumed to have a saturated coefficient of permeability of 1e-8 m/s and a air entry suction value of 110 kPa. The permeability functions are shown in Figure A.8, assuming the $n$ parameter in the Brooks and Corey (1964) function is set equal to 2.

![Figure A.8 Permeability functions used in comprehensive example problem](image-url)
Equation A.6 and the related definitions needed for defining the permeability function are entered into the definitions section as shown in Figure A.9.

DEFINITIONS

{definition of pressure as a function of head}
\[ u_{ww} = 9.81 \quad \text{(unit weight of water, kN/m}^3\text{)} \]
\[ u = (h-y) * u_{ww} \]

{definition of k function}
\[ k_{sat 1} = 1e-6 \quad \text{[m/s]} \]
\[ k_{sat 2} = 1e-8 \quad \text{[m/s]} \]
\[ k_{sat} \quad \text{(used to define ksat in each of the soil types)} \]
\[ u_{b 1} = -10 \quad \text{[kPa]} \]
\[ u_{b 2} = -50 \quad \text{[kPa]} \]
\[ u_{b} \quad \text{(used to define ub in each of the soil types)} \]
\[ n = 2 \]
\[ k = \text{if } u \geq u_{b} \text{ then } k_{sat} \text{ else } k_{sat} * (u/u_{b})^{(-n)} \]

Figure A.9 Definitions section for comprehensive example problem

The boundaries section needs to be modified to include the material properties that have been specified for each region, as shown in Figure A.10.

BOUNDARIES

region 1
\[ k_{sat} = k_{sat 1} \]
\[ u_{b} = u_{b 1} \]
\[ \text{start } (-26,0) \quad \text{natural}(h) = 0 \]
\[ \text{line to } (14,0) \quad \text{value}(h) = 0 \]
\[ \text{line to } (26,0) \quad \text{natural}(h) = 0 \]
\[ \text{line to } (2,12) \quad \text{natural}(h) = 0 \]
\[ \text{line to } (-2,12) \quad \text{natural}(h) = 0 \]
\[ \text{line to } (-6,10) \quad \text{value}(h) = 10 \]
\[ \text{line to finish} \]

region 2
\[ k_{sat} = k_{sat 2} \]
\[ u_{b} = u_{b 2} \]
\[ \text{start } (-2,0) \]
\[ \text{line to } (2,0) \]
\[ \text{line to } (2,10) \]
\[ \text{line to } (-2,10) \]
\[ \text{line to finish} \]

Figure A.10 Complete boundaries section with material properties specified
Define Required Outputs

Three types of outputs are available in FlexPDE; plots, monitors, and histories. The present problem is not a time dependent problem, so no histories can be produced. Monitors can be useful in steady state problems to monitor the results at each re-grid that is performed by the program. Plots are what the program saves at the end of the run.

The outputs of interest in the present simulation are the pore pressure distribution, the head distribution, and the velocity vectors. Contour plots of the head and pressure are specified along with a vector plot of the gradient of \((h \times k)\), representing the velocity of flow of water in the soil. A grid plot is specified as well, which produces a plot of the solution mesh that was generated by FlexPDE.

<table>
<thead>
<tr>
<th>MONITORS</th>
</tr>
</thead>
<tbody>
<tr>
<td>contour(u)</td>
</tr>
<tr>
<td>contour(h)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PLOTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>contour(u) as 'Pore Water Pressure'</td>
</tr>
<tr>
<td>contour(h) as 'Total Head'</td>
</tr>
<tr>
<td>vector(-dx(h)*k,-dy(h)*k) as 'Velocity Vectors'</td>
</tr>
<tr>
<td>grid (x,y) as 'Grid'</td>
</tr>
</tbody>
</table>

Figure A.11 Monitors and plots for comprehensive example problem

Solution of the Problem

The remaining step is to combine all the sections described above and solve the problem. Title and Select sections are added. The Title section simply provides a title that will appear on all the plots and monitors produced. The Select section is used to specify the number of contours on plots, density of the vector grid, and the error to which the program solves the problem. The End statement is place at the end of the descriptor to alert the program that the descriptor is finished. The Initial Values section is used in the present problem to help the convergence of the problem. In this example,
an initial head of 10 m is specified throughout the dam. If no initial value is specified, accurate solution of the problem may not be obtained.

The completed problem descriptor is shown in Figure A.12.

<table>
<thead>
<tr>
<th>TITLE</th>
<th>'Flow through an earth fill dam with low k cutoff'</th>
</tr>
</thead>
<tbody>
<tr>
<td>SELECT</td>
<td>contours = 10</td>
</tr>
<tr>
<td></td>
<td>vectorgrid = 20</td>
</tr>
<tr>
<td></td>
<td>errlim = 0.001</td>
</tr>
<tr>
<td>VARIABLES</td>
<td>h {definition of dependent variable}</td>
</tr>
<tr>
<td>DEFINITIONS</td>
<td>{definition of pressure as a function of head}</td>
</tr>
<tr>
<td></td>
<td>uww = 9.81 {unit weight of water, kN/m^3}</td>
</tr>
<tr>
<td></td>
<td>u = (h-y)*uww</td>
</tr>
<tr>
<td></td>
<td>{definition of k function}</td>
</tr>
<tr>
<td></td>
<td>ksati = 1e-6 {m/s}</td>
</tr>
<tr>
<td></td>
<td>ksat2 = 1e-8 {m/s}</td>
</tr>
<tr>
<td></td>
<td>ksat {used to define ksat in each of the soil types}</td>
</tr>
<tr>
<td></td>
<td>ub1 = -10 {kPa}</td>
</tr>
<tr>
<td></td>
<td>ub2 = -50 {kPa}</td>
</tr>
<tr>
<td></td>
<td>ub {used to define ub in each of the soil types}</td>
</tr>
<tr>
<td></td>
<td>n = 2</td>
</tr>
<tr>
<td></td>
<td>k = if u&gt;= ub then ksat else ksat*(u/ub)^(-n)</td>
</tr>
<tr>
<td>INITIAL VALUES</td>
<td>h = 10</td>
</tr>
<tr>
<td>EQUATIONS</td>
<td>div(k*grad(h)) + s = 0</td>
</tr>
<tr>
<td>BOUNDARIES</td>
<td>region 1</td>
</tr>
<tr>
<td></td>
<td>ksat = ksati</td>
</tr>
<tr>
<td></td>
<td>ub = ub1</td>
</tr>
<tr>
<td></td>
<td>start (-26,0) natural(h)=0</td>
</tr>
<tr>
<td></td>
<td>line to (14,0) value(h)=0</td>
</tr>
<tr>
<td></td>
<td>line to (26,0) natural(h)=0</td>
</tr>
<tr>
<td></td>
<td>line to (2.12) natural(h)=0</td>
</tr>
</tbody>
</table>
Figure A.12 Complete descriptor for comprehensive example problem

Figures A.13 and A.14 provide the plots of head and pressure contours produced by FlexPDE for the descriptor given in Figure A.12. Figure A.15 plots the vector plot produced by FlexPDE. Figure A.16 shows the solution grid that FlexPDE generated for solution of this problem.
Flow through an earth fill dam with low k cutoff

**Figure A.13** FlexPDE output of hydraulic head contours for comprehensive example problem

Flow through an earth fill dam with low k cutoff

**Figure A.14** FlexPDE output of pressure contours for comprehensive example problem
Flow through an earth fill dam with low k cutoff

Figure A.15  FlexPDE output of velocity vectors for comprehensive example problem

Figure A.16  FlexPDE output of grid generated for comprehensive example problem
APPENDIX B
VERIFICATION OF FLEXPDE
FOR SEEPAGE ANALYSIS

B.1 Introduction

As stated in the body of this thesis, seepage analysis using a general partial differential equation solver has been studied extensively by Nguyen (1999). Nguyen (1999) used the program PDEase2D in performing analysis of various seepage problems. PDEase2D is a program similar to, but not identical to, FlexPDE which has been used in the verification examples discussed in this thesis. Descriptor files for all problems in FlexPDE format can be found in Appendix C.

