MATHEMATICAL MODELING OF A HYDROCARBON SPILL ON THE

ICE COVER OF LAKE FRYXELL, ANTARCTICA

A Thesis
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ABSTRACT

Numerous perennially ice-covered lakes exist in the McMurdo Dry Valleys region of Antarctica. Ice cover melting on these lakes and meltwater infiltration are important processes affecting the ecology of these lakes. The three lakes in Taylor Valley, Lakes Bonney, Fryxell and Hoare, have been investigated since 1993 as part of the McMurdo Dry Valleys Long Term Ecological Research (MCM LTER) site.

A Bell 212 helicopter flying in support of the National Science Foundation's Antarctic Research Program crashed on the frozen surface of Lake Fryxell on January 17, 2003. This resulted in the release of approximately 731 Liters (193 gallons) of diesel fuel and amounts of engine oil and hydraulic fluid.

Two physically based models are developed that simulate heat, meltwater flow and solute transport. The first is a transient, one-dimensional, thermodynamic model, which can predict the temperature distribution in the ice cover, melting rate at the surface and at the bottom of ice cover, and ice thickness. The second model simulates unsaturated flow and solute transport and is used to estimate water content distribution and solute transport through the ice cover.
The validation of heat transport model was accomplished by comparing model results with the original measurements of ice temperature at various depth in Lake Fryxell. Because of lack of the field data, validation of the unsaturated flow and solute transport model couldn’t been accomplished, instead of model validation, programming code has been verified by comparing results with results generated by the HYDRUS 1D software, developed by U.S. Salinity Laboratory, USDA.
Dedicated to my parents

посвящено моим родителям
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And last, but definitely not least, my wife for her patience and endurance, and my parents in Bosnia who always believed in me and to whom this work is dedicated.
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CHAPTER 1

INTRODUCTION

1.1 Motivation

A Bell 212 helicopter flying in support of the National Science Foundation's Antarctic Research Program crashed on the frozen surface of Lake Fryxell in Taylor Valley, Antarctica, on January 17, 2003 (Fig. 1). This resulted in the release of approximately 731 Liters (193 gallons) of diesel fuel and small amounts of engine oil and hydraulic fluid. The crash site was at the edge of an extensively melted area with a complex series of interconnecting pools, channels and sub-surface chambers (Alexander et al., 2003). After the crash, the released fluids spread over the surface of the ice via meltwater flowing over and percolating throughout the ice.

Due to weather delays and the time required for investigation, the clean up of the spilled fluids began four days later on January 21, but the aircraft wreckage remained in place until February 2, 2003 (Alexander et al., 2003). The contamination was clearly evident within a 19 meter radius of the crash center, and was particularly concentrated at the impact point. The fuel/oil mixture traveled from the crash site via
surface water in open melt pools, and within subsurface chambers and channels. Cleanup crews used sorbant pads to remove visible contaminants from the ice and water surfaces in open melt pools and from sub-surface chambers accessed with chisels and ice-axes. Cleanup activities ended on February 5, because it was determined that the recovery rate of petroleum product had become minimal for the effort expended. When the cleanup was halted, it was estimated that 45 to 50% of the hydrocarbons had been recovered, thus leaving a maximum of 341 to 379 liters of fuel and oil at the site (Alexander et al., 2003).

Figure 1. Bell 212 wreckage at Lake Fryxell (Photo: Terry Melton, Alexander et al. 2003).

Despite removal by sorbant pads, the oil continued to seep into these melting pools on subsequent days. Because of the extreme variation in permeability of the
lake ice, the predominantly lateral transport of contaminants, and the presence of subsurface chambers, it is highly probable that isolated pools of fuel and oil still exist in the sampling area. During the winter these are most likely immobile, but at the onset of the summer melt in 2003, the dispersal of contaminants were anticipated to resume (Alexander et al., 2003).

1.2 Thesis objectives

The spill was of particular concern because the mostly ice-free MCM Dry Valleys are an environmentally protected area and, since 1993, the focus of Long Term Ecological Research (LTER) studies.

In response to the crash and spill, the Office of Polar Programs at NSF initiated a meeting in June 2003 to discuss future action to assess the ecological implication of the hydrocarbon contamination on Lake Fryxell. Because Lake Fryxell is a long-term monitoring site of the MCM LTER, it was decided to fund a study to investigate the impact of the crash spill. As part of this investigation a modeling exercise was supported to better establish the potential movement of hydrocarbons through the ice cover.

This model would be used to predict whether the contaminants could reach lake water which occurs at a depth of ~0.5m and in what concentration. The work reported here is important as there are few works related to modeling contaminant transport within ice, especially lake ice, and this research represents the first step related to modeling of transport contaminant within lake ice.
• The purpose of this study was to establish the factors and processes affecting melting and refreezing of lake ice, transport of meltwater through ice, and processes related to the transport of hydrocarbons. Although the work was focused in Lake Fryxell, it can be considered a more generic model for polar ice lakes in general.

• This study provides a practical overview of numerical solutions to one-dimensional heat and transport equations using the finite-difference method.

• Based on that method, MatLab codes were utilized to develop a one-dimensional time dependent contaminant transport model. Using this tool we were able to estimate:
  
  o Melting rate at the surface and bottom of ice cover
  
  o Downward movement of melt water
  
  o Downward spreading of hydrocarbons in ice
  
  o Based on the modeling results, the dominant transport parameters were identified.
  
  o Concentrations of hydrocarbons in lake water.
1.3 Thesis outline

The organization of this thesis is presented as follows: The first two chapters are introductory. Chapter 1 consists of motivation and thesis objectives. Chapter 2 contains a brief literature review that is divided into three main groups: 1. previous work on thermodynamics, 2. previous work on meltwater infiltration, and 3. previous work on contaminant transport in ice. Chapter 3 presents the description of study area and the location of crash site. Chapter 4 contains the model description with four subchapters. In the first subchapter is the description of the physical problems of contaminant transport in ice. The second subchapter contains a formulation and analysis of the mathematical model. The subchapter 3 applies the finite-difference method used for model discretization and the last subchapter describes the program structure.

Model validation is presented in Chapter 5 where the results of the heat transport model are compared to measurements of ice temperatures measured at Lake Fryxell. The programming code of the unsaturated flow and solute transport model is verified by comparing its results with results generated by the Hydrus 1D software. Simulation results are presented in Chapter 6. Because insufficient data were available, six modeling variations are illustrated for scenarios sets of input data. A sensitivity analysis is also performed to determine the relative importance of changes in values of various data. A summary of conclusions and recommendations are presented in chapters 7 and 8.
CHAPTER 2

LITERATURE REVIEW

2.1 Previous work on ice thermodynamics

The thermodynamics of ice is a complex process involving heat exchange in both vertical and horizontal directions, but vertical processes tend to dominate. When ice is formed, heat exchange occurs at the ice boundaries. Ice can gain heat when part of solar radiation penetrates into the ice at upper boundary and from oceanic or lake water heat flux at lower boundary. Heat loss from the ice occurs due to thermal radiation, latent heat and turbulent flux.

In the last couple of decades, numerous sea ice but much less fresh water ice thermodynamic investigations have been undertaken. The first work was done by J. Stefan who, around 1890, was interested in melting of the polar cap (Crank, 1984). He was investigating phase-change processes where he found that the characteristic of phase change problems is that, in addition to the temperature field, the location of the interface is unknown. As result of that work, moving-boundary problems are often called Stefan problems. Moving boundaries are defined as time dependent problems
where the position of the boundary between the liquid and the solid phase has to be determined as a function of space and time (Crank, 1984).

The thermodynamic processes occurring in sea ice are described by Maykut and Untersteiner (1971). They developed a one-dimensional thermodynamic model using energy fluxes at the atmospheric and oceanic boundaries. The model included the effects of internal heating due to penetrating solar radiation and internal storage of heat in brine pockets, and allowed for variation in the specific heat and thermal conductivity of the ice with the temperature. Simplifying the model of Maykut and Untersteiner, Semtner (1976) developed a model for climate studies by using coarse resolution by reducing the number of layers to three. To enable faster long time simulations, he eliminated the heat source term in the diffusion equation and fixed the specific heat and conductivities of snow and ice.

Manabe and Stouffer (1980) and Washington and Meehl (1983) conducted the first climate experiments that included feedbacks between the sea ice and the atmosphere, using simpler formulations of sea ice thermodynamics than Semtner. When the CO₂ concentrations were quadrupled (Manabe and Stouffer, 1980), the ice disappeared completely from the Arctic for several summer months each year. However, in a calculation using three levels in the thermodynamic sea ice model, Semtner (1984) showed that phase and amplitude of the seasonal ice cycle are in error for the zero-layer thermodynamic sea ice and that quadrupling CO₂ did not
result in summertime melting of the Arctic sea ice, in contrast to the Manabe and Stouffer (1980) results.

In the work of Gabison (1987), all the thermodynamic processes and air-ice coupling were included with consideration of ice-ocean interface down to a depth of 60m. The actual depth of the oceanic-mixed layer is determined in the model by the intensity of turbulent mixing, unstable water-density stratification, and tidal mixing. Ebert and Curry (1993) presented a one-dimensional thermodynamic model that reproduced the annual cycle of sea ice growth and decay, and addressed many of the uncertainties inherent in the thermodynamic sea ice model of Maykut and Untersteiner (1971). They introduced an albedo parameterization that was highly sensitive to the surface state and melt pond parameterizations and their effects on the ice thermodynamics. Launiainen and Cheng (1998) constructed a model for simulating ice thickness, ice temperature and air-ice interactions. The model includes calculation of the air-ice interface temperature and surface fluxes, heat conduction in the snow, and ice and heat flux and ice thickness variations at the ice-ocean boundary. Light et al. (1998), studying the effects of included particles on the spectral albedo of sea ice, suggested that even apparently “clean” ice contains trace amounts (5-10g/m³) of particles that can reduce albedo by as much as 5-10% in the visible part of the spectrum.

In previous lake-ice studies, Bilello (1964) modeled lake-ice formation by considering the sensible-heat exchange at the water-air interface. Patterson and
Hamblin (1988) simulated the year-round thermal processes including benthic sediment heat fluxes occurring at the lake bottom. Using an energy balance model, Heron and Woo (1994) studied melt processes during decay of a lake-ice cover in the Arctic. Their calculations indicated that the absorption of short-wave radiation within the ice provided 52% of the melt energy, while 33% and 15% came from surface-energy balance and the heat flux at ice-water interface, respectively.

Rogers et al. (1995) developed a numerical model to simulate the heat budget of a shallow, ice covered, mid-latitude lake. Their model included: snowmelt due to rain, benthic sediment heat transfer, formation of snow-ice and variability in snow density, snow conductivity and albedo. A physically-based mathematical model of the coupled lake, lake ice, snow and atmosphere was developed by Liston and Hall (1995) for studying terrestrial atmospheric interactions in high elevation and high latitude regions. The ability to simulate lake-ice freeze-up, break-up, total ice thickness and ice type offers the potential to describe the effects of climate change in these regions.

The only previous work on Antarctic lake ice was presented by Fritsen et al. (1998). They developed a novel method to calculate the liquid water contents of the ice covers at the end of the austral summer. The method consists of analyzing energy budgets of known depth intervals in the ice during the austral autumn when freezing fronts are propagating from the surface to the bottom of the ice cover. Their simulation results show that Lake Bonney ice contained 9.9%, 33.3% and 23.8%
liquid water located at 0.5-1.0, 1.0-2.0, and 2.0-3.5m respectively, below the ice surface near the end of 1993 melting season. For the year 1994, the liquid water contents were 5.7%, 27.3% and 14.3% at the same depths. Liquid water fractions at Lake Hoare were low (<15%) throughout the ice column at the end of the 1985-1986 summer season. In the following summers (1986-1987 and 1987-1988) liquid water contents reached 50 to 70% within the ice interior between 1.8 to 2.8m depths.

In general, based on the previous discussion, it can be concluded that ice thermodynamics has been studied for many years and well observed. The majority of the previous models were used and verified with very coarse time steps and space resolution, using time steps of one or more days, except the model of Launiainen and Cheng (1998). Their model used one hour time steps as does the model presented in this thesis. Smaller time step allows using finer grid what yields better accuracy in simulation results, what is essential for short time contaminant transport model like this one.

2.2 Previous work on meltwater infiltration

Liquid water from melting of seasonal snow covers, melting glaciers and melting of permanently ice covered regions is critical to the hydrogeological cycle in cold regions. Modeling of snow melting and meltwater infiltration in a snowpack has been a subject of research for many years. One-dimensional models have been developed to describe complex processes of meltwater infiltrations. The simplest
theory was developed by Colbeck (1971, 1972, 1975). Colbeck and Anderson (1982) assumed that the relative permeability of snow has a power law dependence on saturation with exponent $n > 1.0$. To model meltwater in subfreezing snow, Illangasekare et al. (1990) presented a two-dimensional model that considered three major processes: water flow through a porous medium under partially saturated conditions, refreezing of meltwater in subfreezing snow and heat conduction. They demonstrated that various assumptions related to density and porosity variations, dimensionality of flow, capillary effects, etc., which have been made by past investigators for ideal situations may not be valid under many circumstances. For instance, Tseng et al. (1994) presented a physically based mathematical model for snow melting and uniform wetting front migration in a layered subfreezing snowpack. They considered changes in hydraulic and thermal properties due to meltwater infiltration. An enthalpy formulation is used to handle the multiple moving boundary problems.

Sellers (2000), in order to concentrate on the role of the moving boundary, considered only the simplest model of an isothermal snowpack in which he ignored bulk heat conduction, grain metamorphosis, refreezing and spatial inhomogeneities. The planar motion of the surface boundary and the propagation of meltwater waves due to an applied time dependent surface heating were simulated numerically.

During 1973-1974 winter, growth characteristics and mechanical properties of ice on two New Hampshire lakes were studied by Gow et al. (1977). This
investigation included ice thickness measurements, identification of ice types, correlation of ice growth with selected meteorological parameters and the examination of thermal cracks and flaws. They concluded that large ruptures in lake ice usually take the form of cracks which can occur any time the ice is thermally or mechanically stressed.

Mader (1992a and 1992b) investigated a water vein system of ice grown in the laboratory, and Lliboutry (1996) investigated stability of a water vein system, ice permeability and percolation of internal meltwater in temperate glacier ice.

Fountain and Walder (1998), investigating water flow through glaciers, concluded that for temperate glaciers nearly all rain and surface meltwater enters the body of the glacier through crevasses and englacial conduits and that the flux through the veins in the ice is probably negligible. Using dye tracers and water level observations at the Storglaciaren glacier, Hooke et al. (1994) determined that water flow speed through conduits is ~0.01-0.09 m/s.

