INTEGRAL METHODS FOR THE SOLUTION OF CONDUCTION PROBLEMS WITH TEMPERATURE DEPENDENT PARAMETERS

by

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Abstract

In this thesis we examine the suitability of two refinements of Goodman's Integral Method for conduction problems with temperature dependent thermal parameters. The results are compared to those produced by standard methods of solution and the advantages and limitations of the integral approach are discussed.

Acknowledgements

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DECLARATION

I declare that the following thesis is a record of research work carried out by me, that the thesis is my own composition, and that it has not been previously presented in application for a higher degree.

Suhama K Abbas

CONTENTS

1.2 Description of Goodman's Integral Method

Goodman presented a simple technique called the heat balance integral method in 1964 for solving one space dimensional heat transfer problems, which may be either linear or nonlinear. Goodman illustrates that the technique can be applied to a wide range of problems. For example he considers problems involving temperature dependent thermal properties, change of phase, and a variety of different boundary conditions. He obtains approximate analytic solutions for situations that do not have formal analytic solutions.

To illustrate the basic idea of the heat balance integral method consider the simple problem of plane flow in a semi-infinite media described by the equations

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < \infty, \quad t > 0 \tag{1.2.1}$$

$$T = T_s, \quad x = 0, \quad t \geqslant 0 \tag{1.2.2}$$

and

$$T = 0, \quad 0 < x < \infty, \quad t = 0. \tag{1.2.3}$$

The exact solution is well known (see Carslaw and Jaeger (1959)) and may be expressed as

$$T = T_s \, \mathrm{erfc}(x/2(\kappa t)^{\frac{1}{2}})$$

where

$$\mathrm{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^{\infty} e^{-\xi^2} d\xi.$$

In the heat balance integral method, a penetration depth $\delta(t)$ is assumed beyond which no heat transfer takes place. Although such a concept is not strictly true for the heat conduction equation (1.2.1) it is a very reasonable approximation since for some prescribed ε and t there exists a $\delta(t)$ such that

$$T(x,t) < \varepsilon \quad \text{for all} \quad x > \delta(t).$$

With the notion of a penetration depth, beyond which nothing of significance takes place, the method is to approximate T, usually by a polynomial, within an integrated form of equation (1.2.1). Integrating equation (1.2.1) over $[0,\delta(t)]$ yields the heat balance integral

$$\frac{d}{dt}\left[\int_0^\delta T dx\right] = \kappa \frac{\partial T}{\partial x}(\delta,t) - \kappa \frac{\partial T}{\partial x}(0,t), \tag{1.2.4}$$

and it is quite natural, although not essential, to take $\frac{\partial T}{\partial x}(\delta,t) = 0$. Note that in the above $T(\delta,t)$ is taken to be the ambient temperature specified in condition (1.2.3). The approximation, or profile, for T over $[0,\delta(t)]$ involves $\delta(t)$ as an unknown parameter which is determined from the ordinary differential equation obtained from equation (1.2.4). For example, if we choose T to be linear then the conditions at $x = 0$ and $x = \delta$ determine the profile,

$$T \simeq \left(1 - \frac{x}{\delta}\right)T_s.$$

Hence the heat balance integral (1.2.4) becomes

$$\frac{d}{dt}\left[\delta\,\frac{T_s}{2}\right] = \frac{\kappa}{\delta}\,T_s$$

and yields a solution for $\delta(t)$, namely,

$$\delta(t) = 2\sqrt{\kappa t}.$$

Clearly, this approximation for T is rather too simple and Goodman recommends the use of quadratic and cubic profiles. In order to determine the form of a polynomial profile it is necessary to create additional boundary conditions. Langford (1973) discusses some of the options available but as we will see the best choice is not always obvious.

For the problem described by equation (1.2.1) to (1.2.3) the profile

$$T \simeq T_s\left\{1 - \frac{x}{\delta}\right\}^n, \quad n \text{ integer},$$

does not seem unreasonable. At $x = 0$, $T = T_s$ as required. At $x = \delta$ not only is $T = 0$ but

$$\frac{\partial^r T}{\partial x^r}(\delta, t) = 0, \qquad 1 \leqslant r \leqslant n-1,$$

a property not uncharacteristic of the error function at a large value of its argument. On substituting this profile into the heat balance integral (1.2.4) a similar first order differential equation is produced for $\delta(t)$, the solution of which is

$$\delta(t) = (2n(n+1)\kappa t)^{\frac{1}{2}}. \qquad (1.2.5)$$

The temperature distribution

$$T \simeq T_s(1 - x/(2n(n+1)\kappa t)^{\frac{1}{2}})^n = \tilde{T} \qquad (1.2.6)$$

and the incident flux

$$-K\left(\frac{dT}{dx}\right)_0 = KT_s(n/2(n+1)\kappa t)^{\frac{1}{2}} = \tilde{f}. \qquad (1.2.7)$$

For small values of n the numerical values obtained are quite good, see Table 1, and are adequate for many practical situations.

Table 1

Estimates of the Temperature and the incident Flux based on a polynomial profile

	$\tilde{T}/T_s$ $x/(\kappa t)^{\frac{1}{2}} = 1/2$	$\tilde{T}/T_s$ $x/(\kappa t)^{\frac{1}{2}} = 1$	$(\kappa t)^{\frac{1}{2}}\tilde{f}/KT_s$
1	0.75	0.5	0.5
2	0.7322	0.5060	0.5774
3	0.7240	0.5041	0.6124
4	0.7193	0.5024	0.6325
exact values	0.7237	0.4795	0.5642

This illustrates the basic approach and in any given situation it is a matter of judgement what degree of polynomial is chosen and how it is determined. It is this aspect of the technique that is also its weakness as we will see in the next section.

1.3 Virtues and Limitations

The integral methods discussed by Goodman, illustrated above, are the same as the techniques proposed by Pohlhausen and Tani for the approximate treatment of boundary layers in fluid dynamics, (see Curle (1962)). A description of these two techniques in a heat transfer setting is provided by Poots (1962). It is possible to cast all such techniques into the framework of the general method of weighted residuals as discussed by Ames (1977). However, such considerations are not the concern of this thesis.

The virtue of Goodman's integral method is that it is simple to apply to a wide range of heat transfer problems and that the accuracy obtained using polynomial profiles of low degree is adequate in many practical situations. The result is in the form of a simple formula which is ideal in many engineering situations. This is the main attraction of this type of approach.

However, the main disadvantage is that there are no systematic procedures for either selecting the profile or improving upon a given profile.

The performance of the method in any given situation is rather unpredictable and this aspect has been demonstrated by Langford (1973).

For the simple problem described in Section (1.2) the results given in equations (1.2.5) to (1.2.7) seem reasonable. However, consider the situation as n becomes large. A little elementary analysis reveals that

$$\lim_{n \to \infty} \tilde{T} = T_s \, e^{-x/(2\kappa t)^{\frac{1}{2}}}$$

and

$$\lim_{n \to \infty} \tilde{f} = KT_s/(2\kappa t)^{\frac{1}{2}}.$$

As the degree of the polynomial profile is increased the approximate solution converges, with the rapidity of $(1/n)$, to the wrong analytic form.

From a practical point of view it may be argued that the asymptotic trends are not important provided the approximation obtained is, in some sense, close to the desired solution.

A counter argument is that without the correct asymptotic properties, and in the absence of the exact solution, the "closeness" of the approximate solution cannot be assessed.

This inadequacy can be overcome by the introduction of some form of sub-division of the penetration depth.

It is the intention in this thesis to examine methods of sub-division for problems involving temperature dependent thermal properties and assess the accuracy obtained. The types of sub-division to be considered are discussed in the next Chapter.