B.2 Steady State Seepage Problems

Results from two steady state seepage problems are presented in this section.

Seepage Verification Example No. B1

The first seepage example is the steady state case of seepage around a cutoff beneath a concrete gravity dam. Heads are specified on the upstream and downstream soil surface of 60 ft and 40 ft respectively. Zero flow boundary conditions are specified at zero elevation, and along vertical boundaries set sufficiently far from the structure. Figure B.1 shows the extended solution grid created by FlexPDE. Figure B.2 shows the area that is analyzed by Seep/W with the FlexPDE solution grid superimposed, also shown are the specified boundary conditions.

The solutions obtained by FlexPDE compare favorably with the Seep/W results. Figure B.3 shows the computed head contours determined using FlexPDE and Seep/W. The
results also compare favorably with the results obtained by Nguyen (1999). Figure B.4 show the pressures computed by the two programs in pounds per square foot. Again, excellent agreement is obtained between the two solution methods. Finally, Figure B.5 and B.6 compare the velocity vectors that are computed by the two solution methods.

Figure B.1  Extended solution grid created by FlexPDE for seepage verification example no. B1

Figure B.2  Close up of solution grid created by FlexPDE for verification example no. B1 with boundary conditions shown
Figure B.3  Comparison of computed head contours for verification example no. B1 (Seep/W results in black, FlexPDE in color)

Figure B.4  Comparison of computed pressure (psf) contours for verification example no. B1
Figure B.5  Velocity vectors for verification example no. B1 as generated by FlexPDE

Figure B.6  Velocity vectors for verification example no. B1 as generated by Seep/W
Seepage Verification Example No. B2

The second steady state seepage verification example is the case of seepage through an earth fill dam with a toe drain on the downstream side. Figure B.7 gives the permeability function assumed for the two materials (i.e., toe drain and dam). The geometry of the problem, and the solution grid generated by FlexPDE are given in figure B.8. The head on the upstream side of the dam is assumed to be 10 m. Zero flux is specified on the bottom and downstream face of the dam. A zero head boundary is applied to the bottom of the toe drain.

The solutions obtained by FlexPDE and Seep/W are virtually identical. Figure B.9 shows the head contours calculated by the two programs. Figure B.10 compares the pressure contours generated by the two programs. Figures B.11 and B.12 show the velocity vectors computed by FlexPDE and Seep/W respectively. The results match extremely closely for all cases, also the results are close to those obtained by Nguyen (1999).

![Figure B.7](image)

Figure B.7  Hydraulic conductivity functions used in verification example no. B2
Figure B.8  Computation grid generated by FlexPDE for verification example no. B2

Figure B.9  Comparison of computed head contours for verification example no. B2 (Seep/W results in black, FlexPDE results in color)

Figure B.10  Comparison of computed pressure contours for verification example no. B2
B.3 Transient Seepage Problem

One transient seepage example problem is included in the main body of this thesis. This section provides a second example for thoroughness.

Seepage Verification Example No. B3

The third seepage verification example is the transient problem of seepage from a lagoon over time. The lagoon is lined with a lower permeability material than the surrounding soil. Figure B.13 shows the permeability functions that were used in this
analysis. The value of $m_s^\infty$, the slope of the soil water characteristic curve, was assumed to be constant at 0.002 $1/kPa$. Figure B.14 shows the problem geometry and boundary conditions used. The soil is assumed to have a constant head of 5 m prior to filling of the lagoon. After filling, the head acting on the liner is 11 m. Figure B.15 shows the computation grid that FlexPDE generated the last time step of the problem. It is important to note that FlexPDE generates new computation meshes as necessary to achieve the specified error; therefore, more than one mesh will generally be used in the solution of a transient problem.

Figures B.16 through B.20 compare the heads computed at various time steps by Seep/W and FlexPDE. Very good agreement is seen at early time steps, and again at later time steps when the problem approaches steady state conditions. However, at mid range times steps, such as 127 hr as shown in Figure B.19, there appears to be large differences in head values even though the trends observed are similar. This is not of too great a concern, when it is considered that the actually differences in head at any given point between the two methods is 0.1 m. These results as observed in using FlexPDE and Seep/W were also seen by Nguyen (1999) in comparing PDEase2D with Seep/W.

Figures B.21 and B.22 compare the location of the phreatic surface beneath the lagoon over the course of time as determined in Seep/W and FlexPDE respectively. The results agree well with each other and show the expected behavior of the water table rising with time due to seepage from the lagoon.
Figure B.13  Hydraulic conductivity functions used in verification example no. B3

Figure B.14  Problem definition for verification example no. B3 lagoon filling, with initial constant hydraulic head of 5 m in soil
Figure B.15  Computation grid generated by FlexPDE for verification example no. B3

Figure B.16  Comparison of computed heads for verification example no. B3
time step 7 hr (Seep/W results in black, FlexPDE results in color)
Figure B.17  Comparison of computed heads for verification example no. B3
time step 15 hr (Seep/W results in black, FlexPDE results in color)

Figure B.18  Comparison of computed heads for verification example no. B3
time step 31 hr (Seep/W results in black, FlexPDE results in color)
Figure B.19  Comparison of computed heads for verification example no. B3
time step 1023 (Seep/W results in black, FlexPDE results in color)

Figure B.20  Comparison of computed heads for verification example no. B3
time step 1023 (Seep/W results in black, FlexPDE results in color)
Figure B.21  Zero pore water pressure lines generated by Seep/W for verification example no. B3 time steps 0 to 1023

Figure B.22  Zero pore water pressure lines generated by FlexPDE for verification example no. B3 time steps 0 to 1023
B.4 Implication

The implication from this review of the research of Nguyen (1999) using FlexPDE is that FlexPDE and PDEase2D will produce essentially the same results. This is the result that would be expected given the genesis of the two programs. The results summarized in this appendix provide sufficient confidence for the use of FlexPDE in solving additional problems in geotechnical engineering.
Seepage Verification Example No. B1

TITLE
'S.S. Seepage around dam cutoff'

SELECT
errlim=0.01
contours=10
vectorgrid=20

VARIABLES
h

DEFINITIONS
k=1e-3
s=0

EQUATIONS
div(k*grad(h))+s=0

BOUNDARIES
region 1
natural(h)=0
start (0, 0)
line to (150,0) to (300,0)
value(h)=40
line to (300,40) to (150,40)
value(h)=40
line to (105,40)
natural(h)=0
line to (105, 35) to (45.5, 35) to (45.5, 20) to (45, 20) to (45,40)
value(h)=60
line to (0,40) to (-150,40) to (-150,0)
natural(h)=0
line to finish
PLOTS
  grid(x,y)
  contour(h)
  grid(x,y) zoom (0.0,150,40)
  contour(h) zoom (0.0,150,150) as 'Total Head'
  vector(-dx(h)*k,-dy(h)*k) zoom (0.0,150,150) as 'Velocity Vectors'

END

Seepage Verification Example No. B2

TITLE
  'S.S. Seepage through an earthfill dam'

SELECT
  errlim=0.001
  contours=10
  vectorgrid =12

VARIABLES
  h

DEFINITIONS
  s=0
  uww=9.81
  u=(h-y)*uww

  \{Linear Interpolation of Permeability Function\}
  seg1=-7
  seg2=((u+100)*(-7+10)/90-10)
  seg3=((u+150)*(-10+11)/50-11)
  seg=if u>=-10 then seg1 else if u>=-100 then seg2 else seg3
  k1=10^seg
  k2=5.083e-4
  kx
  ky