Eicken et al. (2002), using slug tests adapted to the ice environment, measured sea-ice permeability in the northern Chukchi Sea. Permeability values varied over more than two orders of magnitude as the melt season progressed (10^{-11} to 10^{-9} m²). The overall mean was k_s=2.0x10^{-10} m².

According to previous studies, redistribution and fate of snow and ice meltwater are very important processes for the ice energy and mass balance as it affects ice albedo and heat fluxes through the ice cover. Studies of snow meltwater
infiltrations began in the 1970’s, but more recently research related to meltwater percolation in glaciers has been undertaken. Despite its importance in determining the evolution of the meltwater layers at the surface of ice, very little is known about the magnitude and variability of ice permeability and porosity of sea ice, and almost nothing is known about permeability and porosity for the ice cover of perennially covered lakes in Antarctica.

2.3 Previous work on hydrocarbon contaminant transport in cold regions

The exploration and development of the Arctic region as an important petroleum producing area has resulted in a significant number of hydrocarbon, mostly crude oil, spill accidents. As a result, many research projects have been conducted to understand better the behavior and fate of crude oil products in freezing environments. McMinn (1972) conducted an experiment of spreading of small spills of oil on snow and ice in Arctic mid winter conditions. He also examined aging of oil in snow and cleanup techniques. This study provided considerable useful data with regard to oil spreading. Wilson and Mackay (1987) provided excellent qualitative insight into the processes involved in ice formation and melting in the presence of oil, but only a few quantitative results were presented that would be applicable to future spills.

Dickins and Buist (1999) described the state of knowledge regarding the most applicable countermeasures to deal with oil contamination on, in, or below ice.
Countermeasures are discussed in the context of seasonal variations in ice conditions and observations of oil fate and behavior in a variety of different situations.

Fingas and Hollebone (2003) summarized previous key studies related to oil behaviour in ice environments. They concluded that many methods and mathematical algorithms proposed in the literature are based on limited laboratory experiments, some of the algorithms are based only on one series of experiments or even one experiment and there is a need to verify these experiments on a large scale. They recommended that real spills be studied as much as possible. The complex environments of cold water and ice sometimes cannot be replicated in the laboratory or in a test tank with sufficient accuracy to ensure confirmation to the field.

While contamination in Arctic regions is mostly related to crude oil spills, hydrocarbon contaminations in the Antarctic regions are usually due to fuel spills around current or past scientific research stations, typically located on ice-free areas. Lyons et al. (2000a) evaluated the role of fossil fuel burning from scientific activities in Taylor Valley and compared the fluxes of carbon and nitrogen to natural fluxes within the landscape of the valley. Their calculations suggested that the fossil fuel fluxes for particulate organic carbon and elemental carbon are extremely low, whereas NOx flux is potentially important over decades to century time scales. Balks et al. (2002) investigated the effects of hydrocarbon spills on the soil temperature and moisture regimes by comparing the properties of existing oil contaminated sites with those of nearby, uncontaminated, control sites at Scott Base, the old Marble Point Camp in
the Southern Victoria Land coast and Bull Pass in the Wright Valley. They found that where hydrocarbons accumulated at the soil surface, they contributed to increased soil hydrophobicity and decreased surface albedo. Also they concluded that surface warming at the hydrocarbon contaminated soils are closer to optimum temperature for biological activity for longer period then the controls soils.

To assess the extent and intensity of contamination within abandoned Atlas Cove Station, Heard Island, soil and water samples were collected and analyzed for petroleum hydrocarbons and heavy metals (Stark et al., 2003). They found that contamination by heavy metals was evident throughout the area but not at levels of sufficient magnitude to infer a significant potential impact on local ecosystems. In contrast, contamination by hydrocarbons at the site of the old station was found to be extensive and at a level that may cause a significant impact on the environment. Goldsworthy et al. (2003) investigated human impact and soil and water contamination in the four separate research stations in the Larsemann Hills, East Antarctica. They concluded the cumulative impact of the four facilities was an increase in the number of sites contaminated, rather than increased contamination at specific locations due to the additive effect of overlapping sources. Hydrocarbons were the most common contaminants at all four research facilities, and the activities that caused most contamination are the storage and the use of fuel, maintenance and storage of vehicles and waste disposal. Aislabie et al. (2004) reviewed properties of Antarctic soils, the sources and types of hydrocarbons that accumulate in the soils
following fuel spills, the effects of the hydrocarbons on physical, chemical and biological soil properties and current management strategies for dealing with hydrocarbon contamination in soils. They concluded that current understanding of both the abiotic and biotic effects of hydrocarbon spills on Antarctic soils is incomplete and requires scientific investigation in several disciplines. For example, additional information about the chemical composition of contaminants and co-contaminants (both in spilled products and post-weathering), would improve prediction of spill impacts. Their abiotic fates (including volatilization, adsorption, and dissolution) are only partially known: for example, where hydrocarbons darken the soil surface, they contribute to increased soil temperatures during sunny periods, but possible effects on soil moisture and wettability are poorly known.

There is evidence that recent increased Antarctic exploration and scientific research have led to some significant although localized impacts on the environment. Human impacts occur around current or past scientific research stations, typically located on ice-free areas that are predominantly soils. Fuel spills, the most common occurrence, have the potential to cause the greatest environmental impact in the Antarctic through accumulation of aliphatic and aromatic compounds.

Despite recently increased efforts and activities related to studying ecological implication of the hydrocarbon contamination of the McMurdo Dry Valleys environmentally protected areas, very little is known how much life in perennially ice-covered lakes is affected.
CHAPTER 3

STUDY AREA

Taylor Valley, one of the McMurdo Dry Valleys, the largest ice-free area on
the Antarctic continent, is located on the eastern coast of the Ross Sea (Fig. 2). The
three main Taylor Valley lakes (Bonney, Hoare, and Fryxell) have been the subjects of
study since the discovery of the Dry Valleys by members of R.F. Scott's expedition in
1903 (Doran et al. 1996). They have been studied intensely since the International
Geophysical Year (1957/58) (Priscu, 1998). Because of unique and extremely
environmental conditions, in 1993 this ice-free area was selected as a study site
within the National Science Foundation's Long-term Ecological Research (LTER)
Program.

The lakes of the McMurdo Dry Valleys are unique. They are closed basin,
perennially ice-covered, and the biological communities are dominated by
microorganisms (Voytek et al., 1988; Lizotte and Priscu, 1998; Neale and Priscu,
1998). In addition, the chemical evolution of these lakes is closely tied to their
landscape position and their climate histories (Lyons et al. 2000b). Although the lakes
wax and wane in size as the climate changes, some of them could be very old and
have existed since the mid-Pleistocene or older (Hendy, 2000; Lyons et al. 2005).
Lake Fryxell is land-locked near the mouth of the Taylor Valley and is 5.84 km long and up to 2.06 km wide with an area of 7.08 square kilometers and a total volume of 53.6 million cubic meters (Doran et al. 1996). The average annual air temperature at Lake Fryxell is -20.2°C (Doran et al. 2002). The location is usually accessible between early October and early February. It should be mentioned that ice density calculation, using parameters of average ice thickness and mean piezometric thickness from Table 1., gives ice density value of 0.85, what is to low. This can be explained that ice thickness measurements were conducted at different places at different times, and using these values can produce some errors.

This lake is fed by melt waters of surrounding glaciers, principally the Canada and Commonwealth glaciers on the north side of Taylor Valley and a few small cirque glaciers on the south side of the valley. The lake has a complex morphology, including several small islands and stream deltas that feed into it. Approximately 53 percent of the total lake volume is frozen.

Lake Fryxell is chemically stratified lake and is brackish in its salinity. Lake Fryxell is anoxic below 9m and has by most lake standards very high dissolved organic carbon concentrations with values as high as 30mg C liter⁻¹ (Lyons et al. 1998, McKnight et al. 1991).
<table>
<thead>
<tr>
<th><strong>Morphometric parameter</strong></th>
<th><strong>Value</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum length [km]</td>
<td>5.84±0.01</td>
</tr>
<tr>
<td>Maximum breadth [km]</td>
<td>2.06±0.01</td>
</tr>
<tr>
<td>Shore line length [km]</td>
<td>19.30±0.1</td>
</tr>
<tr>
<td>Maximum depth [m]</td>
<td>20.50±0.5</td>
</tr>
<tr>
<td>Average ice thickness [m]</td>
<td>5.50±0.2</td>
</tr>
<tr>
<td>Mean piezometric thickness [m]</td>
<td>4.70±0.2</td>
</tr>
<tr>
<td>Surface area [km²]</td>
<td>7.08±0.02</td>
</tr>
<tr>
<td>Mean depth [m]</td>
<td>7.6±0.63</td>
</tr>
<tr>
<td>Total Lake Volume [10⁶ m³]</td>
<td>53.57±1.21</td>
</tr>
<tr>
<td>Volume of liquid water [10⁶ m³]</td>
<td>25.24±1.23</td>
</tr>
<tr>
<td>Volume of frozen water [10⁶ m³]</td>
<td>28.33±0.20</td>
</tr>
</tbody>
</table>

Note: Depth datum is at piezometric water level in ice drill holes.

Table 1. Morphometric data for Lake Fryxell (Doran *et al.* 1996)
Figure 2. Location of Taylor Valley and Lake Fryxell
(http://huey.colorado.edu/LTER/images/maps/gla-map.html)

The helicopter crash occurred in the northwestern portion of the lake (Fig. 3) at 77°36'41.09824" S, 163°06'47.22831" E, (Alexander et al. 2003). Its closest proximity to the shoreline and moat is 390m.
Figure 3. Bathymetric map of Lake Fryxell and location of crash site (http://huey.colorado.edu/LTER/images/maps/fryxell.jpg)
CHAPTER 4

MODEL DESCRIPTION

A mathematical model of a physical process can be thought of as a simulation of that process, using mathematical tools. Reliability of simulations and predictions depend on how well the model approximates the field situation.

There are four basic steps involved in the development of computer simulations of physical processes (Alexiades and Solomon, 1993):

- Determination of the physical problem
- Formulation and analysis of the mathematical model
- Discretization of the problem
- Development and implementation of algorithms in a computer code.

After developing, a computer code needs to be verified and confirmed by comparing its results with results generated by analytical method or measured data.
4.1 Determination of the physical problem

To develop a mathematical model of hydrocarbon spill on ice, it is necessary to recognize all the physical processes related to the problem such as melting and creation of ice, heat transport through ice, meltwater percolation, geochemical processes, sediments in ice, etc. Permanently ice covered lakes are unusual environments for modeling of hydrocarbon contaminant dispersion. In addition virtually nothing is known about behavior of various hydrocarbons moving through or over fractured masses of ice. Once released in the ice, hydrocarbons like jet fuel can be found as: free phase; dissolved in meltwater - aqueous phase; volatilize into air - gas phase; and sorbed into ice and sediment in ice - sorbed phase.

Observations at the crash site suggest that the predominant factor influencing the dispersal of fuel and oil was the surface topography. The lake ice surface at the crash site was a complex inter-connecting network of melt pools, channels, cracks, fissures and chambers (Alexander et al., 2003). The air temperature, in January, prior to the accident was relatively warm by Antarctic standards (-4.0 to 6.0°C), providing melting conditions which aided the contaminant transport. Such transport through ice can be horizontal or vertical, but the rate will vary depending on the characteristics of the ice along the pathway. However, as contaminants reach barriers such as solid, less permeable ice or subsurface chambers, they may accumulate and form isolated pockets of high hydrocarbon level.
In this work a one-dimensional model is developed based on the transport of contaminant dissolved in meltwater as aqueous phase, and isolated pockets of hydrocarbons as contaminant sources. Because of the complexity of the problem, the model is divided into three parts. The first part of the model considers the thermodynamics of ice covers and simulates ice thicknesses, ice temperatures and the melting and freezing rates. Ice growth and loss are both strongly influenced by atmospheric forcing and factors controlling the surface heat exchange. The model is based on the one-dimensional time dependent heat conduction equation with penetrating solar radiation. Results from this thermodynamic model, i.e. melting rates and ice thicknesses, are then used as boundary conditions for the second part of the model, which is a flow model. The flow model considers time dependent one-dimensional flow in unsaturated porous media. Finally, the third part involves using the mass transport equation for one-dimensional advection, dispersion and diffusion, so that the time dependent distributions of hydrocarbons in the ice can be calculated.

4.2 Formulation and analysis of the mathematical model

4.2.1 One-dimensional thermodynamic lake-ice model

The thermodynamics of lake-ice is a complex process and attention in this work is focused on:

- the surface heat balance, including determination of the surface temperature and melting at the surface,
the heat flux in the ice layer including heat flux, ice growth and ice
melt from below.

4.2.1.1 Surface heat balance and determination of the surface
temperature

For an ice surface, heat is in thermal equilibrium with the atmosphere, the
sum of the fluxes is equal to zero, according to Maykut and Untersteiner (1971):

\[(1 - \alpha) \cdot F_r - I_o + F_L + F_s + F_e + F_c + F_m = 0\] (1)

where \(\alpha\) is albedo [-]; \(F_r\) is incoming shortwave solar flux [Wm\(^2\)]; \(I_o\) is shortwave flux
penetrating into the ice [Wm\(^2\)]; \(F_L\) is longwave flux [Wm\(^2\)]; \(F_s\) is sensible heat flux
[Wm\(^2\)]; \(F_e\) is latent heat flux [Wm\(^2\)]; \(F_c\) is conductive heat flux [Wm\(^2\)]; \(F_m\) is heat flux
[Wm\(^2\)] due to melting or freezing of ice at the surface. Equation (1) can be rewritten
in form:

\[F(T_s) = \sum F + \sum F(T_s) = 0\] (2)

where \(F\) denotes fluxes that do not depend on the surface temperature \(T_s\) [°C], and
\(F(T_s)\) represents fluxes depending on it. Surface temperature can be calculated using
an iterative method and equation (3)

\[T_s^{n+1} = T_s^n - \frac{F(T_s^n)}{F'(T_s^n)}\] (3)

where \(F'(T_s^n)\) denotes the derivative term with respect to \(T_s\) at the \(n\)th step.

If the surface temperature is to exceed the melting point \(T_s = T_m\) the melting is
controlled by the surface heat balance, then the surface heat flux is
\[ F(T_f) = -\rho_i L_f \frac{dH_i}{dt} \]  

where \( \rho_i \) is the ice density [kg m\(^{-3}\)], \( L_f \) is the latent heat of freezing [J kg\(^{-1}\)] and \( dH_i/dt \) is the ice thickness change at the surface.

In model presented in this thesis, instead of calculating surface temperature, measured surface temperatures will be used.

