Techniques and Analyses for Conductivity Measurements in Antarctica

by

Richard E. Ewing
Richard S. Falk
John F. Bolzan
and
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ABSTRACT

An accurate knowledge of the thermal properties of firn and ice within a glacier is essential for any reliable mathematical model of heat transfer. This paper considers the problem of determining the thermal properties of firn at Dome C, Antarctica, for use in such a model.

First, the difficulties in accurately determining thermal properties are discussed. Then a physical experiment which can be performed under field conditions but which will yield a well-posed mathematical problem for determining the unknown properties is presented. Next, two different numerical techniques for solving the mathematical problem are discussed. Finally, some numerical approximations and error estimates are presented for the results of applying our numerical procedure to data from Dome C. Although insufficient data was obtained to fully test our methods, we have established a measurement procedure and a method of analysis which appear to be promising.
TheTABLE

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TECHNIQUES AND ANALYSIS FOR CONDUCTIVITY
MEASUREMENTS IN ANTARCTICA

1. INTRODUCTION

We shall consider the problem of determining the thermal properties of
firn at Dome C, Antarctica, for use in mathematical models for heat transfer
in the glacier. Such models are very valuable for understanding the dynamics
and stability of glaciers [1, 17, 18, 19, 23, 24, 25], the effects of climate
changes at the surface of the ice sheet, and the general process of heat
transfer into the ice sheet. Accurate models could also be used to make
reverse calculations from measured temperature profiles to derive past,
decade-scale, climatic changes [3, 4, 11, 13, 20] and to guide the choice of
locations, techniques and needed accuracies for future field measurements.

The basic model equation that we will consider will be

\[ \rho c \theta_t = \nabla \cdot K \nabla \theta + \nabla \cdot \mathbf{v} \theta + q, \]

(1.1)

for the temperature $\theta$ where $\rho$ is the density, $c$ is the specific heat, and $K$
is the thermal conductivity of the firn or ice and the subscript $t$ denotes
partial differentiation with respect to time. The $\nabla \cdot \mathbf{v} \theta$ term models heat
flow due to the physical transport of the firn. The term $q$ is a measure of
the heat generated internally. As the firn travels downward, densifies, and
changes to ice, the thermal properties, and thus the coefficients in our
model equation change. We shall concentrate on determining $c$ and $K$, assuming
that the other properties are fairly well understood.

As a first step in our modeling process, we shall consider a one-dimen-
sional model equation to describe the temperature distribution as a function
of depth $z$ into the glacier. Then, for $0 < z < D$, we consider

\[ \rho c \theta_t = (K \theta_z)_z + \nu \theta_z + q, \]

(1.2)
where $D$ is the thickness of the glacier. We make the physically motivated assumption that $c$ and $K$ change fairly slowly with depth, and we take small samples from firn cores in the field and determine the coefficients within each sample as a constant. We finally extrapolate the constants determined in this way to obtain spatially varying coefficients $K$ and $c$.

Since our objective is to obtain error estimates for the coefficients determined, we developed a physical measurement apparatus which can produce the type of data necessary for a mathematical analysis of the problem. We shall describe the measurement apparatus, the techniques for obtaining the data, and some problems encountered with the "lab conditions" at Dome C. Next, we shall set up the mathematical model which requires the data we collect. We present results which show that the mathematical problem is well-posed, give estimates for the error incurred when the problem is solved using inexact data, and then describe two different numerical solution techniques. The first method assumes that $c$ is known and determines $K$, while the second determines estimates for both the specific heat and diffusivity simultaneously. We shall then discuss some data obtained by Dr. Bolzan at Dome C, Antarctica, and present the numerical approximations and error estimates obtained through our procedure using this data.

2. **DESCRIPTION OF THE PROBLEM**

An accurate knowledge of the thermal properties within a glacier is essential for any reliable mathematical model to be used to study heat flow. As temperature changes occur at the surface, it is necessary to know the thermal properties of the subsurface material to gauge how the subsurface thermal regime changes. The widely varying thermal properties near the surface are especially important since the temperature changes from climatic variations must pass through the top section of firn before it effects lower regions. Unfortunately, there are many different problems to be overcome in obtaining accurate measurements of the thermal properties of firn and ice from a glacier. In this section we shall describe the difficulties in obtaining accurate field measurements and how these difficulties motivated the techniques we have developed. We then describe the mathematical problem to be solved to obtain the desired thermal properties.
For most materials, in order to measure the thermal conductivity, one sets up an apparatus in a highly controlled laboratory setting which passes a large thermal gradient through a precisely measured sample of the material, allows the material to achieve thermal equilibrium, and then uses a steady-state temperature model to obtain the thermal properties. The process is usually repeated several times in order to obtain very precise values of the unknown properties.

The circumstances surrounding our measurement procedures are very different from those described above. First, exposure to the air and transport involving large temperature variations could dry out or melt the sample or radically change the thermal properties. Therefore the measurements must be made in the field instead of in a controlled laboratory environment. The "laboratory conditions" encountered at Dome C, Antarctica, were far from optimal. Temperatures of the "laboratory" were not within our control and varied diurnally making it very difficult to obtain a static thermal equilibrium. Maintaining a constant voltage from the field batteries necessary for the heating and measuring process was also very difficult.

Next, a large temperature gradient placed across a thin firn sample would melt the sample and no further measurements could be made. Thus, a fairly low temperature gradient and a fairly thick sample are needed. Low thermal gradients are also required for conductivity measurements on saturated rocks at permafrost temperatures as described in [21]. The measurement apparatus used in [21] is similar to ours. However, in [21], controlled laboratory conditions allowed thermal equilibrium to be attained and steady state models to be used. Since we could not allow thermal equilibrium to be reached at Dome C, we required a transient model in our measurement process.

In our experiments with firn samples, there are no transport terms or internal heat generation; thus, under the assumption that \( K \) is a constant within the sample, (1.2) can be written in the form

\[
(2.1) \quad \theta_\tau = A \theta_{zz}, \quad z \in (0, D') \,, \quad t \in (0, T),
\]

where \( D' \) is the thickness of the sample, and \( A = K (pc)^{-1} \) is the local
diffusivity of the medium. The density and specific heat are assumed to be known constants in our first method. Therefore, the determination of a constant \( K \) is equivalent to the determination of the constant \( A \). We can determine an initial temperature through the sample and can measure the boundary temperatures in time. This naturally leads to the mathematical problem: find a constant \( A > 0 \) and \( \theta = \theta(z,t) \) satisfying

\[
\begin{align*}
a) & \quad \theta_t = A \theta_{zz}, \quad \text{ze}(0,D'), \quad t \in (0,T], \\
b) & \quad \theta(0,t) = g_1(t), \quad t \in (0,T], \\
(2.2) & \\
c) & \quad \theta(D',t) = g_2(t), \quad t \in (0,T], \\
d) & \quad \theta(z,0) = f_0(z), \quad \text{ze}(0,D').
\end{align*}
\]

If \( A \) were known, the initial-boundary-value problem in (2.2) would determine a unique \( \theta = \theta(z,t) \). Since \( A \) is unknown, we shall overspecify the boundary data by measuring the heat flux \( H \) at \( z = 0 \) and some time \( t = t^* \). We then add to (2.2) the condition that, for some \( t^* \in (0,T) \),

\[
(2.3) \quad -K \theta_z(0,t^*) = -pcA \theta_z(0,t^*) = H.
\]

The determination of a unique \( A \) from (2.2) and (2.3) for arbitrary data \( g_1, g_2, f_0 \) and \( H \) is not possible. For example, if \( g_1, g_2, \) and \( f_0 \) are 0, then \( H = 0 \) and there is no heat flow. Clearly any \( A > 0 \) would then satisfy (2.2) and (2.3) with zero data. Thus our mathematical problem is not well-posed in the mathematical sense [5, 6, 9, 12, 13, 14, 15, 16]. We are thus faced with three major problems.