EQUATIONS
  div(vector(kx*dx(h),ky*dy(h)))+s=0

BOUNDARIES
  region 1
    kx=k1
ky=k1
natural(h)=0
  start(0.1,0)
  line to (40.0) to (52.0) to (28,12) to (24,12) to (20,10)
value(h)=10
  line to (0,0)
natural(h)=0
  line to finish

region 2
  kx=k2
  ky=k2
value(h)=0
  start(52,0)
  line to (40,0) to (40,-0.5) to (52,-0.5) to finish

PLOTS
  grid(x,y)
  contour(h) as 'Total Head at Kx=Ky'
  contour(u) as 'Pressure at Kx=Ky'
  vector(-dx(h)*kx, -dy(h)*ky) as 'Velocity Vectors at Kx=Ky'

END

Seepage Verification Example No. B3

TITLE
  'Transient Groundwater Seepage Beneath a Lagoon'

SELECT
  contours=5
  errlim=0.001
  vectorgrid=30
  galerkin_error=on

VARIABLES
  h

DEFINITIONS
  s=0
  uww=9.81
  u=uww*(h-y)
  mw=2e-3
{linear interpolation of permeability function;}
k0=if u<-100 then -7 else if u<=0 then (u+100)*(-5+7)/100-7 else -5
k10=10^5k0
k20=k10/2
k1=3600*k10
k2=3600*k20
k

INITIAL VALUES
h=5

EQUATIONS
div(k*grad(h))+s=dt(h)*uww*mw

BOUNDARIES
region 1
k=k1
natural(h)=0
start(0,0)
line to (40,0)
value(h)=5
line to (40,5)
natural(h)=0
line to (40,10) to (6.5,10) to (5.5,11) to (4,11)
value(h)=11
line to (3,10) to (0,10)
natural(h)=0
line to finish

region 2
k=k2
start(0,9)
line to (3.5,9) to (5.5,11) to (4,11) to (3,10) to (0,10)
line to finish

TIME
0 to 1200 by 1e-3

PLOTS
for t=0
contour(h) as 'Head at Elapsed Time of T=0'
for t=7
contour(h) as 'Head at Elapsed Time of T=7'
for t=15
contour(h) as 'Head at Elapsed Time of T=15'
for t=31
countour(h) as 'Head at Elapsed Time of T=31'
for t=127
   contour(h) as 'Head at Elapsed Time of T=127'
for t=1023
   contour(h) as 'Head at Elapsed Time of T=1023'

HISTORIES
history(h) at (0,0) (10,7.5) (20,0) as 'To find the LAST DAY'

END

Two-Dimensional Seepage Verification Example No. 1- initial conditions

TITLE
'Initial Conditions for Transient Seepage Problem for a Earth Dam'

SELECT
   errlim=0.001
   contours=8
   vectorgrid =40
   galerkin_error=on

VARIABLES
   h

DEFINITIONS
   s=0
   uww=9.81
   u=(h-y)*uww
   mw=1e-03

   {Linear Interpolation of Permeability Function;}
   seg1=-7
   seg2=((u+100)*(-7+10)/90-10)
   seg3=((u+150)*(-10+11)/50-11)
   seg=if u>=-10 then seg1 else if u>=-100 then seg2 else seg3
   k1=10^seg
   k2=5.083e-4
   k

INITIAL VALUES
   h=4
EQUATIONS
\[ \text{div}(k \cdot \text{grad}(h)) + s = 0 \]

BOUNDARIES
region 1
- \( k = k_1 \)
- natural(h) = 0.0
- start(0.1,0)
  line to (40,0)
  line to (52,0)
  line to (28,12) to (24,12) to (8,4)
- value(h) = 4.0
  line to (0,0)
- natural(h) = 0.0
  line to finish

region 2
- \( k = k_2 \)
- value(h) = 0.0
- start(52,0)
  line to (40,0) to (40,-0.5) to (52,-0.5) to finish

PLOTS
- grid(x,y)
- contour(h) as 'Total Head at Initial Condition'
- contour(u) as 'Pressure at Initial Condition'
- vector(-dx(h)*k, -dy(h)*k) as 'Velocity Vectors at Kx=Ky'
- transfer(h)

END

Two-Dimensional Seepage Verification Example No. 1

TITLE
'Transient Seepage Problem for a Earth Dam - Reservoir Filling'

SELECT
errlim=0.001
contours=8
vectorgrid =40
galerkin_error=on
smoothinit
VARIABLES

h

DEFINITIONS

s=0
uww=9.81
u=(h-y)*uww
mw=1e-03

\{Linear Interpolation of Permeability Function\}
seg1=-7
seg2=((u+100)*(-7+10)/90-10)
seg3=((u+150)*(-10+11)/50-11)
seg=if u>=-10 then seg1 else if u>=-100 then seg2 else seg3
k1=3600*10^seg
k2=3600*(5.083e-4)
k

transfer('w20404001_01.dat',h0)

INITIAL VALUES

h=h0

EQUATIONS

div(k*grad(h))+s=dt(h)*uww*mw

BOUNDARIES

region 1

k=k1
natural(h)=0.0

start(0.1,0)
line to (40,0)
line to (52,0)
line to (28,12) to (24,12) to (20,10)
value(h)=10.0

start(0,0)
natural(h)=0.0
line to finish

region 2

k=k2
value(h)=0.0

start(52,0)
line to (40,0) to (40,-0.5) to (52,-0.5) to finish
TIME
0 to 200000 by 1e-4

PLOTS
for t=15
  contour(u) as 'Pressure at Elapsed Time of T=15'
  contour(h)
  vector(-dx(h)*k,-dy(h)*k)
for t=255
  contour(u) as 'Pressure at Elapsed Time of T=225'
  contour(h)
  vector(-dx(h)*k,-dy(h)*k)
for t=1023
  contour(u) as 'Pressure at Elapsed Time of T=1023'
  contour(h)
  vector(-dx(h)*k,-dy(h)*k)
for t=4095
  contour(u) as 'Pressure at Elapsed Time of T=4095'
  contour(h)
  vector(-dx(h)*k,-dy(h)*k)
for t=16383
  contour(u) as 'Pressure at Elapsed Time of T=16383'
  contour(h)
  vector(-dx(h)*k,-dy(h)*k)

HISTORIES
history(h) at (23,5) (13,2) (33,8) as 'To find the LAST DAY'

END

Two-Dimensional Seepage Verification Example No. 2

TITLE
'S.S. Seepage through an earthfill dam with free seepage on downstream face'

SELECT
errlim=1.0e-4
contours=5
vectorgrid=10
aspect=1
VARIABLES
  h

DEFINITIONS
  s=0
  uww=9.81
  u=(h-y)*uww
  
  k1=10^(-7)
  k

  exit = staged( 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8, 8.5, 9, 9.5, 10)
  big = 1e5
  blayer = 1

INITIAL VALUES
  h=10

EQUATIONS
  div(k*grad(h))+s=0

BOUNDARIES
region 1
  k=k1
  natural(h)=0.0
    start(0,0)
    line to (40,0)
    line to (52,0)
  natural(h)= if y<exit then big*(h-y) else 0
    line to (28,12)
  natural(h)=0
    line to (24,12) to (22,11)
  value(h)=11.0
    line to (0,0)
  natural(h)=0.0
    line to finish

  feature start "blayer" (52-4*blayer,blayer) line to (28,12-blayer)
  feature start "downslope" (51,0.5) line to (28,12)

PLOTS
  grid(x,y)
  contour(h) as 'Total Head'
    report(exit)
  contour(u) as 'Pressure'
    report(exit)
vector(-dx(h)*k, -dy(h)*k) as 'Velocity Vectors' norm
report(exit)
elevation(u) on "downslope" as "downslope pressure"
report(exit) report(sqrt((2*exit-1)^2+(exit-0.5)^2)) as "exitdist"