CHAPTER 2

Methods of Refinement

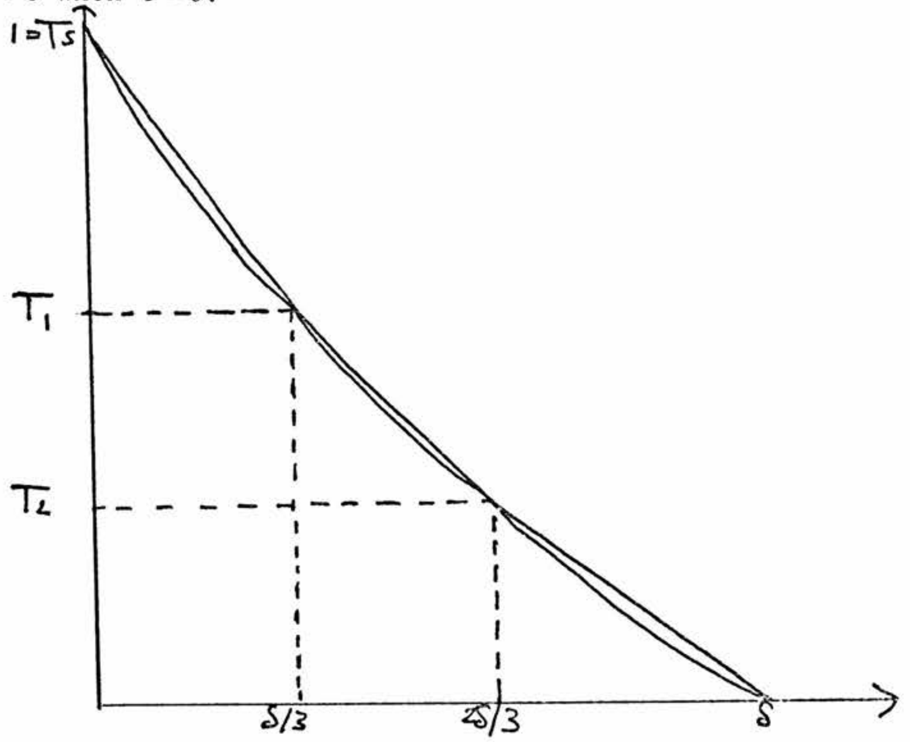
2.1 Equal sub-division of the penetration depth

The heat balance integral method is a simple technique for obtaining reasonably accurate solutions for a variety of problems. In some circumstances it is possible to improve the accuracy of a solution by increasing the degree of the polynomial approximation. Langford (1973) describes ways in which these polynomials can be constructed and his results indicate the difficulty in choosing a suitable polynomial. The convergence properties of polynomial approximations will be referred to in the next chapter. To increase the accuracy of an approximate solution Bell (1978) has used spacial sub-division and in particular equal sub-division of the temperature range assigning a penetration depth to each isotherm. He has shown that this approach works well for melting and freezing problems. In this thesis we will investigate the technique of spacial sub-division for heat conduction with temperature dependent thermal properties. We will consider two approaches. The first is to sub-divide the penetration depth equally. The second is following Bell and sub-dividing the temperature range. With the latter we will consider both finite and semi-infinite regions. For the remainder of this chapter we will present the equations appropriate to these two approaches.

In this section consider the heat equation

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(K(T)\ \frac{\partial T}{\partial x}\right) \tag{2.1.1}$$

in the semi-infinite region where $T = T_s$ at $x = 0$, all t, and $T = 0$ $x > 0$ when $t = 0$.



(Equal sub-division of δ when $n = 3$)

Figure 2.1

As in Chapter 1 a penetration depth $\delta(t)$ is assumed beyond which no heat transfer takes place. Let the interval $[0,\delta]$ be sub-divided into n equal sub-intervals $\left[\frac{i\delta}{n},\ \frac{(i+1)\delta}{n}\right]$, $i = 0,1,\ldots,n-1$.

Integrating the heat equation with respect to x over this interval we get

$$\int_{\frac{i\delta}{n}}^{\frac{(i+1)\delta}{n}} \frac{\partial T}{\partial t}\, dx = K(T_{i+1}) \left.\frac{\partial T}{\partial x}\right|_{\frac{(i+1)\delta}{n}} - K(T_i) \left.\frac{\partial T}{\partial x}\right|_{\frac{i\delta}{n}} \qquad (2.1.2)$$

where $K(T_i)$ is the value of $K(T)$ at $x = i\delta/n$ and is unknown. Using Leibniz rule we can rewrite the left hand side as

$$\frac{d}{dt}\left\{\theta - \frac{(i+1)\delta}{n} T_{i+1} + \frac{i\delta}{n} T_i\right\} \qquad (2.1.3)$$

where
$$\theta = \int_{\frac{i\delta}{n}}^{\frac{(i+1)\delta}{n}} T\, dx.$$

Suppose within this interval the temperature T is approximated by the straight line

$$-\frac{nT_i}{\delta}\left(x - (i+1)\frac{\delta}{n}\right) + \frac{n}{\delta} T_{i+1}\left(x - \frac{i\delta}{n}\right), \qquad (2.1.4)$$

and the gradient by

$$\frac{n}{\delta}(T_{i+1} - T_i), \qquad (2.1.5)$$

where $i = 0,1,\ldots,n-1$. We assume that beyond the penetration depth the gradient is zero. Substituting (2.1.5) and (2.1.4) into (2.1.2) gives

$$\frac{d}{dt}\left[\frac{T_{i+1}\delta}{2n} + \frac{T_i\delta}{2n} - \frac{(i+1)\delta T_{i+1}}{n.} + \frac{i\delta T_i}{n}\right]$$

$$= \frac{n}{\delta}\left[K(T_{i+1})(T_{i+2} - T_{i+1}) - K(T_i)(T_{i+1} - T_i)\right].$$

So

$$\delta \frac{d\delta}{dt} = \frac{-2n^2}{(2i+1)} \frac{K(T_{i+1})T_{i+2} - K(T_{i+1})T_{i+1} - K(T_i)T_{i+1} + K(T_i)T_i}{(T_{i+1} - T_i)} \quad \ldots \quad (2.1.6)$$

for $i = 0,1,\ldots,n-2$.

For the last sub-interval $\left[\frac{(n-1)\delta}{n}, \delta\right]$ we obtain the simpler equation

$$\frac{(n - \frac{1}{2})}{n^2} \delta \frac{d\delta}{dt} = K(T_{n-1}). \qquad (2.1.7)$$

Eliminating δ between (2.1.7) and (2.1.6) produces (n-1) nonlinear equations for the temperatures $T_1,T_2,\ldots,T_{n-1}$. It should be noted that the value of the temperature at $x=0$ is taken to be unity for convenience. A typical equation is

$$-\left(K_i - K_{n-1}\frac{(2i+1)}{(2n-1)}\right)T_i + \left(K_i + K_{i+1} - K_{n-1}\frac{(2i+1)}{(2n-1)}\right)T_{i+1}$$
$$- K_{i+1}T_{i+2} = 0 \qquad (2.1.8)$$

where $K_i = K(T_i)$, etc.

The procedure is now to solve this system of equations numerically, writing the system as

$$A\underline{T} = \underline{b} \qquad (2.1.9)$$

where $\underline{T} = [T_1,T_2,\ldots,T_{n-1}]^T$ and A is a matrix whose coefficients will also depend upon T. A simple iterative method of solution can be devised. Given an estimate of $\underline{T}$ the matrix A can be determined and then a new estimate of $\underline{T}$ can be obtained by solving the above set of equations (2.1.9), using Gaussian elimination.

Suppose $\underline{T}^{(k)}$ is the kth estimate of the vector $\underline{T}$ then $\underline{T}^{(k+1)}$ is obtained from the

$$A^{(k)}\underline{T}^{(k+1)} = \underline{b}$$

where $A^{(k)}$ contains the coefficients given in (2.1.8) evaluated in terms of $\underline{T}^{(k)}$. The iterative procedure stops when

$$\sum_{i=1}^{n-1} \left(T_i^{(k+1)} - T_i^{(k)}\right)^2 \leqslant \text{tolerance}$$

where the tolerance was taken to be 0.00005. For particular K(T) it may be easier to solve the equations given by (2.1.8) in a different way.

For example, when $K = 1 + \frac{1}{2}T$ the equation (2.1.8) becomes, after some rearrangement,

$$a\,T_{i+1}^2 + b\,T_{i+1} + c = 0$$

where

$$a = 1.0$$

$$b = (4n-3)/(2n-1) - 2i - T_{i+2} + T_i - \frac{(2i+1)}{(2n-1)} T_{n-1}$$

and $$c = T_i^2 + 2T_i - 2T_{i+2} - \frac{4i+2}{(2n-1)} - \frac{(2i+1)}{(2n-1)} T_{n-1}$$

which all depend on T_i, T_{i+2} and T_{n-1}. Again a simple iterative procedure can be devised to calculate T_i, $i = 1,\ldots,n-1$ by treating the equation as a quadratic in T_{i+1}.

The significance of this particular choice of K(T) is that it has been studied by other authors, in particular Yang (1958) and in a later chapter we compare Yang's results to those produced by the methods described here.

2.2 Equal sub-division of the temperature range

As an alternative approach we will consider the equal sub-division of the temperature range and assign a penetration depth to each isotherm created.

For the moment we will again consider a semi-infinite region with the same initial and boundary conditions as in the previous section.