1. Find types of data \( f_0, g_1, g_2, H \) and assumptions on \( A \) which allow us to prove that a solution to (2.2) and (2.3) exists, is unique, and depends continuously upon the data.
2. Set up an experiment which can be performed in the field which will yield the data needed in (1).

3. Do a complete error analysis and interpretation of the resulting model problem.

The problem of determining an unknown coefficient is a classical problem which has been considered by several authors in the mathematical literature [5, 6, 9, 15, 16]. In [9] Douglas and Jones treated the determination of a time-dependent coefficient. In [5, 6] Cannon and DuChateau considered some problems similar to that considered here, but with more restrictive data than could be obtained accurately in Antarctica or Greenland. The work presented here is an extension of Cannon's analysis in [5] with less restrictive data assumptions.

In Section 4 and the appendix, we shall treat problem (1) above. In Section 3, we shall describe the experimental apparatus and the experiment which was performed in the field to yield our data. Then in Section 6 we shall consider error estimates from the actual data taken by Dr. Bolzan at Dome C and interpret the results.

3. DESCRIPTION OF THE MEASUREMENT APPARATUS AND PROCEDURE

We shall next describe the experimental apparatus and the experiment which was performed at Dome C, Antarctica, to yield our field data. The physical apparatus consists of a stack of control cylinders of lucite, the sample cylinder, and plates of copper containing thermistors. The stack is shown in Figure 1.

The apparatus was first tested in Antarctica during the 1978-79 field season. By allowing the stack to remain in operation for up to twelve hours to approach steady state conditions, we determined there was excessive heat loss out the sides of the stack and the data was then useless for the designed analysis. The stack was redesigned before the 1979-80 field season by including a thick styrofoam sleeve for better insulation around the stack. This reduced the heat loss out the sides of the stack to a very low level.
Figure 1: Measurement apparatus.
Unfortunately, we were not able to run the experiment to steady state during the 1979-80 field season to quantify this level closely.

The redesigned stack is well-insulated around the top and sides and was set onto the ice floor of the measuring pit. The ice floor served as a heat sink, the heater served as a heat source of about 1 watt when connected across a 12-volt battery, and the thermistors allowed the measurement of the time rate of change of the temperature through the stack. The thermistors allowed us to obtain temperature measurements as a function of time on both sides of the sample and on both sides of each lucite cylinder. Since the thermal properties of the lucite were known, we were able to solve initial-boundary-value problems in the lucite to determine the heat flux at the ends of the sample and to measure the total heat flow through the stack to indicate any appreciable heat loss out the sides through the insulation. The stack was allowed to reach an essentially steady-state temperature distribution before the heater was turned on. The initial temperature was assumed to be linear through the sample and thus determined by the initial temperature measurements taken at the ends of the sample just prior to activating the heater. This thermal equilibrium also yields the following compatibility conditions on the data which are necessary for the numerical error estimates:

\begin{align}
\text{a) } g_1(0) &= f_0(0), \\
g_2(0) &= f_0(D), \\
\text{b) } g_1'(0) &= g_1''(0) = g_2'(0) = g_2''(0) = 0.
\end{align}

In order to obtain as strong a gradient as possible through the ice, and thus better error estimates as described in Section 4, we wanted \( g_1(t) \) to rise rapidly and \( g_2(t) \) to stay nearly constant or rise slowly. This was the motivation for using the ice pit floor as a heat sink during the experiment.

Thermistors were Fenwal CA31J7 disc thermistors, .30" in diameter and .086" thick, with a nominal resistance of 1000 ohms at 25°C. They were calibrated by the Cold Regions Research and Engineering Laboratory in the summer of 1979. In the temperature interval from -40°C to +40°C we take the accuracy of temperatures measured to be ±0.05°C. However, because of the high
resistances of the thermistors (~30,000 Ω) at the temperatures in the stack during a measurement and because of the high resolution of the digital multimeter in this resistance range, the sensitivity is on the order of a few thousandths of a degree.

In order to minimize the effects of electrical noise which were appreciable in the vicinity of the Dome C camp, measurements of the thermal properties of firn were made at a site 5 kilometers away. This necessitated the use of a heated track vehicle to house the electronics and constrained the amount of time for a given run to several hours.

Firm samples were obtained by means of a SIPRE auger and consisted of cylinders 7.52 cm (3") in diameter of various lengths upon removal from the core barrel of the auger. Because of the friability of the firm core and its rapid deterioration upon handling, the firm sample to be measured was inserted into a stiff hollow cardboard tube. This also allowed the upper and lower surfaces to be trimmed parallel to each other and facilitated centering of the sample between the lucite discs. This cardboard tube remained around the sample for the duration of the experiment. After trimming the edges flush with the cardboard tube, the sample was weighed on a triple beam balance to determine the density. The sample was placed between the lucite discs, the entire stack fitted into the styrofoam jacket and the assembly buried about 1 meter below the snow surface so as to minimize the effect of the diurnal surface temperature change on the stack. The bottom copper plate was in thermal contact with the firm, which provided a heat sink. A typical run consisted of turning on the heater and monitoring the electrical resistance of each thermistor at 1-minute intervals for about 2 hours, which was the time needed for the heat pulse to pass through the sample.

A source of error which we have not yet addressed is the effect of possible diagenetic changes in the firm sample during the equilibration period. A sample taken from a depth of 8 meters, then buried at a depth of 1 meter may experience a difference in ambient temperature as high as 25°C. Two days of annealing at an elevated temperature may trigger grain growth, growth of bonds between crystals, and accelerate the sintering process leading to an increase of density and reduction of pore space. The thermal properties of the annealed sample may then be significantly different from the sample in situ. Measurements at different ambient temperatures of samples taken from
the same depth should help decide whether diagenetic effects induced during
the measurement process are significant.

4. WELL-POSEDNESS OF THE MATHEMATICAL PROBLEM

In this section we shall present conditions which, if satisfied, allow
us to show that a solution to our mathematical problem (2.2)-(2.3) exists, is
unique and depends continuously upon the data. We shall then give error
estimates for the mathematical problem based on these assumptions.