### 4.2.1.2 Heat flux in ice

The conservation of heat in the ice layer is given by the one-dimensional transient heat conduction equation,

\[ (\rho c_i) \frac{dT_i(z,t)}{dt} = -\frac{\partial}{\partial z} K_i \left( \frac{\partial T_i(z,t)}{\partial z} \right) + F_{sr}(z,t) \]  

where \( T(z,t) \) is the temperature, \( c_i \) is the heat capacity of ice [J kg\(^{-1}\) °C\(^{-1}\)], \( t \) is the time, \( K_i \) is the thermal conductivity of ice [W m\(^{-1}\) °C\(^{-1}\)], \( z \) [m] is depth measured positive downward from the upper surface and \( F_{sr}(z,t) \) [Wm\(^{-2}\)] is an internal heat source term, such as the solar radiation flux. Part of the solar radiation penetrates into the ice and usually is approximated as a portion of the incident shortwave radiation:

\[ F_{sr} = \kappa \cdot i_o \cdot F_r \cdot (1 - \alpha) \cdot e^{-\kappa z} \]  

Equation (7) was introduced by Maykut and Untersteiner (1971)

\[ \rho c \frac{dT}{dt} = \frac{\partial}{\partial z} K \frac{\partial T}{\partial z} + F_r \cdot i_o \cdot (1 - \alpha) \cdot \kappa \cdot e^{-\kappa z} \]  

where \( i_0 \) is the cloudiness factor, \( \kappa \) [m\(^{-1}\)] is the extinction coefficient, \( \alpha \) is albedo, and \( F_r \) is incoming shortwave solar flux [Wm\(^{-2}\)].
Based on measurements in sea ice by Grenfell and Maykut (1977) $i_0$ is taken as 0.18 and 0.35 for white ice under clear and overcast skies, respectively, and as 0.43 and 0.63 for blue ice or melt ponds under clear and overcast skies.

The albedo of ice cover is defined as the fraction of the incident irradiance reflected from the surface: (Perovich, 1996)

$$\alpha(\lambda) = \frac{F \uparrow (0, \lambda)}{F \downarrow (0, \lambda)}$$  \hspace{1cm} (7)

The total albedo depends on the spectral distribution of the incident irradiance as well as on the spectral albedo of the surface. Thus, a change in cloud conditions, and thereby the incident spectral irradiance, can result in changes in the total albedo (Grenfell and Maykut 1977).

The range of albedo associated with the polar ice pack spans almost the entire range of albedo of different surfaces (Fig. 4). Generally the total albedo is highest for thick, snow-covered (multi-year) ice and lowest for melting or thin ice.

![Bulk Albedo](image)

*Figure 4. Range of total albedo observed for different pack-ice surfaces (Perovich, 1996)*
Grenfell and Perovich (2004) investigated albedo for different types of ice and under different conditions. Spectral and wavelength-integrated albedo were measured from November 1999 through June 2002 at four sites including Tundra, a freshwater lake (Imikpuk Lake) a seawater lagoon (Elson Lagoon) and shorefast sea ice (Chukchi Sea) near Barrow, Alaska (Table 2). They reported that as melt season progressed, albedo decreased at all sites due to the melting of the snow cover and the decay of the ice.

<table>
<thead>
<tr>
<th>Surface Type</th>
<th>$\alpha$ [Clear]</th>
<th>$\alpha$ [Cloudy]</th>
<th>$\Delta\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cold snow</td>
<td>0.851</td>
<td>0.928</td>
<td>0.077</td>
</tr>
<tr>
<td>Melting snow</td>
<td>0.607</td>
<td>0.678</td>
<td>0.071</td>
</tr>
<tr>
<td>Deteriorated melting ice</td>
<td>0.436</td>
<td>0.492</td>
<td>0.056</td>
</tr>
<tr>
<td>Undeteriorated melting ice</td>
<td>0.294</td>
<td>0.332</td>
<td>0.037</td>
</tr>
<tr>
<td>Blue-green ice</td>
<td>0.273</td>
<td>0.309</td>
<td>0.036</td>
</tr>
<tr>
<td>Dirty ice</td>
<td>0.347</td>
<td>0.367</td>
<td>0.020</td>
</tr>
<tr>
<td>Early melt pond</td>
<td>0.239</td>
<td>0.266</td>
<td>0.027</td>
</tr>
<tr>
<td>Late melt pond</td>
<td>0.129</td>
<td>0.141</td>
<td>0.012</td>
</tr>
<tr>
<td>Dry tundra</td>
<td>0.173</td>
<td>0.151</td>
<td>-0.022</td>
</tr>
<tr>
<td>Wet tundra</td>
<td>0.124</td>
<td>0.114</td>
<td>-0.010</td>
</tr>
</tbody>
</table>

$\Delta\alpha$ is the difference [$\alpha$ (Cloudy) — $\alpha$ (Clear)].

Table 2. Total albedo for different surfaces under clear and cloudy sky conditions (Grenfell and Perovich, 2004)

They also concluded that the structure of lake ice was significantly different from that of sea ice because of the lack of sub-millimeter scale inhomogeneity due to brine inclusions. As a result, volume scattering in the fresh ice was significantly smaller, producing lower albedo over areas where snow cover was thin or absent.
McKay et al. (1994) reported spectral measurements of transmission through the ice cover of Lake Hoare in Taylor Valley as well as spectral albedo of the lake ice (Fig. 5).

![Graph showing spectral albedo of various ice conditions](image)

**Figure 5.** Spectral albedo of the Lake Hoare ice cover and beach sand (McKay et al. 1994)

As albedo, the extinction coefficient in ice also depends strongly on wavelength, on the structure of the ice, and on sky conditions (Grenfell and Maykut, 1977), and (Perovich, 1996), and can be defined as a measure of loss due to scattering and absorption. Albedo of ice is typically determined from measurements of incident, reflected, and transmitted light. Transmission measurements are difficult and demanding, and consequently there have been far fewer observations of extinction coefficient than of albedo (Perovich, 1996). Most of the reported sea ice spectral extinction coefficients have been calculated using a two-stream radiative transfer model (Perovich, 1996). The magnitude of the extinction coefficient is largely
a function of the amount of scattering, whereas the wavelength dependence is determined by absorption. Scattering is the dominant process in the ice cover and results primarily from bubbles in the lower layer in ice, from brine inclusions in ice, from irregular structures and defects in the ice, and from the glaze on upper surface. The drained surface layer of multiyear sea ice (white ice scattering) contains an abundance of air inclusions which formed as a result of brine drainage. These air inclusions cause considerable scattering, and extinction coefficients are large (Perovich, 1996). In the interior of white ice there are fewer air bubbles and extinction coefficients are correspondingly smaller. Extinction coefficient values for sea ice are shown in the Table 3 introduced by Grenfell and Maykut (1977). For the lake-ice extinction coefficient value is much smaller comparing to sea ice extinction coefficients. McKay et al. (1994) and Liston and Hall (1995) used value of 0.16 and 0.5 m\(^{-1}\) respectively.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Clear</th>
<th></th>
<th>Cloudy</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Blue</td>
<td>White</td>
<td>Blue</td>
<td>White</td>
<td></td>
</tr>
<tr>
<td>(i_0)</td>
<td>0.43</td>
<td>0.18</td>
<td>0.63</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>(\kappa\text{[m}^{-1})]</td>
<td>1.5</td>
<td>1.6</td>
<td>1.4</td>
<td>1.5</td>
<td></td>
</tr>
</tbody>
</table>

Table 3. Values for \(i_0\) and \(\kappa\) for sea ice (Grenfell and Maykut 1977)

4.2.1.3 Heat flux, ice growth and ice melt from below

At the lower boundary, i.e. the ice bottom, the sum of the lake water heat flux \(F_w\) and conductive flux \(F_c\) is balanced by the release or consumption of the latent of freezing/melting for a thickness change \(dH/dt\) of ice density \(\rho\), or
\[ F_c + F_w + F_r(z) + \rho \cdot L \frac{dH}{dt} = 0 \]  \hspace{1cm} (8)

\( F_w \) can be calculated by \( F_w = K_w \frac{dT_w}{dz_w} \) where \( K_w \) is thermal conductivity of water, \( \frac{dT_w}{dz_w} \) is thermal gradient. The average thermal gradient for Lake Fryxell has been calculated based on measurement of temperature of lake water at various depth over the period from 1995 to 1999 conducted by LTER McMurdo Dry Valleys, Limnology group (http://huey.colorado.edu/LTER/lakedata.html).

**Assumptions**

To formulate the mathematical model one needs to simplify the complex phase change processes such as melting and freezing of lake ice. In addition some reasonable assumptions are needed regarding the heat flux. These assumptions are:

- Heat transfer is isotropic and by conduction and radiation, all other effects are negligible;
- Latent heat is constant and released or absorbed at the phase change temperature;
- Phase change temperature is a fixed known temperature (melting temperature of ice, 0°C);
- Melting is only phase change process, thus condensation, sublimation and evaporation are neglected;
• No variations of thermo-physical properties of ice ($c_i=$ const, $K_i=$ const);

• Density changes with freezing and melting between water and ice are neglected for the formulation of Stefan condition and are assumed to be constant.

4.2.2 One-dimensional meltwater infiltration model

Despite the importance of ablation processes at the lake surfaces in mass loss of water from the lakes (Clow et al. 1988), little is known about the fate of meltwater generated during the melting season in these Taylor Valley lakes. The redistribution of surface meltwater is hence of critical importance for the ice heat and mass balance as it affects ice albedo and heat fluxes through the ice cover. Downward percolation of meltwater into the porous ice matrix has been shown to strongly affect thermal and optical properties of summer sea ice. The ice cover evolution and water mass balance of the sea ice are significantly affected by ice hydrological processes and ice macroscopic properties, in particular permeability (Eicken et al, 2004). Position of the hydrostatic water table within ice or melt ponds largely depends on the surface melting rate and the permeability of underlying ice. The permeability also affects the transport of particulate and dissolved matter through the ice, which influences nutrient supply to biological communities in these lakes.
Modeling of snow melting and meltwater infiltration into a snowpack has been a subject of research for many years. A number of one-dimensional models have been developed to describe the complex processes of meltwater infiltrations into snow, but none of them examine meltwater infiltration into fractured ice (Colbeck, (1972), Illangasekare et al., (1990), Tseng et al., (1994), Launainen and Cheng (1998)).

Alternatively, infiltration of water through soil or water flow through unsaturated porous media has been studied for agricultural purpose, hydrological and hydrogeological investigations and the modeling of contaminant migration in vadose zone (Celia et al. (1990), van Dam and Feddes (2000), Russo et al. (2001), Hansson et al. 2004), Huang et al. (1996)). This thesis develops a model of ice meltwater infiltration into ice that is similar to models related to unsaturated flow in soils.

To quantify water fluxes into unsaturated porous media, and in this case, fractured ice, Darcy's equation commonly is used. For one-dimensional flow Darcy's equation can be written as

\[ q = -K(h) \left[ \frac{\partial(h + z)}{\partial z} + \cos \beta \right] \]  

where \( q \) is water flux in ice [m h\(^{-1}\)], \( K \) is hydraulic conductivity [m h\(^{-1}\)], \( h \) is water pressure head [m], \( \beta \) is the angle between the flow direction and the vertical axis and \( z \) is vertical coordinate [m].
Water balance considerations of an infinitely small ice volume result in the continuity equation for water in ice and is written

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} - S$$

(10)

where $\theta$ is volumetric water content [m$^3$ m$^{-3}$], $t$ is time [h] and $S$ is a sink term.

The combination of equations (9) and (10) provides the general flow equation in variably saturated media, known as Richards’ equation

$$\frac{\partial \theta}{\partial t} = C_{(w)}(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + \cos \beta \right) \right] - S$$

(11)

where $C_{(w)}$ is water capacity $\frac{\partial \theta}{\partial h}$ [m$^{-1}$].

**Assumptions**

Because water flow through ice is highly complex and irregular, some reasonable assumptions are needed for describing flow and the mass transport phenomena. These assumptions are:

- There are no channel flows or flow fingers ahead of the wetting front due to local concentration of water. Thus, the front advances uniformly and Richards’ equations can be applied.
- The medium is homogeneous and isotropic;
- The possible effect of ponding has been neglected. In the case of ponding, the surface flux is assumed to be equal to saturated hydraulic conductivity;
• Water is incompressible ($\rho$=constant);
• Air does not restrict water from filling void space.

4.2.3 One-dimensional solute transport model

The past several decades have seen considerable progress in the understanding and mathematical description of water flow and solute transport processes in the unsaturated zone. A variety of analytical and numerical models are now available to predict water and solute transport processes between the surface and the groundwater table (Simunek et al. (1998), Kroes and van Dam, (2003)).

Whereas in the unsaturated zone the solute transport is predominantly vertical, after entering in the groundwater solutes may move in any direction. The most popular solute transport models are based on the Fickian advection dispersion equation. Three main solute transport mechanisms in unsaturated media are advection, diffusion and dispersion.

Bulk solute transport occurs when solutes are carried along with the moving water. The mean flux of this transport is called **advective flux**, [g m^{-2} h^{-1}]

$$ q_{adv} = qC $$

(12)

where $q$ is considered as Darcy flux [m h^{-1}], which is averaged over certain cross section, and $C$ is solute concentrations in water [kg m^{-3}]. A fundamental difference between fully and partially saturated conditions lies in calculating the cross sectional area where transport occurs, and the volume of water in which solute accumulation
occurs. The cross sectional area of flow under fully saturated conditions is taken as the porosity or effective porosity multiplied by the bulk cross sectional area of porous material. Under partially saturated conditions, the area of flow is taken as that part of the bulk cross sectional area that is actually occupied by liquid, and is interpreted as the product of water content and bulk cross sectional area of porous material.

\[ v = \frac{q}{\theta} \]  

(13)

**Diffusion** is the process of solute transport which is caused by the solute gradient. The solute flux caused by diffusion \( q_{\text{dif}} \) is generally described by Fick's first law:

\[ q_{\text{dif}} = -\theta D_{\text{dif}} \frac{\partial C}{\partial z} \]  

(14)

where \( D_{\text{dif}} \) is the diffusion coefficient \([m^2 \ h^{-1}]\). The diffusion coefficient is very sensitive to the actual water content, as it strongly affects the solute transport path and the effective cross sectional transport area.