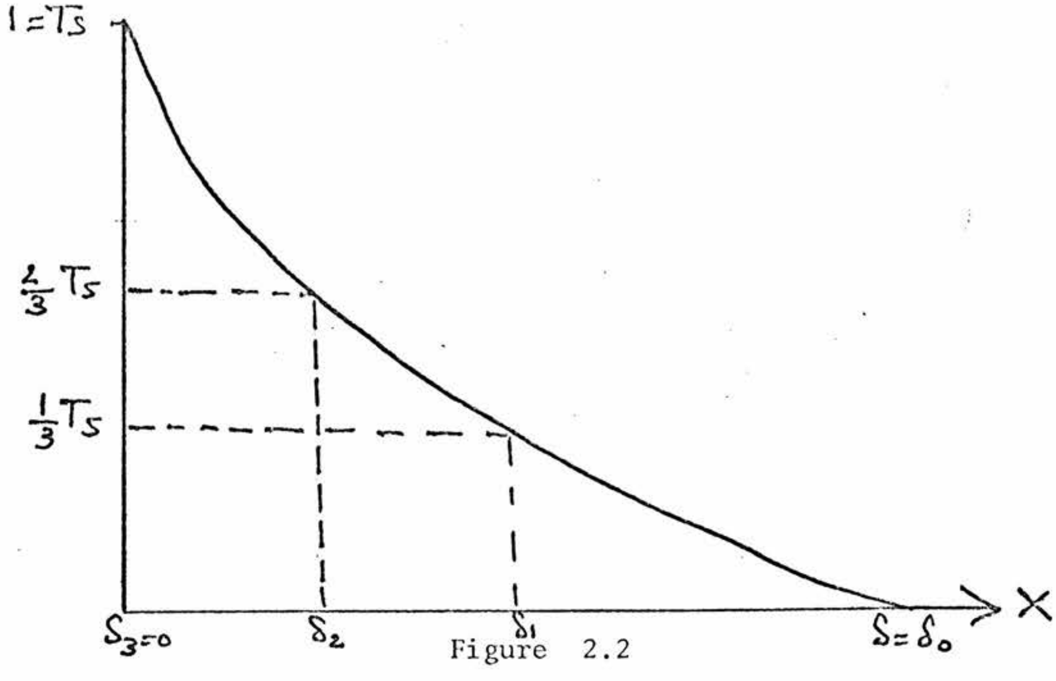


Figure 2.2

(Equal Sub-division of Temperature Range (n=3))

For convenience we denote the penetration depths as δ_i, where the associated isotherm is $\frac{i}{n} T_S$. As in Section 2.1 we will take T_S to be unity. (See diagram for the case n=3)

Again integrating the heat equation over a typical interval $[\delta_{i+1}, \delta_i]$ we get

$$\int_{\delta_{i+1}}^{\delta_i} \frac{\partial T}{\partial t} = K(T_i) \left.\frac{\partial T}{\partial x}\right|_{\delta_i} - K(T_{i+1}) \left.\frac{\partial T}{\partial x}\right|_{\delta_{i+1}} . \qquad (2.2.1)$$

As T_i is known at δ_i (which is unknown) the values $K(T_i)$ are also known in equation (2.2.1), unlike the situation in the previous section.

Following the same procedure as earlier and approximating the temperature over $[\delta_{i+1}, \delta_i]$ by the straight line

$$\frac{i+1}{n} - \frac{(x-\delta_{i+1})}{(\delta_i - \delta_{i+1})} \frac{1}{n}$$

equation (2.2.1) becomes

$$n \frac{d}{dt} \left(\theta - \frac{i}{n} \delta_i + \frac{(i+1)}{n} \delta_{i+1} \right) = \frac{K_i}{\delta_{i-1} - \delta_i} - \frac{K_{i+1}}{\delta_i - \delta_{i+1}} \qquad (2.2.2)$$

where

$$\theta = \int_{\delta_{i+1}}^{\delta_i} T\,dx = \frac{(2i+1)}{2n} (\delta_i - \delta_{i+1}).$$

And simplifying we get

$$\frac{d}{dt} (\delta_i + \delta_{i+1}) = \frac{-2K_i}{\delta_{i-1} - \delta_i} + \frac{2K_{i+1}}{\delta_i - \delta_{i+1}} \quad \text{valid for } i = 1, n-1, \ldots \qquad (2.2.3)$$

noting that $\delta_n = 0$.

Again it is necessary to consider the last interval, $[\delta_1, \delta_0]$ separately as it is assumed that there is no heat flow beyond δ_0.

Following the above procedure and taking

$$\left.\frac{\partial T}{\partial x}\right|_{\delta_0} = 0$$

we obtain

$$\frac{d}{dt}[\delta_0 + \delta_1] = \frac{2K_1}{\delta_0 - \delta_1}. \qquad (2.2.4)$$

Equations (2.2.3) and (2.2.4) give n differential equations in the n unknowns $\delta_0, \delta_1, \ldots, \delta_{n-1}$. It is convenient to work in terms of the interval lengths rather than the penetration depths so we introduce

$$Z_i = \delta_i - \delta_{i+1}, \quad i = 0,1,\ldots,n-1$$

and for the semi-infinite region these differential equations can be reduced to a system of algebraic equations by the similarity transformation

$$Z_i = \lambda_i t^{\frac{1}{2}} \qquad (2.2.5)$$

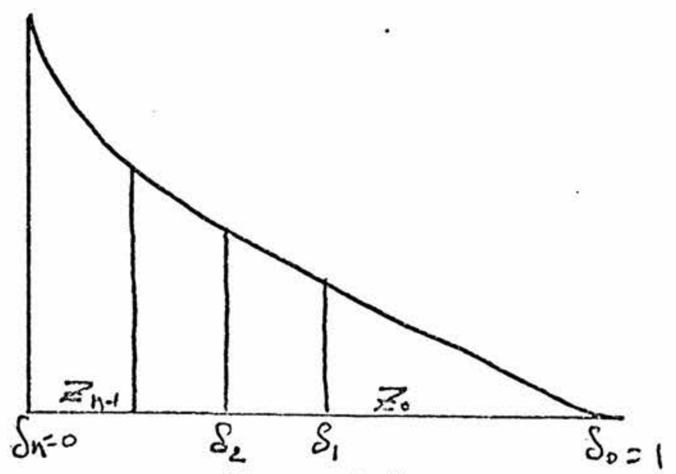


Figure 2.3

Note that

$$\delta_i = Z_{n-1} + Z_{n-2} + \dots + Z_i, \qquad (2.2.6)$$

see Figure 2.3.

In terms of λ_i the equations (2.2.3) and (2.2.4) become

$$\lambda_i^2 + \lambda_i\left[2\sum_{j=i+1}^{n-1}\lambda_j + \frac{4K_i}{\lambda_{i-1}}\right] - 4K_{i+1} = 0 \qquad (2.2.7)$$

together with

$$\lambda_0^2 + \lambda_0\left[2\sum_{j=1}^{n-1}\lambda_j\right] - 4K_1 = 0. \qquad (2.2.8)$$

Treating this nonlinear system as a system of quadratics in λ_i, we can solve for λ_i by iteration given some initial guess at $\lambda_0, \lambda_1, \dots, \lambda_{n-1}$.

The results are discussed later in Chapter 5.

2.3 A Finite Region

Let us consider the heat equation limited as follows

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(K \frac{\partial T}{\partial x}\right) \qquad 0 < x < 1 \qquad (2.3.1)$$

and subject to the initial and boundary conditions:

at $\quad x = 0, \quad T = T_s = 1, \qquad (2.3.2)$

and at $\quad x = 1, \quad T = T_0 = 0, \qquad (2.3.3)$

given $\quad T = 0 \quad$ when $\quad t = 0.$

Since $T = 0$ at $t = 0$, $x > 0$, then either of the proceeding approaches (Section 2.1 or 2.2) can be used until δ, or δ_0 in Section 2.2, reaches the value one.

From that moment δ, or δ_0, remains constant and the previous equations are inappropriate. For the situation described in Section 2.1 the technique breaks down as if δ is constant then all the temperature values T_i become constant. However, for the second approach, Section 2.2, it is merely necessary to modify the system of equations by introducing a new unknown. In the following the additional variable is taken to be the temperature gradient at $x = \delta_0 = 1$. Note that δ_0 is no longer an unknown. For a typical interval $[\delta_{i+1}, \delta_i]$, $i = 1,\ldots,n-1$ the equation is the same as in Section 2.2 namely equation (2.2.3). So consider the last interval $[\delta_1, 1]$, as illustrated in Figure 2.4.