We normalize our problem. Let \( z = 0 \) and \( z = 1 \) be the top and bot-
tom of the sample, let \( g_1 = g_1(t) \) and \( g_2 = g_2(t) \) be the measured tem-
peratures at the top and bottom of the sample, respectively, let \( H \) be the mea-
sured heat flux at the top at some time \( t^* \in (0, T) \), and let \( f_0 = f_0(z) \) be the
initial linear temperature distribution through the sample. We then obtain
the following mathematical problem: find \( A \) and \( \theta = \theta(z, t) \) satisfying

\[
\begin{align*}
(4.1) & \quad \theta(t) = A \theta_{zz} \quad , \quad z \in (0,1), \quad t \in (0, T), \\
(4.2) & \quad f_0(z) = (1 - z) g_1(0) + z g_2(0) .
\end{align*}
\]

We shall seek \( A \) satisfying (4.1) and (4.2) and the additional physical bounds

\[
(4.3) \quad 0 < A_* < A < A^* .
\]
From the field experiment, we see that \( g_1(t) \) increases much faster than \( g_2(t) \). In particular, we have from our experimental data that for \( t^* \) from (4.1.e)

\[
a) \quad g_1(t) > 4g_2(t) \quad , \quad 0 < t < t^* ,
\]

(4.4) and

\[
b) \quad g_1(0) > g_2(0) .
\]

Using Fourier series techniques and techniques from [5, 7], we can obtain a solution, depending upon \( A \), for (4.1) and (4.2) of the form for

\[
0 < z < 1 \quad \text{and} \quad 0 < t < T ,
\]

\[
\theta(z,t;A) = (1 - z) g_1(0) + z g_2(0)
\]

(4.5)

\[
\quad - \int_0^t \frac{\partial M(z, A(t - \tau))}{\partial z} \left[ g_1(\tau) - g_1(0) \right] A d \tau
\]

\[
+ \int_0^t \frac{\partial M(z - 1, A(t - \tau))}{\partial z} \left[ g_2(\tau) - g_2(0) \right] A d \tau
\]

where

(4.6)

\[
M(\xi, \sigma) = \frac{1}{\sqrt{\pi} \sigma} \sum_{n=-\infty}^{\infty} \exp\left[ - \frac{(\xi - 2n)^2}{4\sigma} \right] , \sigma > 0 .
\]

We have emphasized the dependence of \( \theta \) on \( A \) in our notation \( \theta = \theta(z,t;A) \). Next, for \( \alpha \in \mathbb{R} \) we define the continuous function

(4.7)

\[
Q(\alpha) = - \rho \sigma \alpha \theta_z(0,t^*;\alpha) .
\]

We must then find \( A \) such that

\[
Q(A) = H .
\]
We can now obtain the following important lemma.

**Lemma 4.1.** If $\tilde{\alpha} \in [A_*, A^*]$ and $Q$ is defined by (4.7) with $\theta$ satisfying (4.5) and (4.6), we have

$$\frac{dQ}{d\alpha} \left( \tilde{\alpha} \right) > \rho_c \left( [g_1(0) - g_2(0)] + \frac{1}{2} \int_0^{\tau^*} \frac{g_1'(\tau) - 4g_2'(\tau)}{\sqrt{\pi A^*(\tau^* - \tau)}} \, d\tau \right) \equiv G.$$  

**Proof.** Since the details of the proof are intricate we shall defer the proof to Appendix A. The proof techniques contain generalizations of the ideas found in [5].

One consequence of Lemma 4.1 coupled with (4.4) is that for the interval $\tilde{\alpha} \in [A_*, A^*]$, $Q(\alpha)$ is monotone increasing as well as continuous. Thus we can apply the Intermediate Value Theorem to yield the following result:

**Theorem 4.2. Existence and Uniqueness.** If the data $g_1(t)$ and $g_2(t)$ satisfy (4.4), then for any $H$ in the range

$$Q(A_*) < H < Q(A^*),$$

there is one and only one $A$ in the interval

$$A_* < A < A^*,$$

such that $Q(A) = H$. Given this unique $A$, the representation (4.5) and (4.6) gives a unique $\theta(z, t; A)$ such that the pair $A$ and $\theta(z, t; A)$ satisfy (4.1)–(4.2).

We next consider how this solution depends upon measurement errors in the problem. Let

$$\|f\| = \max_{t \in (0, T]} |f(t)|.$$  

Then assume $H$, $g_1$, and $g_2$ are obtained as $H^*$, $g_1^*$, and $g_2^*$ subject to measurement errors of the form
a) \[ |H - H^*| < \varepsilon_0 \quad , \quad \varepsilon_0 > 0, \]

(4.12) b) \[ \|g_1 - g_1^*\| + \|g_2 - g_2^*\| < \varepsilon_1 \quad , \quad \varepsilon_1 > 0, \]

c) \[ \|g_1^* - g_1^*\| + \|g_2^* - g_2^*\| < \varepsilon_1', \quad \varepsilon_1' > 0. \]

Also define \( Q^*(\alpha) \) as the analogue of \( Q \) from (4.7) for the problem with \( g_1, g_2 \) and \( H \) replaced by \( g_1^*, g_2^* \), and \( H^* \).

Using the linearity of the heat equation, we can apply the representations from (4.5) and (4.6) to obtain the following lemma.

**Lemma 4.3.** There exist positive constants \( K_1 \) and \( K_2 \) such that

(4.13) \[ \max_{\alpha \in [A^*, A^*]} |Q(\alpha) - Q^*(\alpha)| \leq K_1 \varepsilon_1 + K_2 \varepsilon_1' \]

where \( \varepsilon_1 \) and \( \varepsilon_1' \) are given by (4.12),

\[ K_1 = 2pcA^*, \quad \text{and} \quad K_2 = pc\left\{3\sqrt{\frac{+}{A^*}} + +^*\right\}. \]

**Proof:** See Appendix A for details.

Let the pair \( (\alpha^*, \theta^*) \) be the unique solution of the problem:

a) \[ \theta^*_t \triangleq a^* \theta^*_z \quad , \quad z \in (0,1), \; t \in (0,T), \]

b) \[ \theta^*(0,t) = g_1^*(t) \quad , \quad t \in (0,T), \]

c) \[ \theta^*(1,t) = g_2^*(t) \quad , \quad t \in (0,T), \]

d) \[ \theta^*(z,0) = (1-z)g_1^*(0) + zg_2^*(0) \quad , \quad z \in [0,1], \]

e) \[ -pc\alpha^*_z(0,\tau) = H^* \quad , \quad \tau \in (0,T), \]
where \( H^* \), \( g_1^* \) and \( g_2^* \) are our measured data satisfying (4.12). Our next theorem shows that the determination of \( A \) depends continuously upon the data in the sense that if \( H^* \), \( g_1^* \) and \( g_2^* \) are close to \( H \), \( g_1 \) and \( g_2 \), respectively, then \( a^* \) from (4.14) is close to \( A \) from (4.1).

**Theorem 4.4.** If \( A \) and \( a^* \) satisfy (4.1) and (4.14), respectively, and (4.12) holds, then

\[
|A - a^*| < G^{-1} \left[ \varepsilon_0 + K_1 \varepsilon_1 + K_2 \varepsilon_1^* \right]
\]

where \( G \), \( K_1 \), and \( K_2 \) are given by (4.8) and (4.13).