In the model presented, \( D_{\text{dif}} \) is calculated using the following equation: (Kroes and van Dam, 2003),

\[ D_{\text{dif}} = D_w \frac{\theta^{1.3}}{\theta_s^2} \]  

(15)

where \( D_w \) is the solute diffusion coefficient in free water \([m^2 \ h^{-1}]\) and \( \theta_s \) is the saturated water content \([m^3 m^{-3}]\).
The variety of water velocities cause some solutes to advance faster than average solute front, and other solutes to advance slower. The overall effect will be that dispersion spreads solute mass beyond the region it normally would occupy due to advection alone. If the time required for solutes to mix in the transverse direction is small compared to the time required for solutes to move in the flow direction by mean advection, the dispersion flux $q_{dis}$ is proportional to the solute gradient

$$q_{dis} = -\partial D_{dis} \frac{\partial C}{\partial z}$$

(16)

where $D_{dis}$ is the dispersion coefficient [m$^2$ h$^{-1}$] and under laminar flow conditions the dispersion coefficient is proportional to the pore water velocity (13) (Domenico and Schwartz, 1990):

$$D_{dis} = L_{dis} |v|$$

(17)

where $L_{dis}$ is longitudinal dispersivity [m]. Dispersivity depends on the scale over which the water flux and solute advection are averaged. In a compilation (Gelhar et al., 1992) of macroscopic dispersivities from 59 field tracer studies (Fig. 6) longitudinal dispersivity clearly increase with the scale of field sites.
The total solute flux $q_{tot}$ is therefore described by sum of all three fluxes:

$$q_{tot} = q_{adv} + q_{dif} + q_{dis} = qC - \theta(D_{dif} + D_{dis}) \frac{\partial C}{\partial z}$$  \hspace{1cm} (18)

Considering conservation of mass in an elementary volume, a one dimensional advective-dispersion solute transport equation can be derived (Zheng and Bennet, 2002) assuming equilibrium-controlled sorption and first order decay

$$\frac{\partial (\theta RC)}{\partial t} = \frac{\partial}{\partial z} \left( \theta D \frac{\partial C}{\partial z} \right) - \frac{\partial}{\partial z} (qC) + q_s C_s - \lambda_1 \theta C - \lambda_2 \rho_b C$$  \hspace{1cm} (19)

where $R$ is retardation factor, $D = D_{dis} + D_{dif}$ is dispersion [$m^2 h^{-1}$], $q_s$ is the flow rate of a fluid source or sink [$m h^{-1}$], $C_s$ is concentration of the fluid source or sink flux [$kg m^{-3}$], $\lambda_1$ and $\lambda_2$ are the reaction rate constants for the dissolved and sorbed phase.
respectively \([h^1]\), \(\rho_o\) is the bulk density of the porous medium \([\text{kgm}^{-3}]\), and \(\tilde{C}\) is the sorbed concentration.

A significant body of research exists for the behavior and the fate of hydrocarbons is known for soil, but much less research has been conducted to understand behavior and fate of hydrocarbon contaminants in ice. Therefore in this work, a number of important assumptions were adopted: chemical, geochemical reactions or biodegradation that cause some attenuations of contaminant transport are not known, thus equation (19) will be simplified involving only advection and dispersion.

\[
\frac{\partial (\theta C)}{\partial t} = \frac{\partial}{\partial z} \left( \theta D \frac{\partial C}{\partial z} \right) - \frac{\partial}{\partial z} (qC)
\]

(20)

4.3 Discretization of the problem

4.3.1 Numerical approximation of thermodynamic lake-ice model

As mentioned earlier, the model presented in this thesis is divided in two parts. The first part presents numerical solutions of one-dimensional thermodynamic model of melting and freezing of lake ice. The melting of ice was first treated by Stefan (Crank, 1984) and after whom problems such as phase change or moving boundary problems are widely referred as Stefan Problems. The characteristic of phase-change problems is that, in addition to the temperature field, the location of the interface is unknown. There are two main methods to resolve moving boundaries: a variable space grid method and fixed grid method. Of all the methods,
Crank (1984), pointed out that the enthalpy method with a fixed grid is the simplest to handle. The most significant advantage of this formulation is that there is no need to track movement of the phase change interface. Its position is determined when the solution is complete.

Alexiades and Solomon (1993) introduced a so-called enthalpy or weak solutions approach, which is based on the fact that the energy conservation law, expressed in terms of energy (enthalpy) and temperature, together with the equations of state, contain all the physical information needed to determine evolution of the phases.

To introduce and explain the basic methodology let us first consider a finite ice slab, \( 0 \leq z \leq l \) (\( l \) = model domain length) with a known initial temperature distribution, \( T_{ini}(z) \). Starting at time \( t=0 \), the slab at \( z=0 \) (ice surface) is imposed with surface temperature and radiation from the sun. At the bottom (\( z=l \)) ice cover is imposed with water temperature. The finite ice slab can be partitioned into \( M \) sub-regions called control volumes, \( V_1, V_2, \ldots V_M \). With each sub-region \( V_j \) a node \( z_j \) is associated as a point inside of \( V_j \), (Fig. 7) where \( \Delta z_j \) is the length of \( j \)th interval.
Figure 7. Space - time grid

A finite-difference discretization of the heat equation (21)

\[ (\rho c)_j \frac{\partial T_j(z,t)}{\partial t} = -\frac{\partial}{\partial z} K_j \left( \frac{\partial T_j(z,t)}{\partial z} \right) \]  

(21)

may be derived that has direct physical meaning, as the discrete heat balance  
(Alexiades and Solomon, 1993) in its primitive form is:

\[ E_i + q_z = 0 \]  

(22)

with \( E_i \) is thermal energy density per unit volume – volumetric enthalpy,

\[ E = \int_{T_{ref}}^{T} \rho c dT = \rho c d(T - T_{ref}) \]  

(23)
where $T_{ref}$ is some convenient reference temperature and $q_z$ is the heat flux.

$$q = -kT_z$$  \hspace{1cm} (24)

Integrating equation (22) over the control volume $V_j$ and over the time interval $[t_n, t_{n+\Delta t_n}]$, we find that

$$
\int_{t_n}^{t_{n+\Delta t_n}} \frac{\partial}{\partial t} \left( A \int_{z_j}^{z_{j+1/2}} E(z,t) \, dz \right) \, dt = - \int_{t_n}^{t_{n+\Delta t_n}} A \int_{z_j}^{z_{j+1/2}} q_z(z,t) \, dz \, dt
$$  \hspace{1cm} (25)

where $A$ is the surface area of the control volume (in one-dimensional models $A=1$).

Dividing the constant cross-sectional area $A$, and integrating the derivatives yields

$$
\int_{z_j}^{z_{j+1/2}} \left. E(z,t) \, dz \right|_{t=t_{n+\Delta t_n}} \bigg|_{t=t_n} = - \int_{t_n}^{t_{n+\Delta t_n}} \left[ q(z_{j-1/2},t) - q(z_{j+1/2},t) \right] \, dt
$$  \hspace{1cm} (26)

Assuming that the time increment $\Delta t_n$ may be so brief that during the time $(t_n, t_{n+\Delta t_n})$ the fluxes are approximately constant, and arbitrarily close to their values at any intermediate time in this interval. Let $t_{n+\varepsilon} := t_n + \varepsilon \cdot \Delta t_n = (1-\varepsilon) \cdot t_n + \varepsilon \cdot t_{n+1}$ be some intermediate time with $0 \leq \varepsilon \leq 1$. Then equation (26) can be approximated by

$$
\{ E(z_j,t_{n+1}) - E(z_j,t_n) \Delta z_j = \Delta t_n \left[ q(z_{j-1/2},t_{n+\varepsilon}) - q(z_{j+1/2},t_{n+\varepsilon}) \right] \}, \quad j = 1, \ldots, M \quad (27)
$$

which constitutes a complete discretization of the conservation law (22). To obtain the finite-difference numerical scheme, equation (27) can be written as

$$
E_j^{n+1} - E_j^n = \frac{\Delta t_n}{\Delta z_j} \left[ q_{j-1/2}^{n+\varepsilon} - q_{j+1/2}^{n+\varepsilon} \right] \quad j = 1, \ldots, M
$$  \hspace{1cm} (28)

The thermal state of the control volume, $V_j$, and the time, $t_n$, are completely determined by the enthalpy $E_j^n$. 

42
Choosing ε = 0, the fluxes can be evaluated at the old time, \( t_n \), and equation (28) can yield an explicit scheme to determine enthalpy approximation at the advanced time step \( t_{n+1} \). For ε = 1 we have a fully implicit scheme, and for ε = 0.5, the Crank-Nicolson numerical scheme.

These schemes require approximations of the fluxes across the faces located at \( z_{j-1/2} \) and \( z_{j+1/2} \). The conductive flux is given by

\[
q = -kT_z \approx -k \frac{\Delta T}{\Delta z} \quad \text{or numerically} \quad q_{j-1/2} = -k_{j-1/2} \frac{T_j - T_{j-1}}{z_j - z_{j-1}}
\]  

(29)

where \( k \) is thermal conductivity. Generally, the conductivity is not constant but a function of the location (liquid or solid phase), and of the temperature \( k = k(z, T) \). Considering this statement, Alexiades and Solomon (1993) introduced the parameter, thermal resistance, defined as the length of the resistance path divided by the thermal conductivity. The resistance between two adjacent control volumes (Fig. 8) is given by

\[
R_{j-1/2} = \frac{0.5\Delta z_{j-1}}{k_{j-1}} + \frac{0.5\Delta z_j}{k_j}
\]

(30)

and the conductive flux (29) is expressed as

\[
q_{j-1/2} = -\frac{T_j - T_{j-1}}{k_{j-1/2}} \quad j = 2, ..., M
\]

(31)

\[\frac{1/2 \Delta z_{j+1}}{k_{j+1}} \quad \frac{1/2 \Delta z_j}{k_j} \]

\[z_{j}, \Delta z_{j+1} \quad z_{j+1/2} \quad \Delta z_{j} \quad z_{j} \]

Figure 8. Resistance of adjacent control volumes
The idea of the enthalpy approach is very simple, direct and physically based. The volume occupied by the phase change material is partitioned into a finite number of control volumes and the energy conservation law is applied to each control volume to obtain a discrete heat balance. Knowing that the enthalpy of the liquid is the sum of the sensible and the latent heat, instead of (23) we have

$$E(z, t) = \begin{cases} \int_{z_{1(t)}}^{z_{2(t)}} \rho c_s dT, & T(z, t) < T_m \quad (S \cdot \text{solid}) \\ \int_{z_{1(t)}}^{z_{2(t)}} \rho c_s dT + \rho L, & T(z, t) > T_m \quad (L \cdot \text{liquid}) \end{cases}$$  \hspace{1cm} (32)$$

The phases are described by liquid fraction of a control volume defined as

$$E(z, t) \leq 0 \quad \Rightarrow \quad \text{solid at } (z, t) \quad \lambda = 0$$
$$0 \leq E(z, t) \leq \rho L \quad \Rightarrow \quad \text{interface at } (z, t) \quad \lambda = E/\rho \cdot L$$
$$E(z, t) \geq \rho L \quad \Rightarrow \quad \text{liquid at } (z, t) \quad \lambda = 1$$  \hspace{1cm} (33)$$

Consider the case in which $c_s$ and $c_L$ = constant then (32) becomes

$$E = \begin{cases} \rho c_s [T - T_m], & T < T_m \\ \rho c_L [T - T_m] + \rho L, & T > T_m \end{cases}$$  \hspace{1cm} (34)$$

or solving for $T$

$$T = \begin{cases} T_m + \frac{E}{\rho c_s}, & E \leq 0 \quad \Rightarrow \quad \text{solid} \\ T_m, & 0 < E < \rho L \quad \Rightarrow \quad \text{interface} \\ T_m + \frac{E - \rho L}{\rho c_L}, & E \geq \rho L \quad \Rightarrow \quad \text{liquid} \end{cases}$$  \hspace{1cm} (35)$$
4.3.1.1 Discretization of initial conditions

To build a time dependent hydrodynamic lake-ice model, a set of initial conditions must be defined. These initial conditions define the initial status of ice thickness and ice temperature. Ice temperature data were provided by LTER McMurdo Dry Valleys, Limnology group (www.huey.colorado.edu/LTER/lakedata.htm). The data are derived from seven thermistors in the Lake Fryxell ice cover. Temperatures were measured at the surface and at the depths 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 m below the surface.

Analyzing the ice temperature gradients when the freezing fronts had reached the bottom of the ice, assuming that the temperature at the solid-liquid interface is 0°C, the ice thickness, as well as the temperature gradient in deeper parts of ice can be estimated. Linear profiles in the empirical data ($R^2=0.9994$) are found during late winter to early spring, (i.e. October 2002) and assuming that this linearity is the same through the entire ice profile, the depth at which the ice temperature was 0°C was then assumed to be thickness of the ice which is 5.5m (Fig. 9). This method is confirmed by analyzing the measured ice thicknesses data of the Lake Fryxell, from 1995 – 1999.

Ice thickness strongly depends on locations of the measurement (Fig. 10), what can be explained by variations of surface albedo, sediment content, etc.
Calculated ice thickness of 5.5m occurs inside of measured interval between 3.4 and 5.75m shown on Fig 10. Ice temperature at various depth are presented by equation (36).

\[ T_j^0 = T_{ini}(z_j), \quad j = 1, ..., M \quad \text{where} \quad T_{ini} = 4.9557 \ z_j - 28.286 \]  

(36)

Figure 9. Temperature profile in the ice cover of Lake Fryxell October 1, 2002.
Figure 10. Lake Fryxell ice thickness through time
(http://huey.colorado.edu/LTER/datasets/lakes/lakeice/icethick.html)

4.3.1.2 Discretization of boundary conditions

Boundary conditions are mathematical statements specifying the dependent variable (temperature) or the derivative of the dependent variable (heat flux) at the boundaries of the problem domain. The correct selection of boundary conditions is a critical step in model design (Anderson and Woessner, 2002).

Treatments of boundary conditions are represented by the following three types of mathematical conditions:

Type 1 Specified temperature (Dirichlet conditions) for which temperature is given.

Type 2 Specified flux boundaries (Neumann conditions) for which the flux across the boundary is given, and
Type 3 Temperature dependent flux boundaries (Cauchy or mixed boundary conditions) for which flux across the boundary is calculated from a given boundary temperature value.