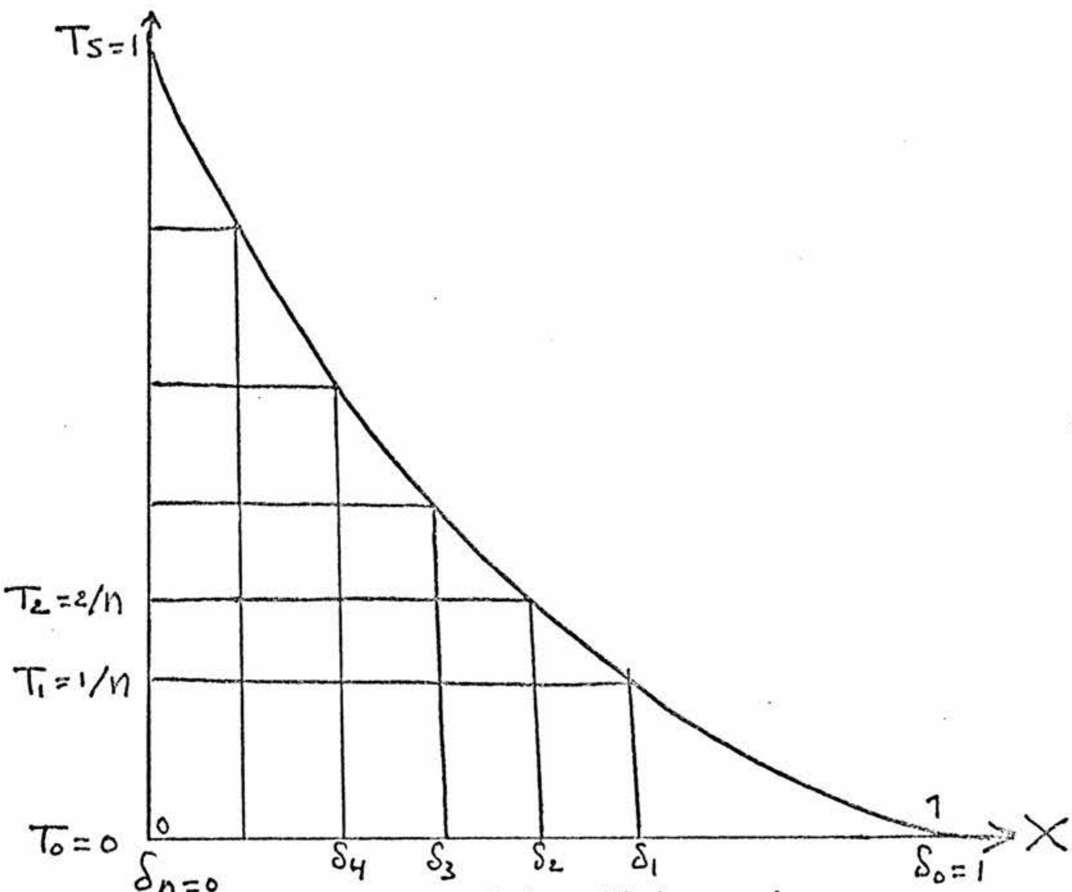


Figure 2.4 Finite region

Then eq (2.2.1) becomes:

$$\frac{d}{dt}\left[\theta + \delta_1 T_1\right] = K_i \left.\frac{\partial T}{\partial x}\right|_1 - K_{i+1} \left.\frac{\partial T}{\partial x}\right|_{\delta_1} \tag{2.3.4}$$

where

$$\theta = \int_{\delta_1}^{1} T\,dx = \frac{(1-\delta_1)}{2} \cdot \frac{1}{n}.$$

Simplifying eq (2.3.4) we get

$$\frac{d}{dt}\left[\delta_1\right] = \frac{2K_1}{1-\delta_1} - 2nf \tag{2.3.5}$$

where f is the flux at $x = 1$. Now, we have n equations in $\delta_1, \delta_2, \ldots, \delta_{n-1}$ and f (n unknowns), and these equations are very different from the equations described earlier because

$$\delta_i = \lambda_i t^{\frac{1}{2}}$$

is not a solution of them. Note $\delta_0 = 1$ in first of (2.2.3).

The (n-1) equations (2.2.3) are differential equations in the (n-1) penetration depths $\delta_1, \delta_2, \ldots, \delta_{n-1}$, and we will solve these numerically. The additional equation (2.3.5), merely provides a way of evaluating the gradient at $x = 1$. Before considering the solution of the equations (2.2.3) together with (2.3.5), let us investigate the steady-state solution of the system of equations. That is let $t \to \infty$ and $\frac{d\delta_i}{dt} \to 0$, $i = 1, \ldots, n-1$. The equations (2.2.3) reduce to

$$\frac{K_i}{\delta_{i-1} - \delta_i} = \frac{K_{i+1}}{\delta_i - \delta_{i+1}}, \qquad i = 1, \ldots, n-1. \tag{2.3.6}$$

The flux at $x = 1$ is constant and given by

$$f = \frac{K_1}{n(1-\delta_1)}. \tag{2.3.7}$$

The δ_i are now constant and we have a system of linear algebraic equations (2.3.6) which are more conveniently written as

$$K_{i+1}\delta_{i-1} - (K_{i+1} + K_i)\delta_i + K_i\delta_{i+1} = 0 \tag{2.3.8}$$

$i = 1, \ldots, n-1$, where $\delta_0 = 1$ and $\delta_n = 0$ and the K_i are known.

This system may again be solved using Gaussian Elimination to give the steady-state values of δ_i. Having determined δ_i the gradient at $x = 1$ can be obtained from (2.3.7). The results obtained in this way for various $K(T)$ will be discussed in Chapter 5. For the steady-state situation we can often obtain the correct solution by simply integrating the equation (2.1.1) so that

$$K(T)\,\frac{dT}{dx} = A, \text{ constant}$$

and integrating again gives

$$\int K(T)\,dT = Ax + B. \qquad (2.3.9)$$

The correct solution, obtained in this way, will be used for comparison in Chapter 5.

It is interesting to check the approach by assuming $K(T) = 1$ for all T. The system of equation reduces to

$$\begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ & & & & & \vdots \\ & & & & & \\ 0 & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \\ \vdots \\ \vdots \\ \delta_{n-1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

and it is easily verified that the solution to this system of equations is

$$\delta_i = 1 - \frac{i}{n},$$

where the associated isotherm is $\left(1 - \frac{i}{n}\right)$. Also, from (2.3.7), $f = 1$. Hence for the simple case of $K(T) = 1$ we obtain the correct steady-state solution which provides some confidence in the use of this approach.

Returning to the general case when $\frac{\partial T}{\partial t} \neq 0$ and T is dependant on t, as well as x, then equations (2.2.3) give a system of equations which are

$$\left.\begin{aligned}
\frac{d}{dt}[\delta_{n-1}] &= \frac{-2K_{n-1}}{\delta_{n-2}-\delta_{n-1}} + \frac{2K_n}{\delta_{n-1}} \\
\frac{d}{dt}[\delta_{n-2}+\delta_{n-1}] &= \frac{-2K_{n-2}}{\delta_{n-3}-\delta_{n-2}} + \frac{2K_{n-1}}{\delta_{n-2}-\delta_{n-1}} \\
& \\
\frac{d}{dt}[\delta_1+\delta_2] &= \frac{-2K_1}{1-\delta_1} + \frac{2K_2}{\delta_1-\delta_2}
\end{aligned}\right\} \qquad (2.3.10)$$

These equations are solved using the Runge-Kutta method, given some starting values for each δ_i.

The starting values are taken from the previous semi-infinite solution, when δ_0 first becomes one. The appropriate NAG Library was used and again the results are discussed in Chapter 5.

CHAPTER 3

Some Convergence Results

3.1 Introduction

Noble (1975) suggested ways in which the heat balance integral method might be implemented in order to provide a more systematic numerical technique. One of Noble's refinements has been exploited by Bell (1978) in the solution of a one-dimensional solidification problem. In a problem involving either melting or freezing the notion of a penetration depth arises naturally. As the point of transition between solid and liquid is usually associated with a particular temperature, Bell sub-divided the temperature range, assigning a penetration variable to each isotherm, and considered the heat balance integral between adjacent isotherms. Computational evidence suggests that the procedure converges to the exact solution as the number of sub-divisions is increased. The technique has been successfully applied to a number of different situations, Bell 1979 and 1982, and the results suggests that discretising the heat balance integral provides a very effective numerical technique for problems in which the temperature distribution contains discontinuities or steep gradients. Its performance when the thermal properties are temperature dependent is one of the concerns of this thesis.