**Proof.** Let \( a \in [A_*, A^*] \) be such that

\[
Q(a) = H^* = Q^*(a^*)
\]

Then applying the triangle inequality, the Mean Value Theorem, Lemmas 4.1 and 4.3, and (4.16), we obtain

\[
|A - a^*| < |A - a| + |a - a^*|
\]

\[
< \max_{a \in [A_*, A^*]} \left[ \frac{1}{Q'(a)} \left[ |Q(A) - Q(a)| + |Q(a) - Q(a^*)| \right] \right]
\]

\[
< G^{-1} \left[ |Q(A) - Q(a)| + |Q(a) - Q(a^*)| \right]
\]

\[
(4.17)
\]

\[
< G^{-1} \left[ |H - H^*| + \max_{a \in [A_*, A^*]} |Q^*(a) - Q(a)| \right]
\]

\[
< G^{-1} \left[ \varepsilon_0 + K_1 \varepsilon_1 + K_2 \varepsilon_1^* \right].
\]

**Corollary 4.5.** If \( a' \) satisfies \( A_* < a' < A^* \) and
\[(4.18) \quad |Q^*(a') - H^*| \leq \varepsilon_2, \]

then

\[(4.19) \quad |a' - A| \leq G^{-1}[\varepsilon_0 + K_1\varepsilon_1 + K_2\varepsilon_1^2 + \varepsilon_2]. \]

\textbf{Proof.} The proof of this result is analogous to that of Theorem 4.4.

Thus any \( a' \) satisfying (4.18) will be close to \( A \) as described in (4.19). The next problem is to show how we can computationally determine an \( a' \in [A_*, A^*] \) satisfying (4.18) for which \( \varepsilon_2 \) is small. This will be done in the next section.

\section{Description of Numerical Methods}

Before we discuss the method for numerically obtaining an approximate solution for (4.14), we describe how the numerical data was obtained. First the recorded resistance data from the thermistors was numerically converted to temperature data and smoothed very slightly staying well within the error bars for the data (see Table 1). This gave us \( g_1^* \) and \( g_2^* \) at one minute intervals for the first hour with \( \varepsilon_1 \) from (4.9.b) approximately \( 0.03^\circ \text{C} \). Then in order to obtain \( H^* \) for (4.9.a), a separate boundary-value problem was solved numerically within the top lucite region where the thermal properties of lucite were known.

A piecewise linear Galerkin spatial discretization was used with a fourth order in time backward differentiation multistep method (see [2, 101]). This method is presented in Appendix B. A special start-up procedure (see [2]) was required. The flux at the bottom of the lucite was then computed and used as \( H^* \), the flux at the top of the sample, in (4.9.a). The numerical results are presented in Table 1.

From Corollary 4.5, if we can find a diffusivity \( a' \in [A_*, A^*] \) such that \( Q^*(a') \) is close to our calculated flux \( H^* \), then \( a' \) will be a good approximation to the unknown \( A \). To determine such an \( a' \) computationally, first find \( a_1 \) and \( a_2 \), \( \varepsilon \in [A_*, A^*] \) for which
(5.1) \[ Q^*(a_1) < H^* < Q^*(a_2). \]

Then pick a sufficiently small error tolerance \( \varepsilon_3 \) and perform an interval-halving routine using \( a_1 \) and \( a_2 \) to start. At each step of the interval-halving routine, pick the mid-point \( \alpha \) of the active interval as a guess for \( \alpha \), numerically solve an initial-boundary-value problem using \( \alpha, g_1^*, \) and \( g_2^* \), and then compare the calculated flux using \( \alpha \) with \( H^* \). The numerical procedures used in each step of this interval-halving routine are the fourth order multistep Galerkin procedures used for the lucite problem. The routine is terminated when \( \alpha \) is determined satisfying

(5.2) \[ | - \rho \frac{\partial \theta}{\partial n} \Big|_{z=0, t^*; \alpha} - H^* | < \varepsilon_3, \]

where \( \frac{\partial \theta}{\partial n} \Big|_{z=0, t^*; \alpha} \) is the computed approximation of the derivative at \( z = 0 \) and \( t = t^* \) of the problem of determining \( \theta(z, t; \alpha) \) satisfying:

a) \( \theta_t = a_n \theta_{zz}, \quad z \in (0, 1), \quad t \in (0, T), \)

b) \( \theta(0, t) = g_1^*(t), \quad t \in (0, T), \)

c) \( \theta(1, t) = g_2^*(t), \quad t \in (0, T), \)

d) \( \theta(z, 0) = (1 - z) g_1^*(0) + z g_2^*(0), \quad z \in [0, 1]. \)

The numerical scheme used satisfies the estimate

\[ \rho \frac{\partial \theta}{\partial n} \Big|_{z=0, t^*; \alpha} - \phi_z(0, t^*; \alpha) | < \varepsilon_4 \]

where \((2, 101)\)

(5.5) \[ \varepsilon_4 = O((\Delta t)^4 + \Delta z). \]
\( \varepsilon_4 \) can be made very small with the proper choice of the spatial mesh size \( \Delta z \) and temporal step size \( \Delta t \). Then, combining (5.2) and (5.4), we see that (4.18) is satisfied with \( a' = a_n \) and \( \varepsilon_2 = \varepsilon_3 + \varepsilon_4 \). Using (4.19), we obtain

\[
|a_n - A| < G^{-1} \left[ \varepsilon_0 + K_1 \varepsilon_1 + K_2 \varepsilon_1' + \varepsilon_3 + \varepsilon_4 \right],
\]

an error bound for the accuracy in our coefficient determination problem. (5.6) is not a "sharp" estimate, but merely an upper bound for the error.

6. INTERSECTING GRAPH TECHNIQUES

So far we have based our method for determining \( A \) (and thus \( K \)) upon the premise that we have a priori knowledge of the specific heat \( c \). In many cases, we may not have accurate estimates of either the specific heat or the thermal conductivity. We next describe an intersecting graph technique used for similar problems, by Cannon and Du Chateau [6]. We will obtain approximate pairs \((K, c)\) for this more difficult problem.

Since we do not have a priori knowledge of \( c \) as before, we shall perform the same method with the flux measured at a fixed \( t = t^* \) for a systematic sequence of values of \( c \) in the anticipated range. Each value of \( c \) will then determine a pair \((c, K)\) through this procedure. If sufficiently many values of \( c \) are chosen at close intervals we will in effect determine the "graph" of the "function" \( K = K(c) \) for the fixed time, \( t^* \). For another choice of \( t = \tilde{t} \) at some distance from \( t^* \) we can repeat the process with the same set of values for \( c \) to obtain a new "graph" of \( K = K(c) \) for the same material. We hope that by taking radically different values of \( t \) we can obtain two curves with different properties. The true parameters, \((c, K)\) should lie on the intersection of the curves determined in this way.

We emphasize that the determination of each "point" \((c, K)\) in this method entails the full numerical method of Section 5. Therefore since several "points" are necessary to determine two curves and their intersection by graphical techniques, this procedure requires considerably more computer time than the previous method. However, if one is uncertain of the values of \( c \), one should always use this method to "check" the proposed values.
We have used this technique for shallow depth samples in Antarctica with good success. The curves are very distinct and smooth and an accurate approximation of \( c \) and \( K \) can be obtained. We found that the values \( c \) given by this method for the shallow Dome C data were somewhat different than expected. The results of these computations are described in Section 7 below.