END

---

**Two-Dimensional Thermal Verification Examples No. 1**

{Solution of Laplacian equation for two dimensional heat flow. Solves simultaneously for the case without a thermal gradient and with a thermal gradient;}

**TITLE**

'Steady state heat flow'

**SELECT**

contours=5
cubic=on
errlim=0.00001

**VARIABLES**

temp (range=-10,10)

**DEFINITIONS**

source=0.0333*(-y)
altemp=temp+source

**EQUATIONS**

dxx(temp)+dyy(temp)=0

**BOUNDARIES**

region 1

start (0,0)
natural(temp)=0 line to (0,-250)
natural(temp)=0 line to (500,-250)
natural(temp)=0 line to (500,0)
value(temp)=-5 line to (250,0)
value(temp)=4 line to finish

**PLOTS**

contour (source)
contour (altemp) export
contour (temp) export
contour (temp) zoom(200,-50,100,100)
grid (x,y)

END

Two-Dimensional Thermal Verification Example No. 3

{Solution of Laplacian equation for the case of a heated strip on permafrost ground}

TITLE
'Steady state heat flow'

SELECT
contours=5
cubic=on
errlim=0.00001

VARIABLES
temp (range=-10,10)

DEFINITIONS
source=0.0333*(-y)
altemp=temp+source

INITIAL VALUES
temp=-5-y/30

EQUATIONS
dxx(temp)+dyy(temp)=0

BOUNDARIES
region 1
start (0,0)
natural(temp)=0 line to (0,-500)
value(temp)=11.6667 line to (500,-500)
value(temp)=-5-y/30 line to (500,0)
value(temp)=-5 line to (50,0)
value(temp)=4 line to finish
PLOTS
  contour (source)
  contour (altemp)
  contour (temp)
  contour (temp) zoom(12.5,-2.5,5,5)
  grid (x,y)
END

Two-Dimensional Thermal Verification Example No. 3

TITLE
  'Heat Flow in a Desert Soil'

SELECT
  smoothinit
  contours=10
  errlim=0.01
  cubic=on
  order=3

VARIABLES
  temp (range=0,50)

DEFINITIONS
  tfunc=table('surftfun.prm') {defines surface temp}

  {thermal properties}
  thet=0.29 {0.03 for dry case}
  theta_solid=1-thet
  source=0

  {thermal conductivity}
  lamb=0.9 {0.45 for dry case}
  vshc_soil=2700000 {1600000 for dry case}

INITIAL VALUES
  temp=15.6 {16.8 for dry case}

EQUATIONS
  div(lamb*grad(temp))=vshc_soil*dt(temp)
BOUNDARIES
region 1
start (0,0)
natural(temp)=0 line to (0.1,0)
value(temp)=15.6 line to (0.1,-0.44)
natural(temp)=0 line to (0.1,-0.44)
value(temp)=tfunc line to finish

feature start (0,-0.01) line to (0.1,-0.01)
feature start (0,-0.02) line to (0.1,-0.02)

TIME
0 to 86400 by 400

MONITORS
For t=0,20000,40000,60000,80000
contour (temp)

PLOTS
contour (temp)
grid (x,y)

HISTORIES
history (temp) at (0.05,-0.09) export

END

Two-Dimensional Thermal Verification Example No. 4

TITLE
'Neuman problem for thaw'

SELECT
smoothinit
erlim=1e-4
c changelim=0.1

VARIABLES
temp

DEFINITIONS
vshc=2 {MJ/m^3} 
lam=0.1 {MJ/day-m-degC}
lf=334 {MJ/m^3}
\( m2i = \text{table('unfroz.prn')} \) \{1/\text{degC}\}

\text{surtemp} = 5

\textbf{INITIAL VALUES}
\text{temp} = -3

\textbf{EQUATIONS}
\( \text{div}(\lambda \text{grad}(\text{temp})) = \text{vshc} \times \text{dt(\text{temp})} + \text{l} \times m2i \times \text{dt(\text{temp})} \)

\textbf{BOUNDARIES}
\text{region 1}
\begin{align*}
\text{start}(0,5) & \quad \text{line to } (0,0) \\
\text{natural(\text{temp})} & = 0 \\
\text{value(\text{temp})} & = -3 \\
\text{natural(\text{temp})} & = 0 \\
\text{value(\text{temp})} & = \text{surtemp} \\
\end{align*}
\text{line to } (0.1,0) \\
\text{line to } (0.1,5) \\
\text{line to finish}

\textbf{TIME}
\text{from 0 to 1200 by 0.01}

\textbf{MONITORS}
\text{for } t = 0.01, 0.02, 0.03, 0.1, 0.2, 0.3, 0.4, 0.5, 1, 2, 5, 10, 15, 20, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200
\text{contour(\text{temp})}
\text{contour(m2i)}
\text{elevation(\text{temp}) from (0.05,5) to (0.05,0) export}

\textbf{HISTORIES}
\text{history(\text{temp}) at (0.05,4.5) (0.05,4) (0.05,3) export}

\textbf{END}

\underline{Two-Dimensional Thermal Verification Example No. 5}

\textbf{TITLE}
'Neuman problem for freeze'

\textbf{SELECT}
\text{smoothinit}
\text{errlim} = 1 \times 10^{-4}
\text{changelim} = 0.1

\textbf{VARIABLES}
\text{temp}

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DEFINITIONS
\[ v_{\text{shc}} = 2 \quad \text{[MJ/m}^3] \]
\[ \lambda = 0.1 \quad \text{[MJ/day-m-degC]} \]
\[ l_f = 334 \quad \text{[MJ/m}^3] \]
\[ m_2i = \text{table('unfroz.prn')} \]
\[ \theta = 0.5 \]
\[ \text{surtemp} = -5 \]

INITIAL VALUES
\[ \text{temp} = 3 \]

EQUATIONS
\[ \text{div}(\lambda \text{grad(temp)}) = (v_{\text{shc}} + l_f m_2i) \frac{\text{dt(temp)}}{} \]

BOUNDARIES
region 1
\[ \text{start}(0,5) \]
\[ \text{naturalt}(\text{temp}) = 0 \quad \text{line to (0,0)} \]
\[ \text{valuer}(\text{temp}) = 3 \quad \text{line to (0.1,0)} \]
\[ \text{naturalt}(\text{temp}) = 0 \quad \text{line to (0.1,5)} \]
\[ \text{valuer}(\text{temp}) = \text{surtemp} \quad \text{line to finish} \]

TIME
\[ \text{from 0 to 1200 by 0.01} \]

MONITORS
\[ \text{for } t = 0 \text{ by 0.1 to 1 by 1 to 20 by 10 to 200 by 100 to 1200} \]
\[ \text{contour (temp)} \]
\[ \text{contour (m2i)} \]
\[ \text{elevation(temp) from (0.05,5) to (0.05,0)} \text{ export} \]

HISTORIES
\[ \text{history(temp) at (0.05,4.5) (0.05,4) (0.05,3) export} \]

END

---

Two-Dimensional Thermal Verification Example No. 6

TITLE
'Thawing of permafrost beneath a warm foundation'

SELECT
smoothinit
VARIABLES
  temp (range=-5,20)

DEFINITIONS
  \{thermal properties\}
  \eta = 0.18

  \{thermal conductivity\}
  \lambda = \begin{cases} 
  2 \times 10^3 & \text{if } temp < 0 \\
  1 \times 10^3 & \text{else} 
  \end{cases} \text{ (ca/hr-m-degC)}

  m_2i = \text{table('unfroz24.prn')}

  vshc_soil = \begin{cases} 
  3.8 \times 10^5 & \text{if } temp < 0 \\
  6.3 \times 10^5 & \text{else} 
  \end{cases} \text{ (cal/m3-degC)}

  l_f = 8 \times 10^7 \text{ (cal/m3)}

  \text{surbound} = \begin{cases} 
  -2 + 0.175 \cdot t & \text{if } t < 100 \\
  15.5 & \text{else} 
  \end{cases}