The appropriate equations are derived in Chapter 2, Section 2.2, and the results for a selection of model problems are presented in

Chapter 5. Also described in Chapter 2 is a procedure in which the penetration depth $[0,\delta(t)]$ is sub-divided equally and the values of T at each sub-division determined numerically. It is the asymptotic properties of this method of refinement, when applied to the problem specified by equations (1.2.1) to (1.2.3), that will be investigated here.

Following the derivation in Chapter 2, $[0,\delta]$ is sub-divided into n equal sub-intervals of length δ/n where

$$T\left\{\frac{i\delta}{n},\ t\right\} = T_i, \qquad i = 0,1,\ldots,n,$$

$$T_0 = T_s \quad \text{and} \quad T_n = 0.$$

Integrating equation (1.2.1) over each sub-interval $\left[\frac{i\delta}{n},\ (i+1)\,\frac{\delta}{n}\right]$, and using Leibniz's rule, as δ is a function of t, yields

$$\frac{d}{dt}\left[\theta - \frac{(i+1)T_{i+1}\delta}{n} + \frac{iT_i\delta}{n}\right]$$

$$= \kappa\,\frac{\partial T}{\partial x}\left\{\frac{(i+1)\delta}{n},\ t\right\} - \kappa\,\frac{\partial T}{\partial x}\left\{\frac{i\delta}{n},\ t\right\}, \qquad (3.1.1)$$

where

$$\theta \int_{\frac{i\delta}{n}}^{\frac{(i+1)\delta}{n}} T\,dx.$$

The temperature T is approximated by the piecewise linear profile

$$\tilde{T} = \tilde{T}_i + \left[x - \frac{i\delta}{n}\right](\tilde{T}_{i+1} - \tilde{T}_i)\frac{n}{\delta},$$

$$\frac{i\delta}{n} \leqslant x \leqslant \frac{(i+1)\delta}{n}, \quad i = 0,1,\ldots,n-1,$$

where $\tilde{T}_i \approx T_i$. The temperature gradients are taken as the piecewise constants

$$\frac{\partial\tilde{T}}{\partial x}\left[\frac{i\delta}{n}, t\right] = \frac{n}{\delta}(\tilde{T}_{i+1} - \tilde{T}_i), \quad i = 0,1,\ldots,n-1,$$

and $\frac{\partial\tilde{T}}{\partial x}(\delta,t) = 0$. Substituting into equation (3.1.1) produces n-1 equations

$$\frac{d}{dt}(\tfrac{1}{2}\delta^2) = -\frac{2n^2\kappa}{(2i+1)}\frac{(\tilde{T}_{i+2} - 2\tilde{T}_{i+1} + \tilde{T}_i)}{(\tilde{T}_{i+1} - \tilde{T}_i)}, \qquad (3.1.2)$$

$0 \leqslant i < n-1$, together with

$$\frac{d}{dt}(\tfrac{1}{2}\delta^2) = \frac{2n^2\kappa}{(2n-1)}, \qquad (3.1.3)$$

arising from the last sub-interval, $(i = n-1)$. Equations (3.1.2) and (3.1.3) are merely special cases of equations (2.1.6) and (2.1.7). Here $K(T)$ is κ, a constant, and are reproduced for convenience. Using (3.1.3) to eliminate the derivative in (3.1.2) produces a system of n-1 linear equations in the n-1 unknowns $\tilde{T}_1, \tilde{T}_2, \ldots, \tilde{T}_{n-1}$. A typical equation is

$$(2n-1)\tilde{T}_{i+2} - (4n - 2i - 3)\tilde{T}_{i+1} + (2n - 2i - 2)\tilde{T}_i = 0, \qquad (3.1.4)$$

$i = 0,1,\ldots,n-2.$

From the last equation $\tilde{T}_{n-2}$ may be expressed in terms of $\tilde{T}_{n-1}$, namely

$$\tilde{T}_{n-2} = (1 + (n - \tfrac{1}{2}))\tilde{T}_{n-1},$$

and from the penultimate equation $\tilde{T}_{n-3}$ may be expressed in a similar way. Continuing the back substitution it is easily verified, by induction, that

$$\tilde{T}_i = \tilde{T}_{n-1} \sum_{K=1}^{n-i} \frac{(n-\frac{1}{2})^{K-1}}{(K-1)!}, \qquad i = 0,1,\ldots,n-2. \qquad (3.1.5)$$

Hence,

$$\tilde{T}_{n-1} = T_s \Big/ \sum_{K=1}^{n} \frac{(n-\frac{1}{2})^{K-1}}{(K-1)!},$$

and using the usual notation, (see Abramowitz and Stegun 1964), the approximate temperature $\tilde{T}_i$ may be written as

$$\tilde{T}_i = T_s \frac{e_{n-i-1}(n-\frac{1}{2})}{e_{n-1}(n-\frac{1}{2})}, \qquad i = 0,\ldots,n-1, \qquad (3.1.6)$$

where

$$e_m(Z) = 1 + Z + \frac{Z^2}{2!} + \ldots + \frac{Z^m}{m!}.$$

3.2 Asymptotic Properties

Clearly as the number of sub-divisions, n, increases the penetration depth δ increases and

$$\delta \sim (2n\kappa t)^{\frac{1}{2}} \quad \text{as} \quad n \to \infty.$$

Also, it is easy to show that $\tilde{T}_{n-1} \to 0$ and $\frac{\partial \tilde{T}}{\partial x}(\delta, t) \to 0$ as $n \to \infty$. However, these two properties are shared by the polynomial approximation (1.2.6) discussed earlier in Chapter 1, Section 1.2 and 1.3.

To validate the approximate solution given by equation (3.1.6) first consider the behaviour of the incident flux as the number of sub-divisions is increased. At $x = 0$ $(i = 0)$

$$-K\left(\frac{\partial T}{\partial x}\right)_0 = K\frac{n}{\delta}(\tilde{T}_1 - T_s),$$

which, using (3.1.3) and (3.1.6), can be expressed as

$$-K\left(\frac{\partial T}{\partial x}\right)_0 = \frac{K(n-\frac{1}{2})^{n-\frac{1}{2}} T_s}{\Gamma(n)\, e_{n-1}(n-\frac{1}{2})(2\kappa t)^{\frac{1}{2}}}. \tag{3.2.1}$$

It is convenient to recast equation (3.2.1) in terms of the incomplete gamma function

$$\gamma(a,Z) = \int_0^Z e^{-s} s^{a-1} ds$$

suppressing the algebraic details the right hand side of equation (3.2.1) becomes

$$\frac{K\,T_s\,I(n)}{(2\kappa t)^{\frac{1}{2}}(1-\gamma(n,n-\frac{1}{2})/\Gamma(n))}, \tag{3.2.2}$$

where

$$I(n) = \frac{(n-\frac{1}{2})^{n-\frac{1}{2}}}{\Gamma(n)e^{n-\frac{1}{2}}}. \tag{3.2.3}$$

The asymptotic behaviour of I(n) is easily deduced from the known behaviour of the functions involved (see Abramowitz and Stegun (1964)) and, omitting details,

$$I(n) \sim \frac{1}{\sqrt{2\pi}}\left(1+\frac{1}{24n}\right), \quad n \to \infty. \tag{3.2.4}$$

In order to determine the behaviour of the denominator a knowledge of the asymptotic properties of the incomplete gamma function is required. There are many potentially useful results and a comprehensive survey is provided by Bowen (1961).

Here it is sufficient to exploit an expansion originally due to Pearson (1934) and a convenient form of Pearson's result is

$$\gamma(m+1,x) = e^{-m}\, m^{m+\frac{1}{2}}\sqrt{\frac{\pi}{2}}\left\{1+\operatorname{erf}\left(\frac{x-m}{\sqrt{2m}}\right)+O(m^{-\frac{1}{2}})\right\}, \tag{3.2.5}$$

where m is large and $0 < x < 2m$.

Using this result in conjunction with Stirling's formula it is easily deduced that

$$\lim_{n \to \infty} \frac{\gamma(n,n-\frac{1}{2})}{\Gamma(n)} = \frac{1}{2}$$

and that this limit is approached with the rapidity of $n^{-\frac{1}{2}}$.

Hence, the approximate incident flux

$$-K\left(\frac{\partial \widetilde{T}}{\partial x}\right)_0 \to K\, T_s/(\pi\kappa t)^{\frac{1}{2}} \quad \text{as} \quad n \to \infty.$$

The estimates of the incident flux formally converge to the exact value and the asymptotic rate of convergence is proportional to $n^{-\frac{1}{2}}$. Such a process has been observed computationally, see Table 2.