We next consider a slightly different computational procedure. The experimental apparatus allows us to determine the flux not at just one time \( t^* \), at \( z = 0 \), but for many times and for both \( z = 0 \) and \( z = 1 \). We can use this extra data to increase the accuracy of the methods presented above. First we can use our first method to obtain better values of \( A_0 \) and \( A_e \) between which to search. Then, numerically, one can determine a satisfying the new, more restrictive bounds which will minimize the functional

\[
J(\alpha) = \sum_{i=1}^{n} |\rho c \alpha \phi_x (0, t_i; \alpha) - H_{0,i}^*|^2 + \sum_{i=1}^{n} |\rho c \alpha \phi_x (1, t_i; \alpha) - H_{1,i}^*|^2,
\]

where \( H_{0,i}^* \) and \( H_{1,i}^* \) are the flux computations from the lucite control cylinders for \( n \) different \( t = t_i \) at \( z = 0 \) and \( z = 1 \), respectively.

7. **NUMERICAL RESULTS FROM DOME C DATA**

In this section we shall present the numerical results obtained by applying our various methods to the data collected by Dr. Bolzan at Dome C, Antarctica. We then discuss data accuracies and corresponding error bounds. After presenting the results we shall compare them to previously known or assumed values of the various thermal properties under consideration and give our interpretation of the similarities and differences.

Only four samples were tested in our measurement apparatus at Dome C during the 1979-80 field season. On one of these test runs, the printer ran out of paper after twenty minutes and the run was aborted. The sample was later retested, but the data obtained was sufficiently anomalous that the results will not be presented. Thus the results of only three runs will be
presented. The general data is given in Table 2. The error in smoothing the data and the values of $H^*$ determined numerically are given in Table 1.

As we have noted earlier the basic numerical model described in Section 5 required the specification of the specific heat of the sample. The temperature variations within all of the samples over the runs fell between the values of $-29.9^\circ C$ and $-37.3^\circ C$. The first numerical results were obtained using an estimate for the specific heat of ice in this temperature range of 0.45 cal/g/$^\circ C$. The numerical results obtained using this value for specific heat and $t^* = 60$ minutes are given in Table 3. To start the numerical procedures we used $A_w^* = 0.1$ and $A^* = 1$ in units of cm$^2$/min. As the procedures ran, better choices of $A_w^*$ and $A^*$ were obtained.

Since we realized that the value of 0.45 for $c$ used in the numerical procedure was only an approximation based on the value for ice, we decided to use the Intersecting Graph Technique described in Section 6 on the same data to estimate both the specific heat and the thermal conductivity simultaneously. This procedure was carried out for each sample using $t^* = 60$ minutes and $\bar{t} = 90$ minutes. The numerical results obtained by using the Intersecting Graph Technique are presented in Table 4. A graph of the "points" $(c, K)$ determined for the $B$ meter sample is given in Figure 2 to illustrate the ideas, and indicate the accuracies (which depend upon the relative slopes of the "graphs") obtained in the Intersecting Graph Technique.

We note that the specific heats determined numerically from the field data were all somewhat higher than the specific heat of ice at the given temperature. The higher values of specific heat give lower values of diffusivity and conductivity. The values of thermal conductivity obtained here agree fairly well with the values presented in Weller and Schwerdtfeger [8, 24]. We also note that the values of diffusivity in units of m$^2$/year presented in Table 4 are very close to the value of 24.6 m$^2$/year obtained using a slight linearization of the model presented by Lax [22]. The diffusivities using $c = 0.45$ and presented in Table 3, however, are much higher than the 24.6 m$^2$/year estimate. We also note that conductivities correlate fairly well with density for this very narrow range of samples. If this correlation
Figure 2. Diffusivity - 8 meter sample.
were understood better and were shown to hold in more widely varying circumstances, it might be utilized to help model diffusivity more accurately over wide variations of densities.

We point out that although the diffusivities obtained from Table 4 are close to the expected values, the specific heats, and thus the thermal conductivities, are somewhat higher than expected. We also note that the thermal conductivity of ice is in the range 0.005 to 0.0022 cal/sec cm°C, and we would expect the conductivity of firn to be somewhat lower.

Next, we briefly discuss error bounds for our methods. We emphasize again that the estimates obtained in (5.6) are not sharp, but are merely upper bounds. The mesh spacings $\Delta z$ and $\Delta t$ were taken such that $\varepsilon_4 = .01$. Since determination of $\varepsilon_0$ involves a numerical solution of an initial boundary-value problem we can argue as Lemma 4.3 that

$$
(7.1) \quad \varepsilon_0 < \varepsilon_5 + K_1[\varepsilon_1 + \|g_0 - g_0^*\|] + K_2[\varepsilon_1 + \|g_0^* - g_0^{**}\|],
$$

where, like $\varepsilon_4$,

$$
(7.2) \quad \varepsilon_5 = 0((\Delta t)^4 + \Delta z) = .01
$$

and $g_0(t)$ and $g_0^*(t)$ are the true and the measured temperatures at the thermistor at the top of the top lucite control cylinder. It is very difficult to obtain the theoretical estimates for the size of the error between $g_0, g_1, g_2$ and the measured (smoothed) data $g_0^*, g_1^*, g_2^*$. Estimates based on the size of the difference quotients and the smoothness of $g_0, g_1$, and $g_2$ are, with our scalings,

$$
(7.3) \quad \varepsilon_1 + \|g_0 - g_0^*\| = .03 \quad \text{and} \quad \varepsilon_1 + \|g_0^* - g_0^{**}\| = .005.
$$

Rough estimates of $K_1$ and $K_2$ from Lemma 4.3 are

$$
(7.4) \quad K_1 = .17 \quad \text{and} \quad K_2 = 20.
$$
Thus, combining (7.1)-(7.4), we obtain

\[(7.5) \quad \varepsilon_0 = 0.1.\]

The error tolerance in the interval-halving routine was \(\varepsilon_3 = 10^{-7}\). Thus (5.6) yields the estimate

\[(7.6) \quad |a_n - A| < G^{-1}[0.22].\]

We can then obtain an approximate error tolerance from an estimate on the size of \(G\).

We shall present an estimate of \(G\) for the 4.8 meter sample. Estimates for the other samples are obtained in an analogous fashion. For this sample

\[(7.7) \quad g_1(0) - g_2(0) = 1.18\]

and

\[(7.8) \quad \int_0^{60} \frac{g_1'(\tau) - 4g_2'(\tau)}{\sqrt{A^2(90 - \tau)}} \, d\tau = 0.553.\]

Thus, from (4.8) we see that

\[(7.9) \quad G^{-1} = 3.58.\]

Then combining (7.6) and (7.9) we obtain the bound on the error tolerance

\[(7.10) \quad |a_n - A| < 0.79.\]

We emphasize that this is an upper bound for the error since (7.9) is a gross upper bound on \((\frac{dQ}{da}(\bar{a}))^{-1}\).

We note that a major factor in the size of our bound is the estimate on \(K_2\). Looking carefully at the source of this bound in the proof of Lemma
4.3, we see that we have overestimated the size of terms \(T_5\) and \(T_6\) of (A20) in Appendix A in order to obtain an error "bound". We note that the kernel \(M(0, \sigma)\) is small for early times where there is some error in the approximation of the derivative while the data are very smooth with almost negligible error in the derivative when \(M(0, \sigma)\) is larger (for \(t \) near \(t^*\)). Thus for our data, the size of the \(K_2 \varepsilon_1\) is much smaller than the bounds provided by (7.3) and (7.4).