INITIAL VALUES
  temp = -y/30

EQUATIONS
  \text{div}(\lambda \cdot \text{grad}(temp)) = (vshc_soil + l_f \cdot \eta \cdot m_2i) \cdot \text{dt}(temp)

BOUNDARIES
  region 1
    \begin{align*}
    \text{start} &= (0,60) \\
    \text{natural}(temp) &= 0 \quad \text{line to (0,0)} \\
    \text{value}(temp) &= 0 \quad \text{line to (50,0)} \\
    \text{natural}(temp) &= 0 \quad \text{line to (50,60)} \\
    \text{value}(temp) &= -2 \quad \text{line to (40,60)} \\
    \text{value}(temp) &= \text{surbound} \quad \text{line to finish}
    \end{align*}

  \text{feature start(0.59.5) line to (50,59.5)} \{\text{features included to aid convergence}\}
  \text{feature start(0.59) line to (50,59)}
  \text{feature start(0.58) line to (50,58)}

TIME
  0 to 4 \times 10^5 \text{ by 0.0001}

MONITORS
  \text{For } t = 0,10000,100000,220000,250000,400000
  \text{contour (temp)}
  \text{contour(m2i)}
Two-Dimensional Thermal Verification Example No. 7

TITLE
'Freezing of a soil around a chilled pipeline'

SELECT
smoothinit
contours=10
erllim=0.002
changelim=1.0
galerkin_error

VARIABLES
temp (range=-5,5)

DEFINITIONS
{thermal properties}
theta=0.377

{thermal conductivity}
lamb=if temp<0 then 0.15552 else 0.1296 {MJ/day-m-C}

m2i=table('unfroz24.prt') {one of many functions attempted as
discussed in Chapter 5;}

vshc_soil=1.95 {MJ/m3-C}
lf=334 {MJ/m3}
surbound=3

INITIAL VALUES
temp=3
EQUATIONS
\[ \text{div}(\lambda \text{grad}(\text{temp})) = (\text{vshc}_\text{soil} + l f \theta \text{m2i}) \cdot \text{dt(\text{temp})} \]

BOUNDARIES
region 1
start (0,1.6) line to (0.1.3)
natural(\text{temp})=0 line to (0.1.0)
value(\text{temp})=-2 arc to (0.15.1.15) to (0.1.0)
natural(\text{temp})=0 line to (0.0) to (1.6.0) to (1.6.1.6)
value(\text{temp})=\text{surbound} line to finish

TIME
0 to 811 by 0.0001

MONITORS
for \( t=1,3,7,15,31,63,127,255,511,730 \)
contour (\text{temp})
contour(\text{m2i})

PLOTS
for \( t=1,3,7,15,31,63,127,255,511,730 \)
contour (\text{temp})
contour(\text{m2i})
grid (x,y)

HISTORIES
history(\text{temp}) at (0.3,1.2) (0.85,1.2) (0.2,0.4) (0.85,0.4) export

END

---

**Three-Dimensional Thermal Verification Example**

**TITLE**
'Thawing of permafrost beneath a warm foundation in three-dimensions'

**SELECT**
smoothinit
contours=10
errlim=0.01
changelim=0.1
aspect=1

**COORDINATES**
cartesian3
VARIABLES

    temp (range=-5,20)

DEFINITIONS

    \{thermal conductivity\}
    \lambda = \begin{cases} 
        2e3, & \text{if } temp < 0 \\
        1e3, & \text{else} 
    \end{cases} \text{ \( \text{cal/hr-m} \)}

EQUATIONS

    \text{div}(\lambda \text{grad}(\text{temp})) = 0

EXTRUSION

    surface "bottom" z=0
    layer "soil1"
    surface "disfeature" z=59
    layer "soil2"
    surface "disfeature2" z=59.5
    layer "soil3"
    surface "top" z=60

BOUNDARIES

    region 1
    surface "bottom" value(\text{temp}) = 0
    surface "top" value(\text{temp}) = 15.5
    \text{start} (0,50)
    \text{line to} (40,50)
    \text{arc (center=0,50) to (0,10)}
    \text{line to finish}

    region 2
    surface "bottom" value(\text{temp}) = 0
    surface "top" value(\text{temp}) = -2
    \text{start} (40,50)
    \text{arc (center=0,50) to (0,10)}
    \text{line to} (0,0) \text{ to} (50,0) \text{ to} (50,50) \text{ to finish}

MONITORS

    \text{contour (temp) on} y=50
    \text{grid (x,z) on} y=50

PLOTS

    \text{contour (temp) on} y=50
    \text{contour (temp) on} y=25
    \text{contour (temp) on} y=10
    \text{grid (x,z) on} y=50
    \text{grid (x,y,z)
    \text{surface(temp) on} z=50

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surface(temp) on z=30

HISTORIES

END

Two-Dimensional Coupled Heat and Mass Verification Example No. 1

TITLE
'Coupled Heat-Mass Transfer in Soil'

SELECT
smoothinit
contours=10
errlim=0.001
changelim=0.1
galerkin_error

VARIABLES
u {soil suction - kPa}
temp {temperature defined in degrees C}

DEFINITIONS
{general definitions}
lv=2450000 {J/kg}
uww=9.81 {unit weight of water 9.81 kN/m^3}
g=9.81 {acceleration due to gravity m/s^2}
rhow=1 {density of water 1000 kg/m^3}
wv=0.018015 {molecular weight of water kg/mole}
r=8.31451 {universal gas constant J/mole-K}
tempk=temp+273.15 {temperature in K}
rh=if u<0 then exp(u*wv*g/(r*tempk)) else 1

pvs=0.1*(6984.505295+tempk*(-188.903931+tempk*(2.133357675+tempk*(-0.01288580973+tempk*(4.393587233e-5+tempk*(-8.02392e-8+tempk*6.1368e-11))))))
{saturated vapor pressure, kPa}

pv=pvs*rh
pvs_slope=table('pvsslope.pn')
gs=2.65 {needs to be changed depending on soil}
h=y+u/uww
{definition of soil properties;}

{swcc – Fredlund and Xing fit;}

\[
\theta = 0.38900 \ast (1 - \ln(1 + \text{abs}(u)/138.1654e-02)/\ln(1 + 10^{6}/138.1654e-02)) \ast
(1/\ln(\exp(1) + (\text{abs}(u)/996.8662e-03)^{159.3530e-01}))^{815.2985e-03}
\]

\[
\text{por} = 0.389
\]

{permeability}

\[
k_1 = (1.5e-10) \ast \exp(28.061 \ast \theta/\text{por} - 12.235 \ast \theta^2/\text{por}^2)
\]

{k}

{water storage function – Fredlund and Xing fit;}

\[
m_{2w} = \text{if } u < 0 \text{ then } (-0.3890/(138.2e-02*ln(1 + \text{abs}(u)/138.2e-02)) - 0.3890*(1-ln(1+100000/138.2e-02)/(\ln(\exp(1)+(\text{abs}(u)/996.86617e-03)^{159.3530e-01}))^{815.2985e-03}*\text{abs}(u)/996.86617e-03)*(\exp(1) + (\text{abs}(u)/996.86617e-03)^{159.3530e-01})*\ln(\exp(1)+(\text{abs}(u)/996.86617e-03)^{159.3530e-01})) \text{ else } 0.0207
\]

{thermal conductivity}

{input one of several methods of defining the thermal conductivity of the soil;}

\[
l_{\text{amb}} = 0.256 + 2.458 *(1-\exp(-22.94*\theta))
\]

{volumetric specific heat capacity}

{input one of several methods of defining the specific heat capacity;}

\[
v_{\text{shc}} = (1-\text{por})*2.16e6 + \theta*4.17e6
\]