In a similar manner, consider the behaviour of approximate temperature $\widetilde{T}_i$, given by equation (3.1.6). In terms of the incomplete gamma function, equation (3.1.6) becomes

$$\widetilde{T}_i = T_s(1-\gamma(n-i,n-\tfrac{1}{2})/\Gamma(n-i))/(1-\gamma(n,n-\tfrac{1}{2})/\Gamma(n))$$

and the behaviour of the denominator has already been determined.

Again, using (3.2.5), where n-i is large,

$$\frac{\gamma(n-i,n-\frac{1}{2})}{\Gamma(n-i)} \sim \frac{e}{2}\left(1-\frac{1}{n-i}\right)^{n-i-\frac{1}{2}}\left\{1+\operatorname{erf}\left(\frac{i+\frac{1}{2}}{\sqrt{2(n-i-1)}}\right)\right\}. \quad (3.2.6)$$

To investigate the limiting form of $\widetilde{T}_i$ it is necessary to focus attention on a fixed point (x,t) where

$$\frac{i\delta}{n} \leqslant x < (i+1)\frac{\delta}{n},$$

or

$$i \leqslant \frac{x}{2}\left\{\frac{2n-1}{\kappa t}\right\}^{\frac{1}{2}} \leqslant i+1 \quad .$$

Let $x/2(\kappa t)^{\frac{1}{2}} = \alpha$ and consider the behaviour of (3.2.6) where

$$i \sim \alpha\sqrt{2n}$$

as $n \to \infty$, so that $i\delta/n \to \alpha$, fixed and finite.

A little analysis reveals that when $i = \alpha\sqrt{2n} + 0(n^{-\frac{1}{2}})$

$$\frac{\gamma(n-i, n-\frac{1}{2})}{\Gamma(n-i)} \to \tfrac{1}{2}\{1 + \operatorname{erf}(\alpha)\},$$

as $n \to \infty$, and, hence that

$$\lim_{n\to\infty} \tilde{T}_i = T_s \operatorname{erfc}(x/2(\kappa t)^{\frac{1}{2}}).$$

Again convergence occurs with the rapidity of $n^{-\frac{1}{2}}$.

Table 2

n	$-(\kappa t)^{\frac{1}{2}}\left(\frac{\partial\tilde{T}}{\partial x}\right)_0 \Big/ T_s$
2	0.4693
4	0.5319
8	0.5407
16	0.5471
32	0.5518
exact	0.5642

3.3 Remarks

As will be observed in the results of Chapter 5, the approximate solution obtained from equations (2.1.6) and (2.1.7) for a non constant K(T) also appears to converge at a rate of $n^{-\frac{1}{2}}$. It is gratifying to be able to formally show this result for a particular simple problem. The analysis provides confidence in the method of sub-division as a means of overcoming the weakness of the original heat balance approach, as discussed in Chapter 1.

A similar analysis for the alternative approach to sub-division given in Section 2 of Chapter 2 has not been attempted. However, the results of Chapter 5 suggest a rate of convergence proportional to n^{-1}. The two forms of sub-division will be compared, in terms of the results of Chapter 5 in Chapter 6.

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CHAPTER 4

Other Suitable Methods

4.1 The Semi-infinite Region

In order to assess the accuracy and performance of the heat balance integral methods, described in Chapter 2, alternative approaches are considered. In the next Section suitable finite-difference methods are reviewed. However, for problems in a semi-infinite region the most obvious approach is to employ the well known Boltzmann transformation. Shampine (1973) has examined this technique in some detail and a more general description is provided by Crank (1975). Here a brief outline of the Boltzmann transformation is presented in the context of the problems to be discussed later.

Again, consider the heat conduction problem defined by the equations

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(K\,\frac{\partial T}{\partial x}\right) \qquad (4.1.1)$$

where $T = T_s$ at $x = 0$, $t \geqslant 0$, and, for convenience, $T = 0$, $0 < x \leqslant \infty$ when $t = 0$. The function K is a continuous function of T only and is always non-negative. Boltzmann (1894) introduced the similarity variable

$$\eta = x/2t^{\frac{1}{2}}. \qquad (4.1.2)$$

Assuming the temperature T can be expressed in terms of η only the left hand side becomes

$$- \frac{\eta}{2t} \frac{dT}{d\eta}$$

and the right hand side becomes

$$\frac{1}{4t} \frac{d}{d\eta} \left(K \frac{dT}{d\eta} \right).$$

Equating the two sides yields the ordinary differential equation

$$-2\eta \frac{dT}{d\eta} = \frac{d}{d\eta} \left(K \frac{dT}{d\eta} \right). \qquad (4.1.3)$$

This transformation is only of use if the initial and boundary conditions are similarly transformed into conditions dependent on η only. The boundary condition at $x = 0$ becomes

$$T = T_s \quad \text{at} \quad \eta = 0$$

and the initial condition requires that $T \to 0$ as $\eta \to \infty$. The procedure is then to solve (4.1.3) numerically and it is usual to reduce the second order equation (4.1.3) to a pair of first order equations by setting

$$f = K \frac{dT}{d\eta}. \qquad (4.1.4)$$

So that

$$-2\eta f/K = \frac{df}{d\eta}. \qquad (4.1.5)$$

A standard Runge-Kutta package is then used to solve this pair of equations. (The result quoted in Chapter 5 were obtained using the NAG Library routine DO2BBF.

To solve a pair of equations two starting values are required and here only one is available. Consequently a trial and error approach is adopted in which a guess is made at the initial value for f and then repeatedly modified until the solution tends to zero at large values of η. The procedure is essentially that of Shampine (1973a) who provides *a priori* bounds for the initial flux in terms of K(T).

For example

$$-2\Delta/(\pi\delta)^{\frac{1}{2}} \leqslant f_{\eta=0} \leqslant -2\delta/(\pi\Delta)^{\frac{1}{2}}$$

and

$$0 < \delta < K(T) < \Delta.$$

The above procedure will break down if K becomes zero. The differential equation (4.1.3) is said to be singular when K vanishes for some value of T. Shampine (1973b) discusses this situation in detail. For such a function K the solution has a front at some value of η, and hence is discontinuous at that point.

The particular case to be investigated in this thesis is when

$$K(T) = T \quad \text{and} \quad T_s = 1.$$

The method of solution will be similar to that outlined by Crank (1975). It is convenient to adopt the transformation

$$\eta = x/t^{\frac{1}{2}},$$

as did Shampine, upon which the transformed equation becomes

$$\frac{d}{d\eta}\left(T\,\frac{dT}{d\eta}\right) = -\,\frac{\eta}{2}\,\frac{dT}{d\eta}\,. \tag{4.1.6}$$

The solution is singular at some value $\eta = \eta_0$. In order to overcome this difficulty let

$$Z = 1 - \eta/\eta_0 \quad \text{and} \quad u = T/\eta_0^2.$$

Rewriting the problem in terms of u and Z gives the equations

$$\frac{d}{dz}\left(u\,\frac{du}{dz}\right) = \frac{(1-Z)}{2}\,\frac{du}{dz} \tag{4.1.7}$$

where $u = 1/\eta_0^2$ at $Z = 1$.

To solve this equation starting values at $Z = 0$ are required. At $Z = 0$, $T = 0$ and as there is no heat flow beyond η_0 the flux is also zero which implies

$$T\,\frac{dT}{d\eta} = 0.$$

In terms of u the conditions are

$$u = 0 \quad \text{and} \quad u\,\frac{du}{dz} = 0 \quad \text{at} \quad Z = 0.$$

Following the earlier approach let

$$\frac{du}{dz} = f/u \tag{4.1.8}$$

and so

$$\frac{df}{dz} = \frac{(1-Z)\,f}{2u}\,. \tag{4.1.9}$$

However, the right hand sides are still indeterminant at $Z = 0$, and hence a starting procedure is necessary.

Suppose u has a small Z expansion of the form

$$u \doteq a_0 Z + a_1 Z^2 + a_2 Z^3 + \ldots \qquad (4.1.10)$$

then the unknown coefficients a_0, a_1, a_2, etc. can be determined by substituting (4.1.10) into (4.1.7) and equating like powers of Z. Omitting the details, equating powers produces the equations

$$a_0(a_0 - \tfrac{1}{2}) = 0,$$

$$6a_0 a_1 - a_1 + \frac{a_0}{2} = 0,$$

$$12a_0 a_2 + 6a_1^2 - \frac{3}{2}a_2 + a_1 = 0,$$

and so on. Ignoring the trivial solution $a_0 = a_1 = \ldots = 0$, the expansion for u about zero is

$$u = \frac{1}{2}Z - \frac{1}{8}Z^2 + \ldots . \qquad (4.1.11)$$

The series is then used to provide starting values for u and f at some small value of Z and the pair of equations is then showed using a standard Runge-Kutta routine.