**Boundary condition at x=0**

In this model, for the upper boundary, type 3 – Cauchy boundary condition has been applied. The surface boundary flux is presented as the sum of the flux calculated by the imposed temperature and the fraction of solar radiation flux penetrated at the surface ice.

\[
q_{n}^{1/2} = -\frac{T_{i}^{n} - T_{s}^{n}}{R_{1/2}} + i_{o} \cdot F_{r} \cdot (1 - \alpha) \cdot \kappa 
\]  

(37)

\[
T_{s}^{n} = T_{s}(x_{n}), \quad n = 0, 1, 2, ..., \quad \text{and} \quad R_{1/2} = \frac{0.5\Delta x}{k_{l}}
\]  

(38)

where \(T_{s}\) is the surface temperature and \(n\) is the time step

**Boundary condition at z=1**

For the lower boundary \((z=1)\) Type 2 – Neumann boundary condition has been applied, where the specified flux is calculated as the sum of the heat flux from lake water and the fraction of the solar radiation at the bottom of ice slab. The total heat flux at the bottom of the lake is calculated by equation (39)

\[
q_{M,1/2}^{n} = -K_{w} \frac{\Delta T_{w}}{\Delta x} + i_{o} \cdot F_{r} \cdot (1 - \alpha) \cdot \kappa \cdot e^{-\chi(z)}
\]

(39)

where \(Z\) is ice thickness, \(K_{w}\) is thermal conductivity of water, \(T_{w}\) is water temperature. A calculation of heat flux from the lake water is based on water temperature
measurements conducted in Lake Fryxell by LTER McMurdo Dry Valleys, Limnology group (http://huey.colorado.edu/LTER/lakedata.html).

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_w$</td>
<td>Thermal conductivity of water [W m$^{-1}$ °C$^{-1}$]</td>
<td>0.56</td>
</tr>
<tr>
<td>$\frac{dT_w}{dz_w}$</td>
<td>Thermal gradient</td>
<td>0.52</td>
</tr>
<tr>
<td>$F_w=\frac{dT_w}{dz_w} K_w$</td>
<td>Heat flux from lake water [Wm$^{-2}$]</td>
<td>0.29</td>
</tr>
</tbody>
</table>

Table 4. Calculations of heat flux at the bottom of ice

4.3.2 Numerical approximation of unsaturated flow equation

The prediction of fluid movement in a variable saturated porous media is an important problem in many fields of sciences and engineering. The theory of flow involving either one or more fluids through porous media is well established and generally accepted in the literature for both saturated and unsaturated conditions (Domenico and Schwartz, 1990, and Simunek et al., 1998). Under unsaturated conditions both fluid and air flow through pores. It is clear that the air filled pores will reduce the effective cross section for liquid flow and will increase tortuosity of the remaining liquid flow path. Hence hydraulic conductivity for unsaturated flow is less than for saturated flow and becomes a function of water content (Mualem, 1976).

In virtually all studies, partially saturated flow is assumed to obey the classical Richards' equation (40). In the last two decades, various numerical routines to solve the Richards' equation have been developed (Celia et al., 1990, and Huang et al.,
Richards' equation is difficult to solve because of its parabolic form in combination with the strong non-linearity of the hydraulic functions which relate water content, water head pressure and hydraulic conductivity.

\[
\frac{\partial \theta}{\partial t} = C_{(w)}(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + \cos \beta \right) \right] - S \tag{40}
\]

To introduce a numerical scheme of the Richards' equation, due to complexity of problem, an established conceptual model is needed. The purpose of building a conceptual model is to simplify the field problem, and organize the associated field data so that the system can be analyzed more readily (Anderson and Woessner, 2002). The first step in formulating the conceptual model is to define the model domain, i.e. to identify the boundaries of the model.

Model domain definition in this problem is based on Archimedes's Law. Water and ice have different densities, and because the ice density is less than the density of water, ice floats in the water. Knowing the ice thickness and differences in densities, the submerged part of the ice can be calculated by

\[
h_s = \frac{\rho_i}{\rho_w} \cdot H \tag{41}
\]

where \(H\) is ice thickness and \(\rho_i\) and \(\rho_w\) densities of ice and water respectively.

It is assumed that unsaturated conditions exist in the part of ice above lake level, and fully saturated conditions exist in the ice under the water surface. Based on
data from the thermodynamic model, the unsaturated thickness is calculated for each
time step and the model parameters are linearly interpolated.

Richards’ equations (40) can be solved by finite element or finite-difference
numerical methods, where the finite element method is advantageous for irregular
geometries in two and there-dimensional flow domains (Wang and Anderson, 1982).
In one dimension, the finite difference method is advantageous because it is relatively
easy to conceive and to implement in numerical routines.

The finite-difference scheme of Richards’ equation (40) can be solved with an
explicit linearization of $K$, $C$ and $S$ (Belmans et al, 1983)

$$
\frac{h_j^{n+1} - h_j^n}{\Delta t^n} = \frac{K_j^{n-\frac{1}{2}} \left( \frac{\Delta h_j^{n+1}}{\Delta z_u} + 1 \right) - K_j^{n+\frac{1}{2}} \left( \frac{\Delta h_j^{n+1}}{\Delta z_l} + 1 \right)}{C_{(w)j} \Delta z_j} - \frac{S_j^n}{C_{(w)j}} \tag{42}
$$

where subscript $j$ is the node number (increasing downward), and superscript $n$ is the
time level.

The model presented in this thesis applies the implicit, finite-difference
numerical scheme of equation (42), with some adaptations from that of van Dam et
al. (1997), that is currently used in SWAP (Soil-Water-Air-Plant environment).

The most important adaptations made here concern the evaluation of the $C_{(w)}$
term. Because of the high non-linearity of $C_{(w)}$, averaging during a time step results in
serious mass balance errors when highly transient conditions are simulated.

A simple but effective adaptation was suggested and analyzed by Celia et al.
\[ \theta_j^{n+1} - \theta_j^n = C_{(w)j}^{n+(1/2)} \left( h_j^{n+1} - h_j^n \right) \]

(43)

Instead of application during a time step, where \( C_{(w)j}^{n+(1/2)} \) denotes the average water capacity during the time step, they applied the following at each iteration step:

\[ \theta_j^{n+1} - \theta_j^n = C_{(w)j}^{n+1,p-1} \left( h_j^{n+1,p} - h_j^{n+1,p-1} \right) + \theta_j^{n+1,p-1} - \theta_j^n \]

(44)

where superscript \( p \) is the iteration level and \( C_{(w)j}^{n+1,p-1} \) is the water capacity evaluated at the pressure head value of the last iteration, \( h_j^{n+1,p-1} \). At convergence, the term \( \left( h_j^{n+1,p} - h_j^{n+1,p-1} \right) \) will be small, which effectively eliminates the remaining inaccuracies in the evaluation of \( C_{(w)} \). The implementation of this mass conservation property requires an iterative solution of the equation matrix.

Figure 11. Spatial and temporal discretization used to solve Richards’ equation
The implicit, backward, finite-difference scheme of equation (42) with explicit linearization (Fig. 11), including the above mentioned adaptations, yields the following discretization of the Richards' equation:

\[
C_{(w)j}^{n+1,p-1} \left( h_j^{n+1,p} - h_j^{n+1,p-1} \right) + \theta_j^{n+1,p-1} - \theta_j^n = 0
\]

\[
= \frac{\Delta t^n}{\Delta z_j} \left\{ K_j^{n} \left( h_{j-1}^{n+1,p} - h_j^{n+1,p} \right) \right. + K_j^{n} \left( h_{j-1}^{n+1,p} - h_j^{n+1,p} \right) \left( h_{j+1}^{n+1,p} - h_j^{n+1,p} \right) - K_j^{n} \left( h_j^{n+1,p} - h_{j+1}^{n+1,p} \right) \left\} - \Delta t^n S_j^n
\]

where \( \Delta t^n = t^{n+1} - t^n \), \( \Delta z_u = z_{j-1} - z_j \), \( \Delta z_l = z_j - z_{j+1} \), and \( \Delta z_l \) is the compartment thickness. The model presented herein uses a block-centered grid, which means that all the nodes, including the top and the bottom node, are in the center of the grid (Fig. 12).

![Block centered finite-difference grid](image)

![Mesh centered finite-difference grid](image)

Figure 12. Finite-difference grid

The numerical discretization equation (45) leads to a tridiagonal nonlinear set of equations, which can be written in matrix form as
where the coefficients $\alpha$, $\beta$, $\gamma$, and $f_j (j=1, 2, \ldots, N, N$ is the number of nodes) are nonlinear functions of the variable $\theta$.

Rearrangement of (45) to (46) results in the coefficients:

$$\alpha = -\frac{\Delta t^n}{\Delta z_j^2} K_j^{n-(1/2)}$$

$$\beta = C_j^{n+1, p-1} + \frac{\Delta t^n}{\Delta z_j^2} K_j^{n-(1/2)} + \frac{\Delta t^n}{\Delta z_j^2} K_j^{n+(1/2)}$$

$$\gamma = -\frac{\Delta t^n}{\Delta z_j^2} K_j^{n+(1/2)}$$

$$f_j = C_j^{n+1, p-1} \cdot h_j^{n+1, p-1} \cdot \theta_j^{n+1, p-1} + \theta_j^n + \frac{\Delta t^n}{\Delta z_j} (K_j^{n-(1/2)} - K_j^{n+(1/2)}) - \Delta t^n S_j^n$$

Because of the nonlinear nature of (45), to obtain solutions of the system of matrix equations (46), an iterative process must be used. This iterative process continues until a satisfactory degree of convergence is obtained. The model presented in this thesis uses the convergence criterion of Huang et al. (1996). They proposed the following criterion for an iterative solution of (45)

$$C_j^{n+1, p} \delta_j^n = |\theta_j^{n+1, p+1} - \theta_j^{n+1, p}| \leq \delta_0$$
where $\delta^p$ is the absolute error at iteration step $p$ and $\delta_y$ is the tolerance.

4.3.2.1 Discretization of initial conditions

The solution of equation (42) requires knowledge of the initial distribution of the pressure head within the flow domain $h(z,t) = h_s(z)$ for $t=0$ and values of hydraulic parameters such as $K_s$ – saturated hydraulic conductivity [$m \cdot h^{-1}$], $\theta_r$ – residual water content [$m^3 \cdot m^{-3}$] and $\theta_s$ – saturated water content [$m^3 \cdot m^{-3}$].

The relation between the water content $\theta$, the pressure head $h$ and the saturated hydraulic conductivity $K_s$ are generally summarized in the retention function, $\theta(h)$, and the unsaturated hydraulic conductivity function, $K(\theta)$. These soil hydraulic functions need to be specified for each distinct layer.

Mualem (1976) derived a predictive model of the $K(\theta)$ relation based on the retention function. Van Genuchten (1980) proposed a more flexible $\theta(h)$ function and combined it with Mualem's predictive model to derive $K(\theta)$. The Van Genuchten function has been used in numerous studies, and forms the basis of several national and international data-bases, and is implemented in numerous unsaturated flow models (Kroes and van Dam, 2003).

The analytical $\theta(h)$ function proposed by Van Genuchten (1980) is:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{(1 + |ah|^n)^m}$$ (52)
where $\theta$ is the saturated water content [$m^3 m^{-3}$], $\theta_r$ is the residual water content in the very dry range [$m^3 m^{-3}$] and $a$ [m$^{-1}$], $n$ [-] and $m$ [-] are empirical shape factors. Parameter $m$ can be calculated by:

$$m = 1 - \frac{1}{n}$$  \hspace{1cm} (53)

Using the above $\theta(h)$ relation and applying the theory of unsaturated hydraulic conductivity by Mualem (1976), the following $K(\theta)$ function results:

$$K = K_s S_e^{\lambda} \left[ 1 - \left( 1 - S_e^{\frac{1}{m}} \right)^2 \right]$$  \hspace{1cm} (54)

where $K_s$ is the saturated hydraulic conductivity [m h$^{-1}$], $\lambda$ is a shape parameter [-] depending on $\partial K / \partial h$, and $S_e$ is the relative saturation defined as:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$  \hspace{1cm} (55)

and $C_{(w)}$ is the water capacity $\frac{\partial \theta}{\partial h}$ [m$^{-1}$] calculated from

$$C_{(w)} = \frac{(\theta_s - \theta_r) \cdot n \cdot m \cdot a \cdot |ah|^{n-1}}{[1 + |ah|^n]^{m+1}}$$  \hspace{1cm} (56)

### 4.3.2.2 Discretization of boundary conditions

An appropriate choice for the top boundary condition during the iterative solution of the Richards' equation may determine the success or failure of a numerical scheme. For the upper boundary, two types of boundary conditions were
applied. The model is designed that the top boundary condition may switch from head controlled to flux controlled, and vice versa.

1. Neumann type – the specified flux \(q_{\text{sur}}\) is applied in the case of ice melting (Surface temperature \(T_s \geq 0^\circ\text{C}\)) and the right hand side of equation (45) transforms to

\[
\frac{\Delta t^n}{\Delta z_1} \left\{ q_{\text{sur}} - K^{n}_{l(1/2)} \left( \frac{h_{1}^{n+1,p} - h_{2}^{n+1,p}}{\Delta z_l} \right) - K^n_{l(1/2)} \right\} - \Delta t^n S_1^n
\]

(57)

which after rearrangements gives the coefficients

\[
\beta \beta_1 = C_{(w)_1}^{n+1,p-1} + \frac{\Delta t^n}{\Delta z_1^2} K^n_{l(1/2)}
\]

(58)

\[
\mathcal{Y}'_1 = -\frac{\Delta t^n}{\Delta z_1^2} K^n_{j(1/2)}
\]

(59)

\[
f_1 = C_{(w)_1}^{n+1,p-1} \cdot h_{1}^{n+1,p-1} - \theta_1^n + \frac{\Delta t^n}{\Delta z_1} \left( -q_{\text{sur}} - K^n_{l(1/2)} \right) - \Delta t^n S'_1
\]

(60)

2. Dirichlet type – the specified head pressure \((h_{\text{sur}})\) is applied for case \(T_s \leq 0^\circ\text{C}\) and the right side of equation (45) transforms to

\[
\frac{\Delta t^n}{\Delta z_1} \left\{ K^n_{l(1/2)} \left( \frac{h_{\text{sur}} - h_{1}^{n+1,p}}{\Delta z_u} \right) + K^n_{l(1/2)} \left( \frac{h_{1}^{n+1,p} - h_{2}^{n+1,p}}{\Delta z_l} \right) - K^n_{l(1/2)} \right\} - \Delta t^n S_1^n
\]

(61)

and after rearrangements gives the coefficients

\[
\beta \beta_1 = C_{(w)_1}^{n+1,p-1} + \frac{\Delta t^n}{\Delta z_1^2} K^n_{l(1/2)} + \frac{\Delta t^n}{\Delta z_1^2} K^n_{j(1/2)}
\]

(62)

\[
\mathcal{Y}'_1 = -\frac{\Delta t^n}{\Delta z_1^2} K^n_{j(1/2)}
\]

(63)
\[ f_1 = C_{(w)}^{n+1,p-1} \cdot h_1^{n+1,p-1} - \theta_1^{n+1,p-1} + \theta_1^n + \frac{\Delta t^n}{\Delta z_1} (K_{i(1/2)}^n - K_{i(1/2)}^n) + \frac{\Delta t^n}{\Delta z_1^2} (K_1^n \cdot h_{sur} - K_{i(1/2)}^n) - \Delta t^n S_i^n \] (64)