{vapor diffusion coefficient}

{input method of defining vapor diffusion coefficient as a function of water content;}

\[
v_{\text{app}} = (0.229e-4)*(1+(\text{tempk})/272)^{1.75}
\]

\[
\beta = (1-\theta/\text{por}) \ast \text{por}
\]

\[
\alpha = \beta^{(2/3)}
\]

\[
v = \alpha \ast \beta \ast v_{\text{app}} \ast w/v/(r^4(\text{tempk}))
\]

{definition of constants for PDE's;
sd1=pv*wv/(rho*w*r*tempk)  {should temp be tempk here???}
sd2=pvs_slope*rh-pv*abs(u)*wv/(rho*w*r*tempk^2)  {ditto???}
d1=1/rhow*(dv*sd1)
d2=1/rhow*(dv*sd2)
d3=dv*sd1
d4=dv*sd2

{definition of surface boundary condition}
heater=if t<10800 then 20+0.003703*t else 60

INITIAL VALUES
u=(-2.035)
temp=20

EQUATIONS
{equations for the coupled heat mass transfer as given by Bhaskar Joshi}

{mass transfer}
l/m2w*div(k*grad(u/uww+y))+l/m2w*div(d1*grad(abs(u)))+
l/m2w*div(d2*grad(temp))=dt(u)

{heat flow}
div(lamb*grad(temp))=lv*div(d3*grad(abs(u)))-lv*div(d4*grad(temp))
 =vshc*dt(temp)

BOUNDARIES

region 1
k=k1
natural(u)=0  natural(temp)=0  start (0,0.2196)
line to (0,0.11615)
natural(u)=0  value(temp)=heater arc to (0.00635,0.1098) to (0.10345)
natural(u)=0  natural(temp)=0  line to (0,0)
natural(u)=0  value(temp)=20 arc to (0.1098,0.1098) to (0.2196)

TIME
from 0 to 1080000 by 0.001

PLOTS
for
t=0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9,1.0,1.1,1.2,1.3,1.4,1.5,1.6,1.7,1.8,1.9,2.0
contour(temp)
contour(pv)
MONITORS
for t=0 by 0.1 to 1 by 1 to 20 by 10 to 200 by 100 to 2000 by 1000 to 10000 by
10000 to 20000 by 100000 to 1080000
contour(temp)
contour(pv)
contour(u)
contour(h)
contour(theta)

HISTORIES
history(theta) at (0.01725,0.00453) (0.0155,0.0182) (0.0138,0.0319)
(0.0121,0.0456) (0.0104,0.0593) (0.0087,0.073) (0.007,0.0867) (0.0053,0.1004) export

END

Two-Dimensional Coupled Heat and Mass Verification Example No. 2

TITLE
'Coupled Heat-Mass Transfer in Soil Undergoing Evaporation'

SELECT
smoothinit
contours=10
errlim=0.0001
ngrid=15
changelim=0.5

VARIABLES
u {suction (ua-uw) in kPa}
temp {temperature defined in degrees C}

DEFINITIONS
{general definitions}
lv=2.45 {MJ/kg}
uww=9.81 {unit weight of water 9.81 kN/m^3}
g=9.81 {acceleration due to gravity m/s^2}
rhow=1 {density of water 1000 kg/m^3}
wv=0.018015 {molecular weight of water kg/mole}
\[ r = 8.31451 \] \{ \text{universal gas constant j/mole-K} \}
\[ \text{tempk} = \text{temp} + 273.15 \] \{ \text{temperature in Kelvins} \}
\[ \text{rh} = \exp(-u \times wv \times g / (r \times \text{tempk} \times uww)) \]

\[ \text{pvs} = 1.36075e5 \times \exp(-5239.7 / \text{tempk}) \times 1000 \]
\{ \text{saturated vapor pressure, kPa} \}
\[ \text{pv} = \text{pvs} \times \text{rh} \]
\[ \text{pvs_slope} = (1.36075e5) \times 5239.7 / (\text{tempk}^{2}) \times \exp(-5239.7 / \text{tempk}) \times 1000 \]
\[ \text{gs} = 2.65 \] \{ \text{needs to be changed depending on soil} \}
\[ h = y + u \times uww \]

\{===============================\}
\{definition of soil properties\}
\{permeability\}
\[ k0 = \text{if} \ u<4 \ \text{then} \ -4.09151 \ \text{else} \ -20 \ \text{else} \ -0.7123 \times u - 1.24231 \]
\[ k1 = 10^{k0} \]
\[ k \]

\{water storage function\}
\{input one of several methods of defining mw as a function of u\}
\[ \text{m2w} = \text{table('m2w.pm')} \]
\{table functions used to speed up solution time\}

\{water content function\}
\{input one of several methods of defining the SWCC of the soil\}
\[ \text{theta} = \text{table('swcc.pm')} \]
\[ \text{theta_solids} = 0.597 \]
\{"solids porosity" decimal value\}
\{needs to be changed depending on soil\}
\[ \text{theta_air} = 1 - \text{theta} - \text{theta_solids} \]
\{air filled porosity\}
\[ \text{por} = 1 - \text{theta_solids} \]
\{porosity\}

\{thermal conductivity\}
\{input one of several methods of defining the thermal conductivity of the soil\}
\[ \text{lamb} = \text{table('lamb.pm')} \times 1e-6 \]

\{volumetric specific heat capacity\}
\{input one of several methods of defining the specific heat capacity\}
\[ \text{vshc} = \text{table('vhsc.pm')} \]

\{vapor diffusion coefficient\}

\{input method of defining vapor diffusion coefficient as a function of water content\}
vapp=(0.2299e-4)*(1+(tempk)/272)^1.75 \quad \{m^2/s\}

beta=(1-(theta/por))\times por
alpha=beta^(2/3)
vap=alpha \times beta \times vapp \times wv/(r*tempk) \quad \{kg\cdot m/kN\cdot s\}

{definition of constants for PDE's}

sd1=pv\times wv/(rhow\times r\times tempk)
sd2=pvs_slope\times rh-pv\times u\times wv/(rhow\times r\times tempk^2)
d1=1/rhow*(vap*sd1)
d2=1/rhow*(vap*sd2)
d3=vap*sd1
d4=vap*sd2

{definition of surface boundary condition}

surtemp=(2.634\times (log10(t+945)/24/3600))^2+1.1455\times (log10((t+945)/24/3600)) +30.12
sursuct=table('sursuct.pm') \quad \{table of suction values calculated using Equation 5.7\}

INITIAL VALUES
u=if y<0.22 then 4 else (12.5*y+1.25)
temp=38.0

EQUATIONS
{equations for the coupled heat mass transfer as given by Bhaskar Joshi}

{mass transfer}
1/m2w*div(k*grad(u/uww-y))+1/(m2w*1000)*div(d1*grad(u)+
d2*grad(temp))=dt(u)

{heat flow}
div(lamb*grad(temp))-lv*div(d3*grad(u))-
lv*div(d4*grad(temp))=vshe*dt(temp)