The integration is performed until $Z = 1$, which corresponds to the origin

$$\eta = 0.$$

The computed value of u at $Z = 1$ provides the value of η_0 as at that point $T = 1$ and hence

$$\eta_0 = \left(\frac{1}{u}\right)^{\frac{1}{2}}.$$

For the results presented in Chapter 5 the starting values were taken as

$$u = 0.4999875 \times 10^{-4}$$

and

$$f = u\,\frac{du}{dZ} = 0.24998125 \times 10^{-4},$$

corresponding to $Z = 10^{-4}$, and again the NAG Library routine DO2BBF was used for the integration of the pair of first order equations.

4.2 The Finite Region

The Boltzmann transformation as described in the previous section can not be used in a finite region because equation (4.1.2) at $x = 1$, say, becomes

$$\eta = 1/2t^{\frac{1}{2}}$$

which does not depend on η only but involves t explicitly. For problems in finite regions it is more usual to use the well known finite-difference methods as Smith (1965) discusses in detail.

Mitchell (1969) describes two and three level schemes for linear and non-linear equations. Crank (1975) discusses the application of some of these methods to the type of problem investigated in this thesis. He also gives computed results for a number of commonly occuring situations.

In order to assess the performance of the heat balance integral methods described in Chapter 2, consider two finite-difference approximations. The first is the simple explicit method.

The simplest approximation of (4.1.1) is

$$\begin{aligned} T_{i,j+1} &= T_{i,j} + rK(T_{i,j})(T_{i+1,j} + T_{i-1,j} - 2T_{i,j}) \\ &\quad \tfrac{1}{4}rK'(T_{i,j})(T_{i+1,j} - T_{i-1,j})^2 \qquad (4.2.1) \end{aligned}$$

where, using the usual notation

$$T_{i,j} \simeq T(ih,jk) \quad \text{and} \quad r = k/h^2.$$

The disadvantage of such an approach is that the method is unstable for certain values of r.

In an attempt to avoid such difficulties the value of r is chosen such that

$$\min_{T} \, (1 - 2rK(T)) \geq 0 \tag{4.2.2}$$

Stability difficulties can be overcome by using an implicit method. For example a Crank-Nicholson approximation could be used. However, as Mitchell (1969) points out, a two level difference approximation is difficult to use computationally when the equation is non-linear.

For the type of equation under investigation in this thesis Mitchell suggests a three level scheme. Equation (4.1.1) is approximated by the difference equation

$$\begin{aligned} T_{i,j+1} - T_{i,j-1} = \tfrac{2}{3}r\Big[\overset{+}{\alpha}\Big\{&(T_{i+1,j+1} - T_{i,j+1}) + (T_{i+1,j} - T_{i,j}) \\ &+ (T_{i+1,j-1} - T_{i,j-1})\Big\} - \bar{\alpha}\Big\{(T_{i,j+1} - T_{i-1,j+1}) \\ &+ (T_{i,j} - T_{i-1,j}) + (T_{i,j-1} - T_{i-1,j-1})\Big\}\Big] \end{aligned} \tag{4.2.3}$$

where $$\overset{+}{\alpha} = K\left(\frac{T_{i+1,j} + T_{i,j}}{2}\right)$$

and $$\bar{\alpha} = K\left(\frac{T_{i,j} + T_{i-1,j}}{2}\right).$$

Lees (1966) proved that the above scheme converges to the exact solution for all values of r.

The main advantage is that the system of equations at $t = (j+1)k$ is linear and easily solved at each time step using the factorisation method described by Phillips and Taylor (1973).

In addition the accuracy of the approximation is comparable with the more complicated Crank-Nicolson approximation.

The one disadvantage is that starting values for both $T_{i,0}$ and $T_{i,1}$, (all i) are required. When the initial condition is zero and the boundary condition at one end, say $x = 0$, is $T = T_s$, values for $T_{i,1}$ can be obtained using the Boltzmann transformation described in the previous section. Details of the starting procedure are given later in the next Chapter.

Another, less satisfactory, approach is to assume that $T_{i,1} = T_{i,0}$ for all i. The consequence of this simpler approach will also be commented upon later.

CHAPTER 5

Results

5.1 Specification of problems

In Chapter 2 we derived the equations for the integral method with two types of sub-division. In this chapter we will present the results obtained for a number of model problems. For all these problems the region considered will be either finite of length unity or semi-infinite. The specification of the problems is as given in Chapter 1 and 2 and for convenience are restated:-

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(K(T)\ \frac{\partial T}{\partial x}\right), \quad 0 < x < \infty \text{ OR } 0 < x < 1,$$

$$T = T_s \quad \text{at} \quad x = 0, \quad \text{all } t,$$

$$T = 0 \quad \text{when} \quad t = 0, \quad 0 < x < \infty \text{ OR } 0 < x < 1,$$

and for the finite region $T = 0$ at $x = 1$, all t.

The problems to be considered are when

$$K(T) = 1 + \tfrac{1}{2}T, \qquad \text{problem I,}$$

$$K(T) = 1/(1 + \tfrac{1}{2}T), \qquad \text{problem II,}$$

$$K(T) = T, \qquad \text{problem III.}$$

Sometimes it will be helpful to see the results of the situation when $K(T) = 1$ and we will refer to this problem as problem IV. Problem IV has a well-known solution, see Chapter 1, Section

(1.2), which will be used for comparison. Problems I and II are very similar and problem I has been solved by Yang (1958) and again his results will be used for comparison. Problem III is very different. There will always be a point x where K(T) is zero and in the semi-infinite region the solution will have a discontinuous gradient. The difficulties when using the Boltzmann transformation have already been discussed in Chapter 4.

In the results that follow the number of sub-divisions used is frequently 2^m, where m is an integer, which aids inspection of the rate of convergence. For example if the results are converging with a rate proportional to n^{-1} (th number of sub-divisions) then the error should decrease by about a factor of 2.

5.2 Semi-infinite Region

A Equal sub-division of $[0,\delta]$

For each of problems I, II and IV the calculated value of δ will tend to infinity as the number of sub-divisions tend to infinity. One way of comparing the results is to compare the gradient at $x = 0$, that is

$$\left.\frac{\partial T}{\partial x}\right|_{x=0}$$

which from equation (2.1.5) is

$$\frac{n}{\delta}\,(T_1 - T_S)$$

where δ is found from equation (2.1.7) and t is taken to be unity. To compare temperatures is more difficult as the intervals created by two different sub-divisions do not coincide as the values of δ are different. Therefore to compare temperatures we need to interpolate the results obtained at particular x and t. The results are given in Tables 3, 4 and 6.

Table 3 Problem I

n	T(1,1)	T(2,1)	$-\left.\frac{\partial T}{\partial x}\right\|_{x=0}$	error
8	0.5712	0.2002	0.4225	0.0091
16	0.5682	0.2059	0.4249	0.0067
32	0.5656	0.2063	0.4267	0.0049
64	0.5643	0.2087	0.4280	0.0036
128	0.5631	0.2096	0.4290	0.0026
256	0.5624	0.2108	0.4297	0.0019
Yang result			0.4315	0.0001
Boltzmann result	0.5608	0.2131	0.4316	

Table 4 Problem II

n	T(1,1)	T(2,1)	$-\left.\frac{\partial T}{\partial x}\right\|_{x=0}$	Error
8	0.3790	0.0849	0.6899	0.0506
16	0.3890	0.0973	0.7040	0.0365
32	0.3911	0.1022	0.7143	0.0262
64	0.3958	0.1075	0.7218	0.0187
128	0.3971	0.1104	0.7273	0.0132
256	0.3991	0.1127	0.7312	0.0093
Boltzmann result	0.4031	0.1185	0.7405	

Table 5 Problem III

n	δ	error	$\left.\frac{\partial T}{\partial x}\right\|_{x=0}$	error
8	1.6479	.0308	0.4527	0.0090
16	1.6311	.0150	0.4482	0.0045
32	1.6235	.0074	0.4474	0.0037
64	1.6198	.0037	0.4449	0.0012
128	1.6179	.0018	0.4443	0.0006
Boltzmann result	1.6161		0.4437	
Shampine result	1.6163		0.4438	

Table 6 Problem IV

n	T(1,1)	T(2,1)	$-\left.\frac{\partial T}{\partial x}\right\|_{x=0}$	Error
8	0.4767	0.1304	0.5406	0.0236
16	0.4786	0.1409	0.5470	0.0172
32	0.4776	0.1440	0.5518	0.0124
64	0.4788	0.1487	0.5552	0.0090
128	0.4785	0.1507	0.5577	0.0065
256	0.4790	0.1531	0.5596	0.0046
Boltzmann result	0.4795	0.1573	0.5642	

The results for Problem III are presented in Table 5.