Usually the \(K_1 \varepsilon_1\) term in (4.11) will dominate with our data. If we assume \(K_2 \varepsilon_1 \ll K_1 \varepsilon_1\) as an "estimate" of our error, we see that (7.5) can be replaced by

\[
(7.11) \quad \varepsilon_0 = 0.025
\]

and (7.7) can be replaced by

\[
(7.12) \quad |a_n - A| = \left(\frac{dQ}{da} (\alpha)\right)^{-1} (.05)
\]

For \(c = .58\) in the 4.8 meter sample we use the results of the interval halving scheme to obtain the estimate

\[
(7.13) \quad \frac{dQ}{da} (.43) = 0.60
\]

Combining (7.12) and (7.13) we obtain the estimate in \(\text{cm}^2/\text{min}\)

\[
(7.14) \quad |a_n - A| = 0.08
\]

Our accuracy is basically limited by the data measurement accuracy and not by the mathematical and computational tools used. We also found that although the numerical methods were somewhat complex, the results indicated the stability of the methods by producing very smooth "curves" in the intersecting graph technique.
### TABLE 1. NUMERICAL COMPUTATION OF $g_1$, $g_2$, AND $H^*$

<table>
<thead>
<tr>
<th>Run Number</th>
<th>Depth (m)</th>
<th>$g_1(t)$</th>
<th>$g_2(t)$</th>
<th>$g_1(t)$</th>
<th>$g_2(t)$</th>
<th>$t=60$ min.</th>
<th>$t=90$ min.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>0.08707</td>
<td>0.00648</td>
<td>0.00983</td>
<td>0.00044</td>
<td>-0.0516</td>
<td>-0.0668</td>
</tr>
<tr>
<td>2</td>
<td>4.8</td>
<td>0.00186</td>
<td>0.00117</td>
<td>0.00006</td>
<td>0.00002</td>
<td>-0.0538</td>
<td>-0.0685</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>0.01030</td>
<td>0.00555</td>
<td>0.00015</td>
<td>0.00009</td>
<td>-0.0560</td>
<td>-0.0721</td>
</tr>
</tbody>
</table>

### TABLE 2. DOME C CONDUCTIVITY RUNS - 1979

<table>
<thead>
<tr>
<th>Sample Number</th>
<th>Depth (m)</th>
<th>Thickness (cm)</th>
<th>Density (g/cm³)</th>
<th>Date Obtained</th>
<th>Date Measured</th>
<th>Duration of Run (min.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>7.48</td>
<td>.395 ± .014</td>
<td>Dec. 17</td>
<td>Dec. 21</td>
<td>110</td>
</tr>
<tr>
<td>2</td>
<td>4.8</td>
<td>7.48</td>
<td>.370 ± .013</td>
<td>Dec. 21</td>
<td>Dec. 23</td>
<td>120</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>7.48</td>
<td>.428 ± .016</td>
<td>Dec. 28</td>
<td>Dec. 31</td>
<td>120</td>
</tr>
</tbody>
</table>

### TABLE 3. CONDUCTIVITY RESULTS USING $c = .45$ cal/g/°C and $t^* = 60$ min.

<table>
<thead>
<tr>
<th>Sample Number</th>
<th>Depth (m)</th>
<th>Density (g/cm³)</th>
<th>Diffusivity (cm²/min)</th>
<th>Diffusivity (m²/yr)</th>
<th>Conductivity (cal/sec cm°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>.395</td>
<td>.615</td>
<td>32.3</td>
<td>0.001822</td>
</tr>
<tr>
<td>2</td>
<td>4.8</td>
<td>.370</td>
<td>.680</td>
<td>35.7</td>
<td>0.001887</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>.428</td>
<td>.591</td>
<td>31.0</td>
<td>0.001897</td>
</tr>
</tbody>
</table>

### TABLE 4. CONDUCTIVITY AND SPECIFIC HEAT RESULTS USING THE INTERSECTING GRAPH TECHNIQUE

<table>
<thead>
<tr>
<th>Depth (m)</th>
<th>Density (g/cm³)</th>
<th>Specific Heat (cal/g°C)</th>
<th>Diffusivity (cm²/min)</th>
<th>Diffusivity (m²/yr)</th>
<th>Conductivity (cal/sec cm°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>.395</td>
<td>.545</td>
<td>.455</td>
<td>23.9</td>
<td>0.001633</td>
</tr>
<tr>
<td>4.8</td>
<td>.370</td>
<td>.565</td>
<td>.456</td>
<td>24.0</td>
<td>0.001589</td>
</tr>
<tr>
<td>8</td>
<td>.428</td>
<td>.490</td>
<td>.502</td>
<td>26.4</td>
<td>0.001755</td>
</tr>
</tbody>
</table>
REFERENCES


APPENDIX A

In this appendix we shall sketch the proof of Lemmas 4.1 and 4.3. We shall rely on many of the ideas of Cannon from [5] in our proofs.

Proof of Lemma 4.1. First we shall differentiate (4.5) to obtain $Q(\alpha)$.
Assuming $g_1$ and $g_2$ are continuously differentiable, we can apply Leibnitz's rule to differentiate (4.5) under the integral sign to obtain on $0 < z < 1,$ $0 < t < T,$

$$\theta_z(z, t; \alpha) = -g_1(0) + g_2(0)$$

$$- \int_{0}^{\tau} \frac{\partial^2 M(z, \alpha(t - \tau))}{\partial z^2} \left[ g_1(\tau) - g_1(0) \right] \alpha d\tau$$

$$(A1)$$

$$+ \int_{0}^{\tau} \frac{\partial^2 M(z - 1, \alpha(t - \tau))}{\partial z^2} \left[ g_2(\tau) - g_2(0) \right] \alpha d\tau .$$

Next use the fact that $M(z - \xi, \alpha(t - \tau))$ satisfies

$$(A2) \quad \frac{\partial M(z - \xi, \alpha(t - \tau))}{\partial \tau} = -\alpha \frac{\partial^2 M(z - \xi, \alpha(t - \tau))}{\partial z^2}, \quad z \neq \xi, \quad t \neq \tau,$$

and integration by parts to see that

$$\theta_z(z, t; \alpha) = -g_1(0) + g_2(0) - \int_{0}^{\tau} M(z, \alpha(t - \tau)) g_1(\tau) d\tau$$

$$+ \int_{0}^{\tau} M(z - 1, \alpha(t - \tau)) g_2(\tau) d\tau + M(z, \alpha(t - \tau)) \left[ g_1(\tau) - g_1(0) \right]^{\tau}_{0}$$

$$(A3)$$

$$- M(z - 1, \alpha(t - \tau)) \left[ g_2(\tau) - g_2(0) \right]^{\tau}_{0} .$$
Next using the fact that \( \lim_{\tau \to t} M(x - \xi, \alpha(t - \tau)) = 0, \ x \neq \xi, \) and the Lebesgue Dominated Convergence Theorem to take the limit as \( z \) tends to zero we obtain

\[
Q(\alpha) = -\rho c a \theta_z(0, +\ast; \alpha) \\
= \rho c a [g_1(0) - g_2(0)] \\
+ \int_0^{+\ast} \left[ M(0, \alpha(\tau - \tau)) g_1(\tau) - M(-1, \alpha(\tau - \tau)) g_2(\tau) \right] d\tau.
\]

(A4)