BOUNDARIES
region 1
k=k1
start (0,0.3)
natural(u)=0 \quad natural(temp)=0 \quad line to (0,0)
natural(u)=0 \quad value(temp)=38.0 \quad line to (0.01,0)
natural(u)=0  natural(temp)=0  line to (0.01,0.3)
value(u)=sursuct  value(temp)=surtemp  line to finish

feature start (0,0.2999) line to (0.01,0.2999)
feature start (0,0.2998) line to (0.01,0.2998)
feature start (0,0.2997) line to (0.01,0.2997)
feature start (0,0.2996) line to (0.01,0.2996)
feature start (0,0.2995) line to (0.01,0.2995)
feature start (0,0.299) line to (0.01,0.299)
feature start (0,0.2985) line to (0.01,0.2985)
feature start (0,0.298) line to (0.01,0.298)
feature start (0,0.2975) line to (0.01,0.2975)
feature start (0,0.297) line to (0.01,0.297)
feature start (0,0.2965) line to (0.01,0.2965)
feature start (0,0.296) line to (0.01,0.296)
feature start (0,0.295) line to (0.01,0.295)
feature start (0,0.294) line to (0.01,0.294)
feature start (0,0.293) line to (0.01,0.293)
feature start (0,0.292) line to (0.01,0.292)
feature start (0,0.291) line to (0.01,0.291)
feature start (0,0.290) line to (0.01,0.290)
feature start (0,0.2875) line to (0.01,0.2875)
feature start (0,0.285) line to (0.01,0.285)
feature start (0,0.280) line to (0.01,0.280)
feature start (0,0.275) line to (0.01,0.275)
feature start (0,0.270) line to (0.01,0.270)
feature start (0,0.260) line to (0.01,0.260)
feature start (0,0.250) line to (0.01,0.250)

TIME
from 0 to 1728000 by 0.01

MONITORS
for t=0 by 0.1 to 2 by 1 to 20 by 10 to 200 by 100 to 2000 by 1000 to 100000 by 10000 to 1728000
grid(x,y)
grid(x,y) zoom(0.025,0.05,0.05)
contour(temp)
contour(pv)
contour(u)
contour(h)
elevation(u) from (0.005,0.3) to (0.005,0)

PLOTS
HISTORIES
  history(temp) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.3)
  history(u) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.275) (0.005,0.3)
  history(sd1) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.25) (0.005,0.3)
  history(sd2) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.25) (0.005,0.3)
  history(pv) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.25) (0.005,0.3)
  history(log10(k)) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.3)
  history(rh) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.3)
  history(m2w) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.3)
  history(theta) at (0.005,0.1) (0.005,0.2) (0.005,0.25) (0.005,0.3)

END

---

**Comprehensive Example Problem — Steady State Seepage**

**TITLE**

'Comprehensive Pipeline Example — Steady State Seepage'

**SELECT**

errlim=1e-3

**VARIABLES**

h

**DEFINITIONS**

uww=9.81
u=(h-y)*uww

{definition of soil water characteristic curve}
theta1=table('theta1.prn')

{definition of theta 2 from fredlund and xing fit equation}
theta2=if u<0 then thetasat*(1-(ln(1+abs(u)/ur))/(ln(1+1000000/ur))))* 
     (1/(ln(exp(1)+(abs(u)/af)^nf)^mf)) else thetasat

theta
{definition of k-functions}
k1=table('k1.prn')
\{definition of k2 using campbell's equation;\}
ksat=1e-6
p=3
k2=ksat*(\theta_2/\theta_{sat})^p

k

s=0
surflux=-1e-8

INITIAL VALUES
h=y

EQUATIONS
div(k*\nabla(h))+s=0

CONSTRAINTS

BOUNDARIES
region 1 \{outer system boundaries-material properties as undisturbed soil\}
k=k1
\theta=\theta_1

start (0,2)
natural(h)=0 \ line to (0,1.7)
natural(h)=0 \ arc to (0.15,1.55) to (0,1.4)
natural(h)=0 \ line to (0,0)
value(h)=0 \ line to (2.0)
natural(h)=0 \ line to (2,2)
natural(h)=surflux \ line to finish

region 2 \{boundary of disturbed soil\}
k=k2
\theta=\theta_2

start (0,2)
line to (0,1.7)
arc to (0.15,1.55) to (0,1.4)
line to (0.13) to (0.25,1.3) to (0.25,2)
line to finish

MONITORS
contour (h)
contour (u)
contour (\theta)
Comprehensive Verification Example – Steady State Heat Flow

TITLE
'Comprehensive Pipeline Example - Heat Flow, Determination of Initial Conditions'

SELECT

VARIABLES
temp

DEFINITIONS
rhoice=0.918
rhow=1
I=334 \{MJ/m^3\}

\{basic material properties\}
\n\ntheta=thetaice+thetau
satw=(thetau)/n
sati=(thetaice)/n
gs=2.65
voidrat=n/(1-n)
wu=satw*voidrat/gs
wi=rhoice*sati*voidrat/gs
drydens \{kg/m^3; dry density of soil\}

\{thermal properties\}
\ncs=837 \{j/kg-degC\;
\nvshc1=drydens*(cs+4184*wu+2100*wi) \{J/m^3-degC\;
\nvshc=vshc1/1e6 \{MJ/m^3-degC\;
\nlambsolids=8.54
\nlambfroz=2.176
\nlambwater=0.573
fsolids=0.27265
funfroz=1
ffroz=0.6015
lamb1=(fsolids*thetasolid*lambsolids+ffroz*thetaice*lambfroz+
funfroz*thetau*lambwater)/(fsolids*thetasolid+ffroz*thetaice+
funfroz*thetau)
lamb=lamb1/1e6 [MJ/s-m-degC]
s=0

EQUATIONS
div(lamb*grad(temp))+s=0

BOUNDARIES
region 1 {outer system boundaries-m.p as undisturbed soil}
drydens=1550
n=0.35
  start (0,2)
  natural(temp)=0 line to (0,1.7)
  natural(temp)=0 arc to (0.15,1.55) to (0,1.4)
  natural(temp)=0 line to (0,0)
  value(temp)=2 line to (2,0)
  natural(temp)=0 line to (2,2)
  value(temp)=5 line to finish

region 2 {boundary of disturbed soil}
drydens=1450
n=0.40
  start (0,2)
  line to (0,1.7)
  arc to (0.15,1.55) to (0,1.4)
  line to (0,1.3) to (0.25,1.3) to (0.25,2)
  line to finish

PLOTS
  contour (temp)

END

Comprehensive Verification Example – Transient Heat Flow

TITLE
'Comprehensive Pipeline Example - Heat Flow'
SELECT
  smoothinit
errlim=0.005
contours=8
VARIABLES
temp

DEFINITIONS
rhoice=0.918
rhow=1
lf=334  \{MJ/m^3\}

\{unfroz curves\}
m2i
unfroz1=table('unfroz1.pnm')
unfrozfrac1=unfroz1/0.35
m2i1=table('m2i1.pnm')

thetasat=0.4
af=400
nf=3
mf=1
cf=2.2
unfroz2=if temp<0 then thetasat*(1-(ln(1+(cf*1110*abs(temp))/180)/(ln(1+
  cf*1110*273/180))))*(1/(ln(exp(1)+((cf*1110*abs(temp))/af)^nf)^mf))
else thetasat
unfrozfrac2=unfroz2/0.40
m2i2=if temp<0 then -(thetasat*cf*(37/6)/(((1+37/6*cf*abs(temp))* (ln(1+
  3367/2*cf))*(ln(exp(1)+(1110*cf*abs(temp)/af)^nf)^mf))) -thetasat*(1-
  ln(1+37/6*cf*abs(temp))/ln(1+3367/2*cf))/(ln(exp(1)+(1110*cf*abs(temp)/af)^nf)^mf*(1110*cf*abs(temp)/af)^nf*nf/((exp(1)+
  (1110*cf*abs(temp)/af)^nf)*ln(exp(1)+(1110*cf*abs(temp)/af)^nf))))
else 0
unfrozfrac

\{basic material properties\}
n
thetasolid=1-n
thetau0=table('last seepage.p03')
thetaice0=0
thetau=thetau0*unfrozfrac
thetaice=thetaice0+(thetau0-thetau)*1.089
theta=thetaice+thetau
satw=(thetau)/n
sati=(thetaice)/n
gs=2.65
voidrat = n/(1-n)
wu = satw * voidrat / gs
wi = rhoice * sati * voidrat / gs
drydens = {kg/m^3: dry density of soil}