For the lower boundary condition, \textit{free drainage} condition represented by Neumann type – specified flux \((q_{bot})\) is applied and the equations are similar to the equation for upper boundary

\[ \frac{\Delta t^n}{\Delta z_N} \left( K_{N-(1/2)}^n \left( \frac{h_{N-1}^{n+p} - h_N^{n+1,p}}{\Delta z_{N-1}} \right) + K_{N-(1/2)}^n + q_{bot} \right) - \Delta t^n S_N^n \] (65)

\[ \alpha \alpha_N = -\frac{\Delta t^n}{\Delta z_N^2} K_{N-(1/2)}^n \] (66)

\[ \beta \beta_j = C_{(w)N}^{n+1,p-1} + \frac{\Delta t^n}{\Delta z_N^2} K_{N-(1/2)}^n \] (67)

\[ f_j = C_{(w)N}^{n+1,p-1} \cdot h_N^{n+1,p-1} - \theta_N^{n+1,p-1} + \theta_N^n + \frac{\Delta t^n}{\Delta z_N} (K_{N-(1/2)}^n + q_{bot}) - \Delta t^n S_N^n \] (68)

with assumption that \( q_{bot} = -K_{N(1/2)}^n \) (69)

4.3.3 \textbf{Numerical approximation of transport equation}

The simplified transport equation (70) involving advection and mechanical dispersion in one dimension, can be approximated by a system of finite-difference equations, such that

\[ \frac{\partial (\alpha \xi)}{\partial t} = \frac{\partial}{\partial z} \left( \theta D \frac{\partial C}{\partial z} \right) - \frac{\partial}{\partial z} (qC) \] (70)
An explicit, central finite-difference scheme of (65) can be approximated at nodal point \( j \) by

\[
\frac{\theta_j^{n+1} C_j^{n+1} - \theta_j^n C_j^n}{\Delta t^n} = \frac{1}{\Delta z_j} \left[ \frac{\theta_j^{n-(1/2)} D_j^{n-(1/2)} (C_{j-1} - C_j^n)}{\Delta z_u} - \frac{\theta_j^{n+(1/2)} D_j^{n+(1/2)} (C_j^n - C_{j+1})}{\Delta z_l} \right] - \frac{q_j^{n-(1/2)} \cdot C_j^{n-(1/2)} - q_j^{n+(1/2)} \cdot C_j^{n+(1/2)}}{\Delta z_j}
\]

(71)

where superscript \( n \) denotes the time level, subscript \( j \) the node number, and subscripts \( j-(1/2) \) and \( j+(1/2) \) refer to linearly interpolated values at the upper and lower cell interface. A general formula for the interface concentration may be expressed as

\[
C_{j+(1/2)} = (1 - \omega) C_j + \omega C_{j+1}
\]

(72)

where \( \omega \) is a spatial weighting factor. The most obvious choice of \( \omega \) is 0.5 and resulting formulation is referred as the "central in space weighting scheme". However, the central weighting scheme tends to create artificial oscillations, and, because of that, an alternative upstream spatial weighting scheme was used. It can be expressed as follows: \( \omega = \begin{cases} 0 & \text{if } v > 0 \\ 1 & \text{if } v < 0 \end{cases} \) or in terms of interface concentration

\[
C_{j+(1/2)} = \begin{cases} C_j & \text{if } v > 0 \\ C_{j+1} & \text{if } v < 0 \end{cases}
\]

where \( v \) is velocity [\( \text{m} \text{h}^{-1} \)].
The explicit scheme is simple to implement in a computer code, however, it is subject to instability. To ensure stability, the time step \( \Delta t_j \) should meet the following criterion (van Dam et al. 1997)

\[
\Delta t_j \leq \frac{\Delta z_j^2 \theta^n_j}{2D^n_j}
\]  

(73)

4.3.3.1 Discretization of initial and boundary conditions

The solution of equation (42) requires specifying the initial solute concentrations in the water \( C(z,t) = 0 \) for \( t=0 \).

For the upper boundary condition, the solute concentration of meltwater needs to be specified. \( C(0,t) = C_0 \) for \( t>0 \)

For the bottom boundary condition, the flux through the bottom is used and the solute flux \( J_{bot} \) [g m\(^{-2}\)] is calculated by

\[
J_{bot} = q_{bot} \cdot C_N
\]  

(74)

and for free drainage condition \( C_N = C_{N-1} \) is assumed.

4.4 Development and implementation of the algorithms

This chapter describes overall structure of model. The computer program of the model is written in MatLab programming language. The model is divided into two main programs and several subprograms. Main programs are independent of each other and can be used separately.
The first program “IceMelt” presents a one-dimensional thermodynamic lake-ice model and basic structure of the “IceMelt” program is illustrated in Fig 13. The model simulates heat transport in one dimension. Using the model results, one can estimate:

- Melting rate at the surface of ice cover
- Melting and freezing rate at the bottom of ice cover and
- Ice cover thickness.

The second program is called “USFST” (UnSaturated Flow and Solute Transport). It numerically solves Richards’ equation for unsaturated flow, and the advection-dispersion equation for solute transport. The governing flow and transport equations are solved numerically using finite-difference methods. Program output consists of water content, head pressure, solute concentrations and solute flux at the bottom of profile at the end of each time step. Fig. 14 shows flow chart of “USFST” program.

Appendixes A and B contain original program code for “IceMelt” and “USFS” programs.
Figure 13. Flow chart of "IceMelt" program
Figure 14. Flow chart of "USFST" program
CHAPTER 5

MODEL TESTING

The two major components of the model are tested separately. The validation of heat transport is accomplished by comparing model results with empirical measurements of ice temperature at various depths in Lake Fryxell. The unsaturated flow and solute transport model was not validated because lack of field data. Instead of validation program code is verified by comparing model results with results generated by the Hydrus 1D software, which is a software package for simulating the one-dimensional movement of water, heat and multiple solutes in variably saturated media. It was developed by U.S. Salinity Laboratory, USDA (Simunek et al. 1998).

A sensitivity analysis was performed to observe the changes in the model-generated data caused by change of input parameters. The purpose of a sensitivity analysis is to quantify the uncertainty in the model caused by uncertainty in the estimates of parameters (Anderson and Woessner, 2002). A sensitivity analysis is typically performed by changing one parameter at a time within the plausible range.
5.1 Validation of the heat transport component

The finite-difference solution of the heat equation using enthalpy formulation, adopted in this model was tested based on the measured ice temperature data at Lake Fryxell, provided by LTER McMurdo Dry Valleys, Limnology group (http://huey.colorado.edu/LTER/lakedata.html). These data came from seven thermistors set up in Lake Fryxell ice cover. Temperatures were measured at surface and at depths 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0m below the surface for the period from October 1, 2002 to October 24, 2003.

The solar radiation data are provided by LTER McMurdo Dry Valleys Meteorology group (http://huey.colorado.edu/LTER/meteordata.html). The initial ice thickness of 5.5m was calculated based on the ice temperature distribution, as explained in chapter 4.3.1.1. The model parameters used for the thermodynamic “IceMelt” model are shown in Table 5. Figures 15-20 show that the models results are similar to the measured values with an R² above 0.99. A relatively small discrepancy can be found at depth intervals from 2.0 to 3.0m. Measured temperatures at 2.5 and 3.0m are slightly lower that modeled, which is difficult to explain, because of ice at that depth contains zones with sediments composed of sand and gravel sized particles. These sediments absorb heat energy, thereby increasing the temperature of the ice, which is opposite of what the simulated results show. One possibility is that lower boundary condition is incorrectly applied. Model assume constant heat flux from lake water, what is based on measurements of water
temperature in summer time. It is unknown how much is heat flux in winter time. It should be mentioned that the measured high temperature values at 0.5m shown on Fig.15 obviously were not actual ice temperature, but probably errors due to the fact that the thermistor was either exposed to air or due to a system malfunction.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_i$</td>
<td>Thermal conductivity of ice [W m$^{-1}$ °C$^{-1}$]</td>
<td>2.22</td>
</tr>
<tr>
<td>$K_w$</td>
<td>Thermal conductivity of water [W m$^{-1}$ °C$^{-1}$]</td>
<td>0.564</td>
</tr>
<tr>
<td>$c_i$</td>
<td>Heat capacity of ice [J kg$^{-1}$ °C$^{-1}$]</td>
<td>2092</td>
</tr>
<tr>
<td>$c_w$</td>
<td>Heat capacity of water [J kg$^{-1}$ °C$^{-1}$]</td>
<td>4187</td>
</tr>
<tr>
<td>$L_f$</td>
<td>Latent heat of freezing [J kg$^{-1}$]</td>
<td>0.334x10$^6$</td>
</tr>
<tr>
<td>$\rho_i$</td>
<td>Ice density [kg m$^{-3}$]</td>
<td>917</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Surface albedo of ice [-]</td>
<td>0.3</td>
</tr>
<tr>
<td>$k_i$</td>
<td>Extinction coefficient [m$^{-1}$]</td>
<td>0.3</td>
</tr>
<tr>
<td>$l_0$</td>
<td>Bulk fraction of the incident radiation [-]</td>
<td>0.35</td>
</tr>
<tr>
<td>$T_m$</td>
<td>Melting temperature of ice [°C]</td>
<td>0.0</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>Time step of model [s]</td>
<td>3600</td>
</tr>
<tr>
<td>$F_{bot}$</td>
<td>Lake heat flux [W m$^{-2}$]</td>
<td>0.2961</td>
</tr>
<tr>
<td>$Z$</td>
<td>Initial ice thickness [m]</td>
<td>5.5</td>
</tr>
</tbody>
</table>

Table 5. Parameters used for “IceMelt” model validation
Figure 15. Ice temperature distribution at 0.5m

Figure 16. Ice temperature distribution at 1.0m
Figure 17. Ice temperature distribution at 1.5m

Figure 18. Ice temperature distribution at 2.0m
Figure 19. Ice temperature distribution at 2.5m

Figure 20. Ice temperature distribution at 3.0m
5.2 Verification of the Unsaturated Flow and Solute Transport program code

The unsaturated flow and solute transport program code was verified by comparing modeled results with results generated by the Hydrus 1D model. The example selected here is water infiltration in a homogeneous soil column. Table 6 shows the parameters used for this modeling exercise. For the upper boundary condition, the model uses two types of conditions, a specified head pressure and a specified flux. The specified flux at the surface represents precipitation, which is similar to a condition of ice surface melting. For the lower boundary condition, a free drainage condition was chosen, which is the best representation of ice floating on the lake surface.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta )</td>
<td>Porosity or saturated water content ([\text{cm}^3 \text{ cm}^{-3}]),</td>
<td>0.36</td>
</tr>
<tr>
<td>( \theta )</td>
<td>Residual water content ([\text{cm}^2 \text{ cm}^{-3}])</td>
<td>0.034</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>Parameter in soil retention function ([\text{cm}^{-1}])</td>
<td>0.016</td>
</tr>
<tr>
<td>( N )</td>
<td>Parameter in soil retention function</td>
<td>1.3</td>
</tr>
<tr>
<td>( K_s )</td>
<td>Saturated hydraulic conductivity ([\text{cm day}^{-1}])</td>
<td>16</td>
</tr>
<tr>
<td>( H )</td>
<td>Initial head pressure ([\text{cm}])</td>
<td>-500</td>
</tr>
<tr>
<td>( \Delta t )</td>
<td>Time Step ([\text{day}])</td>
<td>0.01</td>
</tr>
<tr>
<td>Time</td>
<td>Period of simulation ([\text{day}])</td>
<td>183</td>
</tr>
<tr>
<td>( D_w )</td>
<td>Solute diffusion coefficient in free water ([\text{cm}^2 \text{ day}^{-1}])</td>
<td>16</td>
</tr>
<tr>
<td>( L_{dis} )</td>
<td>Longitudinal dispersivity ([\text{cm}])</td>
<td>5</td>
</tr>
<tr>
<td>( Z )</td>
<td>Depth of the soil column profile ([\text{cm}])</td>
<td>100</td>
</tr>
<tr>
<td>( q_{sur} )</td>
<td>Surface infiltration rate ([\text{cm day}^{-1}])</td>
<td>various</td>
</tr>
</tbody>
</table>

Table 6. Model input parameters
These results show good agreement with the HYDRUS 1D results, although relatively small differences appear at the bottom of the profile.

Figure 21. Head pressure profile
Figure 22. Water content profile

Figure 23. Concentration profile
CHAPTER 6

RESULTS AND DISSCUTION

Due to the lack of appropriate and precise data on lake ice characteristics such as ice porosity, permeability, and water retention parameters of the ice, the model results are presented and discussed for various scenarios. Basically, multiple simulations were made varying one parameter at a time within a plausible range of values while holding the other constant at their baseline values. This method yields the sensitivity of the model to each parameter, independent of others.

As mentioned in Chapter 4.2.3, geochemical reactions or biodegradation or other processes that cause attenuation of contaminant transport are not included in these models. For this reason, at the initial concentration, relative concentration of hydrocarbons of 1µg/cm³ is used. It is assumed that there is an infinite source of contamination at the surface and the diffusion coefficient in water for benzene ($D_w=1.02\times10^{-9}\text{m}^2/\text{s}$)* is used as a surrogate for all the hydrocarbons.

* CRC Handbook of Chemistry and Physics, 85th edition, 2004-2005
6.1 Simulation I

From the previous research one can conclude that the optical properties of ice are important parameters in thermodynamic ice models. For this reason this simulation presents the modeling results of ice surface melting and ice thickness with changing ice surface albedo.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_i$</td>
<td>Thermal conductivity of ice [W m$^{-1}$ °C$^{-1}$]</td>
<td>2.22</td>
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<td>$K_w$</td>
<td>Thermal conductivity of water [W m$^{-1}$ °C$^{-1}$]</td>
<td>0.564</td>
</tr>
<tr>
<td>$c_i$</td>
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<td>2092</td>
</tr>
<tr>
<td>$c_w$</td>
<td>Heat capacity of water [J kg$^{-1}$ °C$^{-1}$]</td>
<td>4187</td>
</tr>
<tr>
<td>$L_f$</td>
<td>Latent heat of freezing [J kg$^{-1}$]</td>
<td>0.334x10$^{6}$</td>
</tr>
<tr>
<td>$I_0$</td>
<td>Bulk fraction of the incident radiation [-]</td>
<td>0.35</td>
</tr>
<tr>
<td>$k_i$</td>
<td>Extinction coefficient [m$^{-1}$]</td>
<td>0.3</td>
</tr>
<tr>
<td>$\rho_i$</td>
<td>Ice density [kg m$^{-3}$]</td>
<td>917</td>
</tr>
<tr>
<td>$T_m$</td>
<td>Melting temperature of ice [°C]</td>
<td>0.0</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>Time step of model [s]</td>
<td>3600</td>
</tr>
<tr>
<td>$F_{bot}$</td>
<td>Lake heat flux [W m$^{-2}$]</td>
<td>0.2961</td>
</tr>
<tr>
<td>$Z$</td>
<td>Initial ice thickness [m]</td>
<td>5.5</td>
</tr>
</tbody>
</table>

Table 7. Parameters used for “IceMelt” model

Fig. 24 shows that by decreasing the ice surface albedo by 0.1, ice surface melting is increased by 5cm and the modeled ice thickness decreases by 15cm (Fig. 24). Comparing the temperature profile at the various depths, (Fig. 14-19) the modeling results show the best agreement to the measured temperatures using an albedo = 0.3. Therefore, for the next simulations of meltwater infiltration, the surface melting rates obtained using albedo=0.3 will be used. It should be mentioned here
that surface albedo might be decreased due to surface darkening by the hydrocarbons spill, resulting in more melting at surface.