Thus, differentiating (A4) with respect to \( \alpha \) and letting \( \sigma = \alpha(\tau - \tau) \),

\[
Q'(\alpha) = -\rho c a \theta_z(0, +\ast; \alpha) - \rho c a \frac{\partial}{\partial \alpha} \theta_z(0, +\ast; \alpha) \\
= \rho c a [g_1(0) - g_2(0)] \\
+ \int_0^{+\ast} \left[ M(0, \sigma) + \frac{\partial}{\partial \sigma} M(0, \sigma) \alpha(\tau - \tau) \right] g_1(\tau) d\tau \\
- \int_0^{+\ast} \left[ M(-1, \sigma) + \frac{\partial}{\partial \sigma} M(-1, \sigma) \alpha(\tau - \tau) \right] g_2(\tau) d\tau.
\]

(A5)

Now, using (4.6), we see that, for \( \sigma > 0 \)

\[
\frac{\partial}{\partial \sigma} M(z, \sigma) = -\frac{1}{2} \frac{1}{\sqrt{\pi \sigma}} \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{(z - 2n)^2}{4 \sigma} \right] \\
+ \frac{1}{\sqrt{\pi \sigma}} \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{(z - 2n)^2}{4 \sigma} \right] \frac{(z - 2n)^2}{4 \sigma^2}.
\]

(A6)

We then write the integral terms from (A5) in the form (noting \( \frac{\partial}{\partial \sigma} M(z, \sigma) = M_0(z, \sigma) \))
\[ \int_0^{\infty} \left[ [M(0, \sigma) + \sigma M_\sigma(0, \sigma)] g_1^2(\tau) - [M(-1, \sigma) + \sigma M_\sigma(-1, \sigma)] g_2^2(\tau) \right] d\tau \]

(A7)

\[ = \int_0^{\infty} \left[ [M(0, \sigma) + \sigma M_\sigma(0, \sigma)] [g_1^2(\tau) - g_2^2(\tau)] \right. \]

\[ + \left. [M(0, \sigma) - M(-1, \sigma) + \sigma M_\sigma(0, \sigma) - \sigma M_\sigma(-1, \sigma)] g_2^2(\tau) \right] d\tau. \]

Next, using (4.6) and (A6) we see that

\[ M(0, \sigma) - M(-1, \sigma) + \sigma M_\sigma(0, \sigma) - \sigma M_\sigma(-1, \sigma) \]

\[ = \frac{1}{2} \int_0^{\infty} \left\{ \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{4n^2}{4\sigma} \right] \right\} - \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{(1-2n)^2}{4\sigma} \right] \}

(A8)

\[ + \frac{1}{\sqrt{\pi\sigma}} \left[ \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{4n^2}{4\sigma} \right] \right] \frac{n^2}{\sigma} \]

\[ - \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{(1-2n)^2}{4\sigma} \right] \frac{(1-2n)^2}{4\sigma} \]

\[ = T_1 + T_2. \]

Now we note that

(A9) \[ \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{4n^2}{4\sigma} \right] = 1 + 2 \sum_{n=1}^{\infty} \exp \left[ -\frac{4n^2}{4\sigma} \right] \]

and, by a shift of index on part of the sum,

(A10) \[ \sum_{n=-\infty}^{\infty} \exp \left[ -\frac{(1-2n)^2}{4\sigma} \right] = 2 \exp \left[ -\frac{1}{4\sigma} \right] + 2 \sum_{n=1}^{\infty} \exp \left[ -\frac{(1-2n)^2}{4\sigma} \right]. \]
Thus we see that, using the mean value theorem,

\[ \sum_{n=\infty}^{\infty} \exp \left[ - \frac{4n^2}{4\sigma} \right] - \sum_{n=\infty}^{\infty} \exp \left[ - \frac{(1 - 2n)^2}{4\sigma} \right] \]

\[ = 1 - 2 \exp \left[ - \frac{1}{4\sigma} \right] + 2 \sum_{n=1}^{\infty} \exp \left[ - \frac{n^2}{\sigma} \right] \left\{ 1 - \exp \left[ - \frac{1}{4\sigma} \right] \right\} \]

(A11)

\[ > 1 - 2 \exp \left[ - \frac{1}{4\sigma} \right] + 2 \sum_{n=1}^{\infty} \exp \left[ - \frac{n^2}{\sigma} \right] \left\{ 1 - \exp \left[ - \frac{1}{4\sigma} \right] \right\} \]

\[ > 1 - 2 \exp \left[ - \frac{1}{4\sigma} \right] + 2 \sum_{n=1}^{\infty} \exp \left[ - \frac{n^2}{\sigma} \right] \left\{ 1 - \exp \left[ - \frac{1}{4\sigma} \right] \right\} \]

\[ > 1 - 2 \exp \left[ - \frac{1}{4\sigma} \right] + 2 \sum_{n=1}^{\infty} \exp \left[ - \frac{n^2}{\sigma} \right] \left\{ 1 - \exp \left[ - \frac{1}{4\sigma} \right] \right\} \]

By the same argument,

\[ \sum_{n=\infty}^{\infty} \exp \left[ - \frac{4n^2}{4\sigma} \right] \frac{n^2}{\sigma} - \sum_{n=\infty}^{\infty} \exp \left[ - \frac{(1 - 2n)^2}{4\sigma} \right] \frac{(1 - 2n)^2}{4\sigma} \]

(A12)

\[ = - \frac{1}{2\sigma} \exp \left[ - \frac{1}{4\sigma} \right] + 2 \sum_{n=1}^{\infty} \left\{ \frac{n^2}{\sigma} \exp \left[ - \frac{n^2}{\sigma} \right] \right\} \]

\[ \left\{ 1 - \exp \left[ - \frac{1}{4\sigma} \right] \right\} \left\{ 1 - \exp \left[ - \frac{1}{4\sigma} \right] \right\} \]

Consider the function

\[ y(x) = xe^{-x} \]
From elementary calculus, we see that $y(x)$ attains its maximum of $\exp(-1)$ at $x = 1$ and that $y(x)$ is decreasing for $x > 1$ and increasing for $x < 1$. For $\sigma$ fixed, define $N_0(\sigma) > 1$ such that

$$N_0^2 > \sigma \quad \text{and} \quad (N_0 - 1)^2 < \sigma.$$  

(A13)

Then for $n > N_0$, we have $4n^2 < (-1 - 2n)^2$ and

$$\exp\left[-\frac{4n^2}{4\sigma}\right] \times \frac{4n^2}{4\sigma} > \exp\left[-\frac{(-1 - 2n)^2}{4\sigma}\right] \times \frac{(-1 - 2n)^2}{4\sigma}.$$  

(A14)

Hence we can bound $T_2$ from (A8) by shifting the index in the sum and dropping positive terms on the right hand side as follows

$$T_2 > \frac{2}{\sqrt{\pi \sigma}} \left\{ \sum_{n=1}^{N_0-1} \frac{n^2}{\sigma} \exp\left[-\frac{4n^2}{4\sigma}\right] - \sum_{n=0}^{N_0-1} \frac{(-1 - 2n)^2}{4\sigma} \exp\left[-\frac{(-1 - 2n)^2}{4\sigma}\right] \right\}$$  

$$> \frac{2}{\sqrt{\pi \sigma}} \left\{ \sum_{n=1}^{N_0-1} \left(\frac{n^2}{\sigma} + \frac{(-1 - 2n)^2}{4\sigma}\right) \exp\left[-\frac{(-1 - 2n)^2}{4\sigma}\right] \right\}$$  

(A15)

$$- \frac{(1 - 2N_0)^2}{4\sigma} \exp\left[-\frac{(1 - 2N_0)^2}{4\sigma}\right]$$  

$$> - \frac{2}{\sqrt{\pi \sigma}} \exp\left[-\frac{(1 - 2N_0)^2}{4\sigma}\right]$$  

$$> - \frac{2}{\sqrt{\pi \sigma}} \exp\{-1\} = - \frac{2}{e \sqrt{\pi \sigma}}$$

where we have dropped the sum of positive terms on the right-hand side.