{thermal properties}
cs = 837  {j/kg-degC}
vshc = drydens * (cs + 4184 * wu + 2100 * wi)  {j/m^3-degC}
vshc = vshc / 1e6  {MJ/m^3-degC}

λsolids = 8.54
λfroz = 2.176
λwater = 0.573

fsolids = 0.27265
funfroz = 1
ffroz = 0.6015

λ1 = (fsolids * thetasolid * λsolids + funfroz * thetaice * λfroz +
      funfroz * thetau * λwater) / (fsolids * thetasolid + funfroz * thetaice +
      funfroz * thetau)
λ = λ1 / 1e6  {MJ/s-m-degC}

s = 0
surtemp = 3 + 5 * (sin(2 * 3.1416 * t / 3153600))  {or 3 deg C for 1st run}

INITIAL VALUES
  temp = table('last heat flow 1.p01')  {import initial conditions from steady stat analysis}

EQUATIONS
  div(λ * grad(temp)) + s = (vshc + λf * thetau * m2i) * dt(temp)

BOUNDARIES
  region 1 {outer system boundaries-m.p as undisturbed soil}
    drydens = 1550
    n = 0.35
    m2i = m2i1
    unfrozfrac = unfrozfrac1
    start (0,2)
    natural(temp) = 0  line to (0.17)
    value(temp) = -3  arc to (0.15, 1.55) to (0.14)
    natural(temp) = 0  line to (0,0)
    natural(temp) = 0  line to (2,0)
    natural(temp) = 0  line to (2.2)
    value(temp) = surtemp  line to finish

  region 2 {boundary of disturbed soil}
drydens=1450
n=0.40
m2i=m2i2
unfrozfrac=unfrozfrac2
  start (0,2)
  line to (0,1.7)
  arc to (0.15,1.55) to (0,1.4)
  line to (0,1.3) to (0.25,1.3) to (0.25,2)
  line to finish

TIME
  from 0 to 31536000

MONITORS
  for t=0 by 0.1 to 2 by 1 to 50 by 10 to 200 by 100 to 2000 by 1000 to 20000 by 10000 to 100000 to 31536000
  contour (temp)
  contour (theta)
  contour (m2i)

PLOTS
  for t=100, 1000, 10000, 100000, 1000000, 2592000, 10000000, 15552000, 31536000
  contour (temp)

HISTORIES
  history (temp) at (0.2,1.5) (0.2,1) (0.2,0.5) (1,1.5) (1,1) (1,0.5) export
  history (lamb) at (0.2,1.5) (0.2,1) (0.2,0.5) (1,1.5) (1,1) (1,0.5)
  history (vshc) at (0.2,1.5) (0.2,1) (0.2,0.5) (1,1.5) (1,1) (1,0.5)
  history (surtemp)

END

---

Comprehensive Verification Example – Parametric Heat Flow

TITLE
  'Comprehensive Pipeline Example - Heat Flow'

SELECT
  smoothinit
  errlim=0.01

VARIABLES
  temp
DEFINITIONS
rhoice=0.918
rhow=1
lf=334 \{MJ/m^3\}

\{unfroz curves\}
m2i

unfroz1=table('unfroz1.prn')
unfrozfrac1=unfroz1/0.35
m2i=table('m2i1.prn')

thetasat=0.4
af=1000 \{or 400\} \{parameters tested!!\}
f=2 \{or 3.4\}
mf=1 \{constant\}
cf=2.2 \{or 1.0\}

unfroz1=if temp<0 then thetasat*(1-(ln(1+(cf*1110*abs(temp))/180))/(ln(1+cf*1110*273/180)))*(1/(ln(exp(1)+(cf*1110*abs(temp)/af)^nf)^mf))
else thetasat

unfrozfrac1=unfroz2/0.40
m2i=if temp<0 then -(thetasat*cf*(37/6))/((1+37/6*cf*abs(temp))* (ln(1+3367/2*cf)*(ln(exp(1)+(1110*cf*abs(temp)/af)^nf)^mf))-thetasat*(1-
ln(1+37/6*cf*abs(temp))/ln(1+3367/2*cf))/ln(exp(1)+(1110*cf*abs(temp)/af)^nf)^mf*(1110*cf*abs(temp)/af)^nf*nf/(abs(temp)*((exp(1)
+(1110*cf*abs(temp)/af)^nf)*ln(exp(1)+(1110*cf*abs(temp)/af)^nf))
else 0

unfrozfrac

\{basic material properties\}

n
thetasolid=1-n
thetau0=0.3
thetai0=0
thetau=thetau0*unfrozfrac
thetai=thetai0+(thetau0-thetau)*1.089
theta=thetai+thetau
satw=(thetau)/n
sati=(thetai)/n
gs=2.65
voidrat=n/(1-n)
wu=satw*voidrat/gs
wi=rhoice*sati*voidrat/gs
drydens \{kg/m^3; dry density of soil\}

\{thermal properties\}
\(cs=837\)  \(\text{[j kg-degC]}\)
\(vshc_1=\text{drydens}(cs+4184*wu+2100*wi)\)  \(\text{[j m}^3\text{-degC]}\)
\(vshc=vshc_1/1e6\)  \(\text{[MJ/m}^3\text{-degC]}\)

\(\text{lambsolids}=8.54\)
\(\text{lambfroz}=2.176\)
\(\text{lambwater}=0.573\)

\(\text{fsolids}=0.27265\)
\(\text{funfroz}=1\)
\(\text{ffroz}=0.6015\)

\(\text{lamb}_1=(\text{fsolids*thetasolid*lambsolids+ffroz*thetaice*lambfroz+}
\text{funfroz*thetau*lambwater})/(\text{fsolids*thetasolid+ffroz*thetaice+}
\text{funfroz*thetau})\)

\(\text{lamb}=(\text{lamb}_1/1e6)\)  \(\text{[MJ/s-m-degC]}\)

\(s=0\)
\(\text{surtemp}=3\)

**INITIAL VALUES**
\(\text{temp}=3\)

**EQUATIONS**
\(\text{div(lamb*grad(temp))}+s=(vshc+lf*thetau0*m2i)*dt(temp)\)

**CONSTRAINTS**

**BOUNDARIES**
\(\text{region 1 \{outer system boundaries-m.p as undisturbed soil}\}
\(\text{drydens}=1450\)
\(\text{n}=0.40\)
\(\text{m2i}=m2i\)

\(\text{unfrozfrac}=\text{unfrozfrac1}\)
\(\text{start (0,2)}\)
\(\text{natural(temp)=0} \quad \text{line to (0,1.7)}\)
\(\text{value(temp)=-3} \quad \text{arc to (0.15,1.55) to (0,1.4)}\)
\(\text{natural(temp)=0} \quad \text{line to (0,0)}\)
\(\text{natural(temp)=0} \quad \text{line to (2,0)}\)
\(\text{natural(temp)=0} \quad \text{line to (2,2)}\)
\(\text{value(temp)=surtemp} \quad \text{line to finish}\)

**TIME**
\(\text{from 0 to 31536000}\)

**MONITORS**
\(\text{for t=0 by 0.1 to 2 by 1 to 50 by 10 to 200 by 100 to 2000 by 1000 to 20000 by}
\text{10000 to 1000000 by 10000000 to 31536000}\)
contour (temp)
contour (theta)
contour (m2i)

PLOTS
for t=100, 1000, 10000, 100000, 1000000, 15552000, 31536000
contour (temp)

HISTORIES
  history (temp) at (0.5,1.55) (0.25,1.55) export
  history (lamb) at (0.2,1.5) (0.2,1) (0.2,0.5) (1,1.5) (1) (1.0.5)
  history (vshc) at (0.2,1.5) (0.2,1) (0.2,0.5) (1,1.5) (1) (1.0.5)
  history (surtemp)

END