Figure 24. Cumulative ice surface melting

Figure 25. Simulated ice thickness
6.2 Simulation II

This simulation considers variations in saturated water content or porosity. There are few data for the porosity of lake ice cover in the literature. For this simulation saturated water content values obtained from work of Fritsen et al. (1998) are used. Their calculations show that at the depth of 0.5 to 1.0m in the ice cover the water content was in the range of 7.6 to 22.3%, and for these simulations values of 10 and 20% are adopted. Other parameters used for this simulation are listed on the Table 8.

The simulation results are shown in Figures 26 to 30, where the first two figures show concentration profiles as a function of time. As was expected lower porosities gave higher concentrations of solutes and the contaminants reach the bottom boundary much faster (Fig. 27 and 28). As a result, the solute flux at the bottom of the model domain is slightly higher for the porosity of 10% (Fig. 30).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$ [cm$^{-1}$]</td>
<td>0.05</td>
<td>$L_{idh}$ [cm]</td>
<td>2</td>
</tr>
<tr>
<td>$n$ [-]</td>
<td>1.5</td>
<td>$D_w$ [m$^2$/s]</td>
<td>$10^{-9}$</td>
</tr>
<tr>
<td>$k_1$ [m$^2$]</td>
<td>$10^{-9}$</td>
<td>$\alpha$ [-]</td>
<td>0.3</td>
</tr>
</tbody>
</table>

All other parameters are listed in Table 7

Table 8. Input parameters used for Simulation II
Figure 26. Concentration profiles as a function of the time for $\theta_s=0.1$

Figure 27. Concentration profiles as a function of the time for $\theta_s=0.2$
Figure 28. Concentration at the middle of the model domain as a function of the time

Figure 29. Concentration at the bottom of the model domain as a function of the time
Figure 30. Cumulative solute flux at the bottom of the model domain
6.3 Simulation III

The next two simulations present a review of the variation in water retention parameters. The numerical solution of unsaturated flow, based on Richards' equation is primarily used for modeling of water movement in the vadose zone with intergranular porosity where unsaturated hydraulic parameters are highly nonlinear functions of pressure head. To obtain unsaturated hydraulic conductivity values, the model implements the soil hydraulic functions of van Genuchten (1980) and Mualem (1976) by equations (52) and (54), respectively, where \( a \) and \( n \) are water retention parameters. It is difficult to predict values for \( a \) and \( n \) in case of unsaturated flow modeling in fractured ice and for that reason two plausible values are used. Parameter \( a \) is the inverse of the air-entry value or bubbling pressure (Simunek et al. 1998), and for this simulation values of 0.02 and 0.05 are used. The other input parameters are listed in Table 9.

Model results show that by decreasing parameter \( a \), the solute concentration in the profile is also decreased, but the flux at the bottom of the model is increased. Due to decreasing parameter \( a \), water flow velocities are increased, therefore the solute residence time is smaller, and because of that, solute concentrations in the profile are smaller. The solute flux at the bottom of the model is larger because solute movement is much faster and more solute reach the bottom of the profile.
Table 9. Input parameters used for Simulation III

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_e$ [-]</td>
<td>0.2</td>
<td>$L_{dis}$ [cm]</td>
<td>2</td>
</tr>
<tr>
<td>n [-]</td>
<td>1.5</td>
<td>$D_w$ [m$^2$/s]</td>
<td>$10^9$</td>
</tr>
<tr>
<td>$k_s$ [m$^2$]</td>
<td>$10^{-9}$</td>
<td>$\alpha$ [-]</td>
<td>0.3</td>
</tr>
</tbody>
</table>

All other parameters are listed in Table 7

Figure 31. Concentration profiles as a function of the time for $a=0.05$
Figure 32. Concentration profiles as a function of the time for $a=0.02$

Figure 33. Concentration at the middle of the model domain as a function of time
Figure 34. Concentration at the bottom of the model domain as a function of time

Figure 35. Cumulative solute flux at the bottom of the model domain
6.4 Simulation IV

The second water retention parameter $n$ is related to the pore size distribution index. For fine textured soils like clays, $n$ is relatively small, 1.0-1.5, and for sand the value of $n$ is around 2.5 (Simunek et al. 1998). Similarly, as for the parameter $a$, it is unknown which value better represents lake ice conditions, therefore, for this simulation, values of 1.5 and 2.5 are used. The other input parameters are listed on the Table 10. From the simulation results, it is obvious that parameter $n$, like parameter $a$, has a significant influence on the simulation results, and lower values of parameter $n$ produce higher values of solute flux at the bottom of the model domain.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_0$ [-]</td>
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<td>$L_{dis}$ [cm]</td>
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</tr>
<tr>
<td>$a$ [cm$^{-1}$]</td>
<td>0.05</td>
<td>$D_w$ [m$^2$/s]</td>
<td>$10^{-9}$</td>
</tr>
<tr>
<td>$k_s$ [m$^2$]</td>
<td>$10^{-9}$</td>
<td>$\alpha$ [-]</td>
<td>0.3</td>
</tr>
</tbody>
</table>

All other parameters are listed in Table 7

Table 10. Input parameters used for Simulation IV
Figure 36. Concentration profiles as a function of the time for $n=1.5$

Figure 37. Concentration profiles as a function of the time for $n=2.5$
Figure 38. Concentration at the middle of the model domain as a function of the time

Figure 39. Concentration at the bottom of the model domain as a function of the time
Figure 40. Cumulative solute flux at the bottom of the model domain
6.5 Simulation V

Despite its importance, very little is known about the magnitude and variability of ice permeability. Eicken et al. (2002) measured sea-ice permeability using slug tests adapted to the ice environment. Permeability values vary over more than two orders of magnitude as the melt season progressed (10^{-11} to 10^{-9} m^2). The overall geometric mean is \( k_s = 2.0 \times 10^{-10} \) m^2. In this simulation two values of permeability are applied, 10^{-9} and 10^{-10} m^2. The other input data are listed in Table 11. Results, as expected, show that lower values of permeability produce lower solute fluxes at the bottom of the profile. Travel times and concentrations inside of the model domain are less for the higher value of permeability.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta ) [-]</td>
<td>0.2</td>
<td>( L_{dis} ) [cm]</td>
<td>2</td>
</tr>
<tr>
<td>a [cm^{-1}]</td>
<td>0.05</td>
<td>( D_w ) [m^2/s]</td>
<td>10^{-9}</td>
</tr>
<tr>
<td>n [-]</td>
<td>1.5</td>
<td>( \alpha ) [-]</td>
<td>0.3</td>
</tr>
</tbody>
</table>

All other parameters are listed in Table 7

Table 11. Input parameters used for Simulation V
Figure 41. Concentration profiles as a function of the time for $k_s = 10^{-10} \text{m}^2$

Figure 42. Concentration profiles as a function of the time for $k_s = 10^{-9} \text{m}^2$
Figure 43. Concentration at the middle of the model domain as a function of the time

Figure 44. Concentration at the bottom of the model domain as a function of the time
Figure 45. Cumulative solute flux at the bottom of the model domain
6.6 Simulation VI

This simulation considers the variation in model results depending on dispersivity values. Dispersivity depends on the scale over which the water flux and solute advection are modeled. For a small scale model like this one, dispersivity values are in the range of a few centimeters. For this simulation dispersion values of 0.5 and 5.0 cm were applied. Higher values of dispersion produce faster spreading of contaminant through the ice, which means that the residence time of the solutes and the concentrations are less.

<table>
<thead>
<tr>
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<th>Parameter</th>
<th>Value</th>
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</thead>
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<td>$\theta$ [-]</td>
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<td>$\alpha$ [-]</td>
<td>0.3</td>
</tr>
<tr>
<td>a [cm$^{-1}$]</td>
<td>0.05</td>
<td>$D_w$ [m$^2$/s]</td>
<td>$10^{-9}$</td>
</tr>
<tr>
<td>n [-]</td>
<td>1.5</td>
<td>$k_i$ [m$^2$]</td>
<td>$10^{-9}$</td>
</tr>
</tbody>
</table>

All other parameters are listed in Table 7

Table 12. Input parameters used for Simulation VI
Figure 46. Concentration profiles as a function of the time for $L_{dis} = 0.5 \text{cm}$

Figure 47. Concentration profiles as a function of the time for $L_{dis} = 5.0 \text{cm}$
Figure 48. Concentration at the middle of the model domain as a function of the time

Figure 49. Concentration at the bottom of the model domain as a function of the time
Figure 50. Cumulative solute flux at the bottom of the model domain
CHAPTER 7

SUMMARY AND CONCLUSIONS

In this thesis two one-dimensional models are developed, the first to simulate heat transport and the second to simulate unsaturated flow and solute transport in polar lake ice cover. For practical reasons, the models are separated in two independent programs, but they could be incorporated in one program.

As part of the model development, the governing equations for both models are presented as well as the numerical solutions and the discretization of the model domain. Both models are developed using finite-difference methods with the combination of implicit and explicit solutions.

The finite-difference solution of the heat transport equation is tested based on measured ice temperature data from Lake Fryxell, provided by LTER McMurdo Dry Valleys, Limnology group (http://huey.colorado.edu/LTER/lakedata.html). The "IceMelt" model results correlate well to measured values, which is confirmation that initial and boundary conditions were selected correctly. The second model dealing with unsaturated flow and solute transport was not as successful as the first one. The modeling of unsaturated flow and solute transport by itself was successful, as is confirmed by code verification comparing the model results to those of the HYDRUS
1-D model. It remains a question how well a numerical solution of Richards’ equation can simulate meltwater infiltration through ice. Primarily, because numerical solution of the Richards’ equation is used for simulating in a medium with intergranular porosity. Despite its importance, very little is known about meltwater percolation, magnitude and variability of ice permeability, ice porosity, and most importantly, much less is known about solute transport in ice.

This work is not an attempt to develop a state of the art model. This study is only the first step in establishing the feasibility of this approach as a useful tool, and this approach needs to be confirmed or rejected by future researchers. Several limitations were made evident in this study that should be considered in the future applications of the model. This model only covers a portion of the ice above the lake level, as solute movement in the saturated portion of ice was not an object of this investigation. Another limitation of this model is that the possible effect of water ponding has been neglected. In case of ponding, the surface flux is assumed to be equal to saturated hydraulic conductivity.

Based on the simulation results, the following conclusions can be made:

- Results from the “IceMelt” model show good agreement with measured temperatures and the amount of the ice melted at the summer (~30cm at the surface and ~20cm at the bottom) is compensated during the winter by freezing of lake water at the bottom. Clow et al (1988) demonstrated similar empirical data for Lake Hoare.
- Small variations of parameters $a$ and $n$ can cause huge variations in the results of concentration distributions and for this reason the biggest uncertainty in the modeling results is related to these two parameters. Almost nothing is known about parameters $a$ and $n$ in natural ice. Before further modeling is accomplished, there is a need to quantify these parameters in ice.

- Simulations show that in the worst case scenario, one part per mil of the initial concentration of the solute can reach the bottom of the unsaturated zone in just 14 hours. Using a lower permeability value by one order of magnitude, the travel time is 8.3 days.

- According to modeling results, using the initial concentration of 1.0 $\mu$g/cm$^3$ and parameters that produce the slowest movement, the cumulative flux at the lake hydrostatic level is 1.1$\mu$g/cm$^2$ of the contaminant, a value of 6.2 $\mu$g/cm$^2$ is obtained using parameters that produce the fastest contaminant movement.

- Considering the fact that ice is heterogeneous porous media, it can be concluded that the actual volume of the contaminant at the lake level can be any value between these two values.
CHAPTER 8

RECOMMENDATIONS FOR FUTURE WORK

As described previously, this study is the first step in building a complete model of contaminant spreading in ice covered water surfaces and for that reason several improvements can be recommended.

- A more detailed model needs more accurate input data. Ice optical properties are critically important input parameters, and future work should provide data related to seasonal changes of albedo and the extinction coefficient.

- To validate the heat transport model, it is necessary to have accurate measurements of temperature throughout the ice cover, together with the measurement of ice thickness for the period of simulation.

- Other important parameters are related to meltwater percolation. It is obvious that porosity and permeability are not constant over time because of internal melting induced by the movement of meltwater
throughout the ice. Field work such as tracer studies and \textit{in-situ} ice permeability measurements need to be made to provide these data.

- Consider the possibility of using an airpermeameter for measuring intrinsic permeability at the field.

- The treatment of solute transport in this model considers only advection and dispersion, yet other processes like absorption, degradation by microorganisms, retardation need to be incorporated and field data supporting their use be collected.

Once these activities are accomplished, a more sophisticated model can be developed. From the previous research and field observations, it is known that at times lateral water movement is more dominant than vertical water movement, therefore, two or three dimensional model should be considered.

To simulate heterogeneity and the ponding effect, surface albedo and permeability values should be assigned randomly inside of a plausible range of values. As a improvement, a new model should include the ability to change porosity as a result of internal melting.

It should be considered the possibility of using more sophisticated commercial software such as "FRACTRAN" or "FRAC3DVS". Developed at the University of Waterloo, the "FRAC3DVS" program is a three-dimensional, numerical finite-element model for steady-state/transient, variably-saturated flow and advective-dispersive
solute transport in porous or discretely-fractured porous media. Its application to this problem might be quite beneficial.