Combining the above estimates, we see that
\[ T_1 + T_2 > \frac{1}{2} \sqrt{\frac{\pi}{\sigma}} \left[ 1 - 2 \exp\left(-\frac{1}{4\sigma}\right) + \frac{2}{\sigma} \sum_{n=1}^{\infty} n \exp\left(-\frac{(n + \frac{\sigma}{n})^2}{4}\right) \right] \]

We note that we have grossly underestimated \( T_1 + T_2 \) in (A16) so our estimate will be far from sharp. Given an upper bound on \( \sigma \) from the particular problem, a much better estimate could be obtained using the first inequality in (A16). We also note that we can obtain the non-strict bound

\[ (A17) \quad dM(0, \alpha) + M(0, \alpha) = \frac{1}{\sqrt{\pi \sigma}} \sum_{n=-\infty}^{\infty} \left( \frac{1}{2} + \frac{n^2}{\sigma} \right) \exp\left(-\frac{n^2}{\sigma}\right) > \frac{1}{2} \sqrt{\frac{\pi}{\sigma}} . \]

Combining (A7), (A8), (A16), and (A17), we see that if \( T_3 \) is the term on the left side of (A7), we have

\[ (A18) \quad T_3 > \int_{0}^{*} \frac{1}{2 \sqrt{\pi \sigma}} \left[ g_3(\tau) - 4g_2(\tau) \right] d\tau . \]

Thus from (A5), (A7), and (A18), we obtain for \( A_\alpha < \alpha < A^* \),

\[ (A19) \quad Q'(\alpha) > \rho c \left[ g_1(0) - g_2(0) + \int_{0}^{*} \frac{g_3(\tau) - 4g_2(\tau)}{\sqrt{4 \sigma^2 + (t^* - \tau)^2}} d\tau \right] \]

which was to be shown.

We shall next use similar techniques to obtain a proof for Lemma 4.3.
Proof of Lemma 4.3. We note that using (A1) and the definition of $Q^*$ using (4.14) we can see that for $A_* < \alpha < A^*$ and $\sigma = \alpha(t^* - \tau)$,

$$Q(\alpha) - Q^*(\alpha) = -\rho c \alpha \{ g_1(0) - g_1^*(0) - g_2(0) + g_2^*(0) \}$$

$$+ \rho c \int_0^{t^*} [M(0, \sigma) (g_1'(\tau) - g_1^*(\tau)) - M(-1, \sigma) (g_2'(\tau) - g_2^*(\tau))] d\tau$$

(A20) $$= -\rho c \alpha \{ g_1(0) - g_1^*(0) - g_2(0) + g_2^*(0) \}$$

$$- \rho c \int_0^{t^*} [M(0, \sigma) (g_1'(\tau) - g_1^*(\tau)) - g_2'(\tau) + g_2^*(\tau)] d\tau$$

$$- \rho c \int_0^{t^*} [M(0, \sigma) - M(-1, \sigma)] (g_2'(\tau) + g_2^*(\tau)) d\tau$$

$$= T_4 + T_5 + T_6.$$

We note that from (A8), (A9), and (A10),

$$M(0, \sigma) - M(-1, \sigma) = \frac{1}{2 \sqrt{\pi \sigma}} \left[ 1 + 2 \left\{ \sum_{n=1}^{\infty} \exp \left[ -\frac{n^2}{\sigma} \right] \right\} - 2 \sum_{n=0}^{\infty} \exp \left[ -\frac{(1 - 2n)^2}{4 \sigma} \right] \right] \frac{1}{2 \sqrt{\pi \sigma}}$$

(A21)

since the term in brackets $\{ \cdot \}$ is negative. We also see that
\[ M(0, \sigma) = \frac{1}{2 \sqrt{\pi \sigma}} \left[ 1 + \sum_{n=1}^{\infty} \exp \left[ -\frac{n^2}{\sigma} \right] \right] \]

(A22)

\[ \leq \frac{1}{2 \sqrt{\pi \sigma}} \left[ 1 + 2 \int_{0}^{\infty} \exp \left[ -\frac{x^2}{\sigma} \right] dx \right] \]

\[ \leq \frac{1}{2 \sqrt{\pi \sigma}} \left[ 1 + \sqrt{\pi \sigma} \right]. \]

Combining the above estimates we see that

\[ |Q(\alpha) - Q^*(\alpha)| \leq \rho c \left[ A*2 \varepsilon_1 + \int_{0}^{*} \left( \frac{3}{2 \sqrt{\pi \alpha(t^* - \tau)}} + 1 \right) d\tau \varepsilon_1 \right] \]

(A23)

\[ \leq 2 \rho c A* \varepsilon_1 + \rho c \left[ 3 \sqrt{\alpha(t^* + \tau)} \right] \varepsilon_1, \]

which was to be shown.
APPENDIX B

In this appendix we shall present the fourth order time-stepping procedure that was used for our numerical results. Let $S_h$ denote the space of continuous piecewise linear functions defined on a uniform mesh of width $h = \Delta z$ on $[0, 1]$ and vanishing at $z = 0$ and $z = 1$. We shall consider a family of such spaces for $0 < h < 1$. Let $(\phi, \phi) = \int_0^1 \phi^2 \, dx$ be the standard $L^2$ inner product.

Let $\Delta t > 0$ be the stepsize in time, $N_T = T/\Delta t \in \mathbb{Z}$, $t^n = n\Delta t$, and $\phi_n = \phi(t^n)$. We shall present a fourth-order in time backward differentiation multistep time-stepping procedure for our Galerkin spatial method. We assume that a start-up procedure of sufficiently high order (see [21]) has been used to obtain approximations $W_0, W_1, \ldots, W_N$ for $n > 3$ of the solution of (4.14).

We then define $W: \{0 = t_0, t_1, \ldots, t_{N_T} = T\} \to S_h$ by

$$
\left( \frac{W_{n+1} - W_n}{\Delta t}, V \right) + \frac{12}{25} \alpha \left( \frac{3}{3z} W_{n+1}, \frac{3}{3z} V \right)
$$

(B1)

$$
= \frac{1}{\Delta t} \left( \frac{23}{25} W_n - \frac{36}{25} W_{n-1} + \frac{16}{25} W_{n-2} - \frac{3}{25} W_{n-3}, V \right)
$$

for all $V \in S_h$. Since $S_h$ is a finite-dimensional subspace of $H_0^1$, the first order Sobolev space, the equation (B1) can be considered only for a specific basis for $S_h$ and (B1) reduces to a system of $N$ linear equations in $N$ unknowns where $N$ is the dimension of $S_h$. 

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