After the solute transport problem is solved, there still remains the problem of how to deal with the other possible contaminant movement, such as transfer of the free phase or the transport of contaminants sorbed into sediment in ice-sorbed phase. This is also an issue that will require future work.
APPENDIX A
"ICEMELT" PROGRAM CODE

This appendix holds program codes written in MATLAB used in this thesis. The first is main program code for "IceMelt" model with function for converting input temperature and radiation data into hourly values.

```matlab
% File_name=IceMelt.m % Main program for "IceMelt" problem % Copyright Marinko Karanovic

clear all
l=7; %Model domain length
N=8; %Number of nodes

%Initial %temperature
T=[-25.81 -20.85 -15.89 -10.94 -5.0 -0.1 0.1 0.1];%Node size [m]
Ts,Temp,arad,dt]=calc_hour;
[rows cols] = size(Ts)
n=rows;

%Setting of the model parameters
ro=917; t=0; melt=0; ks=2.22; kl=0.564; Cps=2092; Cpl=4187;
L=0.334E6; albedo=0.3; extin=0.3; cloud=0.35; tot_mel=0; Tn=T; Tm=0;
heat_w=-0.2961;

%Memory allocation
TT = zeros(n, N);
deltax = zeros(n, N);
lambdax = zeros(n, N);
tot_melt=zeros(n,1);

for i=1:N
    if T(i)<Tm
        E(i)=ro*Cps*(T(i)-Tm);
    else
        if T(i)>Tm
```
\[
E(i) = \rho_0 \cdot C_{pl} \cdot (T(i) - T_m) + \rho_0 \cdot L;
\]

end

end

for \( z = 1 \) to \( n \)

\( t = t + dt; \)

for \( i = 1 \) to \( N \)

if \( E(i) < \rho_0 L \)

\( \lambda(i) = 0; \)

else if \( E(i) < \rho_0 \cdot L \)

\( \lambda(i) = E(i)/(\rho_0 \cdot L); \)

else

\( \lambda(i) = 1; \)

end

end

\( \lambda_{	ext{max}}(z, i) = \lambda(i); \)

end

rad = \text{extin} \cdot \text{cloud} \cdot (1 - \text{albedo}) \cdot \text{arad}(z);

if \( T_s(z) > 0 \)

\( \text{melt} = \text{rad} \cdot (dt/(L \cdot \rho_0)); \)

\( \text{dx}(1) = \text{dx}(1) - \text{melt}; \)

\( \text{tot_melt} = \text{tot_melt} + \text{melt}; \)

end

\( \text{tot_melt}(z) = \text{tot_melt}; \)

\( k(1) = k_s; \)

\( R_m = 0.5 \cdot \text{dx}(1)/k(1); \)

\( q_m = (-T(1) - T_s(z))/(R_m) + \text{rad}; \)

for \( i = 2 \) to \( N \)

\( k(i) = 1/(\lambda(i)/(k_1) + (1 - \lambda(i))/k_s); \)

end

\( x = \text{dx}(1) \cdot 0.5; \)

for \( i = 1 \) to \( N - 1 \)

\( \text{rad}(i) = \text{extin} \cdot \text{cloud} \cdot (1 - \text{albedo}) \cdot \text{arad}(z) \cdot \exp(-\text{extin} \cdot x); \)

\( \text{R}(i) = 0.5 \cdot \text{dx}(i)/k(i) + 0.5 \cdot \text{dx}(i+1)/k(i+1); \)

\( q(i) = (-T(i+1) - T(i))/(R(i)) + \text{rad}(i); \)

\( x = x + \text{dx}(i) \cdot 0.5 + \text{dx}(i+1) \cdot 0.5; \)

end

\( \text{rad}(N) = \text{extin} \cdot \text{cloud} \cdot (1 - \text{albedo}) \cdot \text{arad}(z) \cdot \exp(-\text{extin} \cdot x); \)

\( q(N) = \text{heat}_w - \text{rad}(N); \)

\( E_n(1) = E(1) + (dt/(\text{dx}(1))) \cdot (q_m - q(1)); \)

for \( i = 2 \) to \( N \)

\( E_n(i) = E(i) + (dt/(\text{dx}(i))) \cdot (q(i-1) - q(i)); \)

end

for \( i = 1 \) to \( N \)

if \( E_n(i) \leq 0 \)

\( T_{n}(i) = T_m + E_n(i)/(\rho_0 \cdot C_{ps}); \)

else if \( E_n(i) < \rho_0 \cdot L \)

\( T_{n}(i) = T_m; \)

else

\( T_{n}(i) = T_m + (E_n(i) - \rho_0 \cdot L)/(\rho_0 \cdot C_{pl}); \)

end

end

\( T_T(z, i) = T_{n}(i); \)

\( \text{deltax}(z, i) = \text{dx}(i); \)

end
lambda(1)=0; E=En; T=Tn;
time = t/(3600*24);
melt=0;
end

function [Ts,Temp,arad,dt]=calc_hour;
%This function loads text files with measured data for Ice temperature
%and Shortwave radiation and converting them into hourly values.
clear all
data = load('ice_temp2002.txt');
 n=9330; %Number of the time steps
dt=3600; %Duration of the time step [s]

[rows cols] = size(data);
Ts=zeros(n,1); %Surface Temperature
Temp=zeros(n,cols-1); %Temperatures at 0.5, 1.0, 1.5, 2.0, 2.5 and
3.0m depth
arad=zeros(n,1); %Shortwave radiation

k=1;
for i=1:n
   Ts(i)=data(k,1);
   k=k+3;
end
for j=2:cols
   for i=1:n
      Temp(i,j-1)=data(k,j);
      k=k+3;
   end
end
rad = load('radiation2002.txt');
[rows cols] = size(rad);
k=1;
for i=1:n
   arad(i)=rad(k,1);
   k=k+4;
end
APPENDIX B
"USFST" PROGRAM CODE

This appendix contain main program code for “USFST” model with function for load input data and function for calculation of the unsaturated flow parameters.

```matlab
clear all
teta0=0.02;  %residual water content
tetas=0.1;  %water content or porosity
bot=0;      %if bot=0 free drainage, bot=1 forced head presure,
            %bot=2 water level

alpha_t=2;  %longitudinal dispersivity
co=0;       %Initial concentration

acnp=0;
toler=1E-3;

[hbot,htop,h,t1,qin,unsat,melt,np]=input;
timet=t1;
dz=unsat(1)/np;   %node size
dt=0.02;          %time step (days)
z=0:dz:(unsat(1)-dz);
for i=1:np
  p=-h(i);
  [k(i),th(i),c(i),Se(i)]=unsat_calc(p);
end

it=0;
h_0d=h;
hold=th;
for i=1:np
  cl(i)=co;
end
clold=cl;
t1=timet;
conc=zeros(timet,np);
head=zeros(timet,np);
```
theta=zeros(timet,np);
flux=zeros(timet,l);
zz=zeros(timet,np);
while t+dt<=t1
  t=t+dt;
  gg=fix(t+1);
  if gg>1 & unsat(gg)~=unsat(gg-1)
    dz=unsat(gg)/np;
    ss=melt(gg)/np;
    for i=2:np-1
      koef=(np-i)*ss;
      h(i)=(1-koef)*h(i)+koef*h(i+1);
      cl(i)=(1-koef)*cl(i)+koef*cl(i+1);
      th(i)=(1-koef)*th(i)+koef*th(i+1);
    end
  end
  thdif=1;
  rzz=dt/dz^2;
  rz=dt/dz;
  while abs(thdif)>toler
    for i=2:np-1
      melt(gg)=0;
      km=0.5*(k(i-1)+k(i));
      kp=0.5*(k(i)+k(i+1));
      aa(i)=-rzz*km;
      bb(i)=c(i)+rzz*(kp+km);
      cc(i)=-rzz*kp;
      dd(i)=c(i)*h(i)+th(i)-thold(i)+rz*(km-kp);
    end
    if qin(gg)==0
      aa(1)=0;
      acnp=0;
      bb(1)=c(1)+rzz*k(1)+rzz*(0.5*(k(1)+k(2)));
      cc(1)=-rzz*(0.5*(k(1)+k(2)));
      dd(1)=c(1)*h(1)+th(1)-thold(1)+rz*(k(1)-0.5*...k(2)))+rzz*k(1)*htop;
    else
      aa(1)=0;
      if t>=1420
        acnp=1;
      end
      bb(1)=c(1)+rzz*(0.5*(k(1)+k(2)));
      cc(1)=-rzz*(0.5*(k(1)+k(2)));
      dd(1)=c(1)*h(1)+th(1)-thold(1)-rz*((-qin(gg)-thold(1)*...melt(gg))+(0.5*(k(1)+k(2))));
    end
    km=0.5*(k(np-1)+k(np));
    aa(np)=-rzz*km;
    cc(np)=0;
    bb(np)=c(np)+rzz*(km+k(np));
    if bot==0
      bb(np)=c(np)+rzz*(km);
      qbot=-k(np);
      dd(np)=c(np)*h(np)+th(np)-thold(np)+rz*(km+qbot);
    else if bot==1

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\[
\begin{align*}
\text{dd}(np) &= \text{c}(np) \times \text{h}(np) + \text{th}(np) - \text{thold}(np) + rz^*(km-k(np)) + \ldots \\
&\quad - rzz^*(k(np))^*\text{hbot} \\
\text{else} & \\
\text{dd}(np) &= \text{c}(np) \times 0 + \text{th}(np) - \text{thold}(np) + rz^*(km-k(np)) + \ldots \\
&\quad - rzz^*(k(np))^*0 \\
\end{align*}
\]

end

end

for i=2:np

\[
\begin{align*}
\text{bb}(i) &= \text{bb}(i) - \text{aa}(i) \times \text{cc}(i-1)/\text{bb}(i-1) \\
\text{dd}(i) &= \text{dd}(i) - \text{aa}(i) \times \text{dd}(i-1)/\text{bb}(i-1) \\
\end{align*}
\]

end

\[
\text{dd}(np) = \text{dd}(np)/\text{bb}(np) \\
\text{for i=2:np} \\
\text{j=np-i+1;} \\
\text{dd}(j) = (\text{dd}(j) - \text{cc}(j) \times \text{dd}(j+1))/\text{bb}(j) \\
\text{end}
\]

for i=1:np

\[
\begin{align*}
\text{h}(i) &= \text{dd}(i) \\
\text{h}_j(i) &= \text{h}(i) \\
\text{p} &= \text{h}(i) \\
\text{[k}(i), \text{th}(i), \text{c}(i), \text{Ks}] &= \text{unsat}_\text{calc}(p) \\
\text{sumt} &= \text{th}(i) + \text{c}(i) \times (\text{h}(i) - \text{h}_\text{old}(i))/\text{tetas-tetar} \\
\text{thdif} &= \text{th}(i) - \text{sumt} \\
\text{end}
\end{align*}
\]

if abs(thdif) > toler

\[
\text{th}(i) = \text{th}(i) + \text{c}(i) \times (\text{h}(i) - \text{h}_\text{old}(i))
\]

end

\[
\text{h}_\text{old} = \text{h}; \\
\text{it} = \text{it} + 1;
\]

end

\[
\text{cl}(1) = \text{acnp};
\]

for i=2:np-1

\[
\begin{align*}
\text{dif} &= \text{dw} \times \text{thold}(i) \times (7/3)/\text{tetas}^2 \\
\text{velm} &= \text{abs}(-0.5^*(\text{k}(i-1)+\text{k}(i)) \times ((\text{h}(i) - \text{h}(i-1))/\text{dz}) - 1)/\text{thold}(i)) \\
\text{velp} &= \text{abs}(-0.5^*(\text{k}(i+1)+\text{k}(i)) \times ((\text{h}(i+1) - \text{h}(i))/\text{dz}) - 1)/\text{thold}(i+1)) \\
\text{disp} &= \text{velm} \times \text{alpha}_t \\
\text{disp} &= \text{velp} \times \text{alpha}_t \\
\text{Dm} &= \text{dif} + \text{disp} \\
\text{Dp} &= \text{dif} + \text{disp} \\
\text{qcm} &= (-0.5^*(\text{k}(i-1)+\text{k}(i)) \times ((\text{h}(i) - \text{h}(i-1))/\text{dz}) - 1)^* \\
&\quad - 0.5^*(\text{cl}(i)+\text{cl}(i-1))) \\
\text{qcp} &= (-0.5^*(\text{k}(i)+\text{k}(i+1)) \times ((\text{h}(i+1) - \text{h}(i))/\text{dz}) - 1)^* \\
&\quad - 0.5^*(\text{cl}(i)+\text{cl}(i))) \\
\text{tdm} &= 0.5^*(\text{thold}(i-1) + \text{thold}(i)) \times \text{Dm} \\
\text{tdp} &= 0.5^*(\text{thold}(i+1) + \text{thold}(i+1)) \times \text{Dp} \\
\text{cn}(i) &= rz^* \times (\text{qcm} - \text{qcp}) + rzz^* \times \text{tcm} \times (\text{cl}(i-1) - \text{cl}(i)) - rzz^* \times \text{tdp} \times (\text{cl}(i) - \text{cl}(i+1) + \text{thold}(i) \times \text{cl}(i))/\text{th}(i) \\
\text{end}
\]

\[
\text{cn}(np) = \text{cn}(np-1);
\]

for i=2:np

\[
\text{cl}(i) = \text{cn}(i);
\]

end

\[
\text{z} = 0;\text{dz} = (\text{unsat}(gg) - \text{dz})
\]
for i=1:np
    conc(gg,i)=c1(i);
    head(gg,i)=h(i);
    theta(gg,i)=th(i);
    zz(gg,i)=z(i);
end
flux(gg)=flux(gg)+(c1(np)*-0.5*(k(np-1)+k(np))*...
     (((h(np)-h(np-1))/dz)-1))*dt;
thold=th;
if qin(gg)==0
    h(1)=htop;
end
end

function [hbot,htop,h,t1,qin,unsat,melt,np]=input;
np=51 %number of nodes
a = load('res_hour_fin.txt');
[r c] = size(a);
qin=zeros(r,1);
unsat=zeros(r,1);
melt=zeros(r,1);
for i=1:r
    qin(i)=a(i,1)*0.917*100;  % (cm)
    unsat(i)=a(i,2)*0.1*100;   % (cm)
    melt(i)=a(i,1)*100;        % (cm)
end
t1=r;
htop=-500;   % (cm)
hbot=-500;   % (cm)
hini=-500;   % (cm)
h=hini*ones(1,np);
h(np)=hbot; % (cm)

function [k,th,c,Se]=unsat_calc(p);
tetar=0.02;%residual water content
tetas=0.1;%water content or porosity
a=0.05;
n=1.5;
Ks=1969;%Saturated hydraulic conductivity (cm/d)
m=1-1/n;
th=tetar*(tetas-tetar)*(1+abs(a*p)^n)^-m;
Se=(th-tetar)/(tetas-tetar);
k=Ks*Se^0.5*(1-(1-Se^(1/m))^m)^2;
c=((tetas-tetar)*n*m*a*abs(a*p)^n(n-1))/((1+abs(a*p)^n)^{m+1});
LIST OF REFERENCES


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