Firstly we observe that for Problems I, II and IV the gradient at $x=0$ appears to converge to the correct value with the speed of $n^{-\frac{1}{2}}$. This is consistent with our earlier remarks in Chapter 3. It is more difficult to be specific about the behaviour of the temperature at a fixed point. The results in Table 6 for $x=1$ illustrate the problem. Since these values are obtained by interpolation the error can vary by the fact that $x=1$ will not always fall in the same position in an interval. If we assume that the values of the temperature at the end points of each sub-interval are correct then the error due to interpolation may easily be assessed. For example, investigating the results in Table 6 and assuming the values T_i computed are correct the error due to linear interpolation is, at $x=1$,

$$\frac{-(1-x_0)(x_1-1)x_1 e^{-x_1^2/4}}{4\sqrt{\pi}} \leqslant \text{error} \leqslant \frac{-1(1-x_0)(x_1-1)x_0 e^{-x_0^2/4}}{4\sqrt{\pi}}$$

where x_0 and x_1 are the end points of the sub-interval containing $x=1$. Using this formula to correct the values in Table 6 produces the revised results given in Table 7.

These results are in line with our analysis in Chapter 3, but the main conclusion is that the interpolated results can vary significantly as n varies simply due to the position of x. Hence, it can be misleading to make too many conclusions from the values of the temperature.

Table 7

"Corrected" Results - Problem IV

n	T(1,1)	Error
8	0.4753	42
16	0.4764	31
32	0.4774	21
64	0.4780	15
128	0.4785	10
256	0.4788	7
	0.4795	

In contrast the results in Table 5 suggest a different type of behaviour. For Problem III the idea of a penetration depth is appropriate and as $n \to \infty$ δ will tend to a fixed limit. The results, although inconclusive, suggest a rate of convergence of order n^{-1}.

B Equal sub-division of the temperature range

The solution of equations (2.2.7) and (2.2.8) gives the value of $\delta_0, \delta_1, \ldots, \delta_{n-1}$ for a specified n. Again compare the gradient at $\delta_n = 0$ that is

$$\left.\frac{\partial T}{\partial x}\right|_{\delta_{n=0}} = \frac{1}{n\delta_{n-1}} :$$

In order to compare the temperature at a fixed point, we interpolated the results. The results are given in Tables 8, 9 and 11 for Problems I, II and IV. The results for Problem III are given in

Table 10. As in the earlier results it is convenient to take the time t equal to unity.

Table 8 Problem I

n	T(1,1)	T(2,1)	$-\left.\frac{\partial T}{\partial x}\right\|_{\delta_n=0}$	Error
4	0.5777	0.2073	0.4180	0.0137
8	0.5709	0.2115	0.4226	0.0091
16	0.5664	0.2130	0.4261	0.0055
32	0.5641	0.2134	0.4283	0.0033
64	0.5626	0.2137	0.4293	0.0023
128	0.5618	0.2135	0.4316	0.0000
Boltzmann result	0.5608	0.2131	0.4316	

Table 9 Problem II

n	T(1,1)	T(2,1)	$-\left.\frac{\partial T}{\partial x}\right\|_{\delta_n=0}$	Error
4	0.4032	0.0804	0.6838	0.0567
8	0.4028	0.1020	0.7064	0.0341
16	0.4043	0.1108	0.7209	0.0196
32	0.4040	0.1153	0.7296	0.0109
64	0.4039	0.1172	0.7336	0.0069
128	0.4037	0.1180	0.7370	0.0035
Boltzmann result	0.4031	0.1185	0.7405	

Table 10 Problem III

n	δ_0	Error	$-\left.\frac{\partial T}{\partial x}\right\|_{\delta_n=0}$	Error
4	1.6798	.0637	0.4632	0.0194
8	1.6467	.0306	0.4537	0.0100
16	1.6311	.0150	0.4487	0.0050
32	1.6236	.0075	0.4464	0.0027
64	1.6198	.0037	0.4452	0.0015
128	1.6180	.0019	0.4439	0.0002
Boltzmann result	1.6161		0.4437	
Shampine result	1.6163		0.4438	

Table 11 Problem IV

n	T(1,1)	T(2,1)	$-\left.\frac{\partial T}{\partial x}\right\|_{\delta_n=0}$	Error
4	0.4851	0.1388	0.5337	0.0305
8	0.4845	0.1434	0.5454	0.0188
16	0.4831	0.1529	0.5531	0.0111
32	0.4818	0.1552	0.5580	0.0062
64	0.4809	0.1567	0.5600	0.0042
128	0.4803	0.1572	0.5621	0.0021
Boltzmann result	0.4795	0.1573	0.5642	

The remarks made earlier about the interpolated results are also relevant to these quoted in Tables 8, 9 and 11. It is unwise to attempt to deduce too much from the behaviour as n increases.

However, from the estimates of the gradient at $x = 0$ the results for all four problems suggest that the rate of convergence is better than previously observed in Tables 3, 4, 5 and 6. For Problem III the speed at which the values converge for both the penetration depth, δ_0 and the gradient at $x = 0$ appears to be proportional to n^{-1}. The results for the other three problems is less conclusive. The rate is better than $n^{-\frac{1}{2}}$ but clearly not n^{-1}.

5.3 Results for the Finite Region

As described in Chapter 2, Section 2.3, the results for the semi-infinite region are used as starting values for the solution of the problems in a finite region. To illustrate the procedure consider Problem I. When $n = 4$ for the semi-infinite problem, equations (2.2.7) and (2.2.8), the penetration depth is found to be

$$\delta_0 = (2.8044)t^{\frac{1}{2}} = \mu_0 t^{\frac{1}{2}}.$$

Hence, the corresponding problem for a finite region is started at time $t = t_0$ where

$$t_0 = (2.8044)^{-2} = 0.1272.$$

The penetration depth of a typical temperature T_i is $\delta_i(t) = \mu_i t^{\frac{1}{2}}$ and the starting value is taken as

$$\mu_i / \mu_0 .$$

Note in the notation of Chapter 2, Section 2.2

$$\mu_i = \lambda_i + \lambda_{i+1} + \ldots + \lambda_{n-1}.$$

Consequently, for a different value of n the starting time t_0 is different. The Runge-Kutta routine described in Chapter 2, Section 2.3, is run for a time $t - t_0$. The results for each problem are given in Tables 12 to 15 and the value of t is also given. The value of t chosen represents a mid-time solution. Large time solutions will be considered shortly.

Table 12 Problem I

(Values of the position of the 3 temperatures 0.75, 0.5 and 0.25 at total time t = 0.15)

n \ T	0.75	0.5	0.25
4	0.2311	0.4551	0.6986
8	0.2247	0.4476	0.6947
16	0.2213	0.4432	0.6924
32	0.2196	0.4410	0.6915
improved estimate	0.2179	0.4388	0.6906

Table 13 Problem II

(Values of the position of the 3 temperatures 0.75, 0.5 and 0.25 at total time t = 0.2)

n	0.75	0.5	0.25
4	0.2278	0.4539	0.6824
8	0.1796	0.3837	0.6373
16	0.1658	0.3607	0.6173
32	0.1615	0.3532	0.6103
improved estimate	0.1572	0.3457	0.6033

Table 14 Problem III

(Values of the position of the 3 temperatures 0.75, 0.5 and 0.25 at total time t = 0.4)

n	0.75	0.5	0.25
4	0.3409	0.6151	0.8414
8	0.3296	0.6003	0.8315
16	0.3243	0.5927	0.8245
32	0.3218	0.5889	0.8204
improved estimate	0.3193	0.5851	0.8163

Table 15 Problem IV

(Values of the position of the 3 temperatures 0.75, 0.5 and 0.25 at total time t = 0.2)

n	0.75	0.5	0.25
4	0.2079	0.4255	0.6773
8	0.2034	0.4206	0.6760
16	0.2010	0.4178	0.6752
32	0.1997	0.4163	0.6749
improved estimate	0.1984	0.4148	0.6746

Again Problem IV may be used to assess accuracy and convergence properties. To find the values of the correct temperature T at δ_i we substitute into the exact solution given by Carslaw and Jaeger,

$$T = 1 - x - \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{\sin n\pi x}{n} e^{-n^2\pi^2 t}$$

at total time $t = 0.2$.

The results are given in Table 16 and the values of T correspond to the values given in Table 15.

Table 16 Problem IV

n	0.75	Error	0.5	Error	0.25	Error
4	0.7383	.0117	0.4884	.0116	0.2477	.0023
8	0.7438	.0062	0.4937	.0063	0.2488	.0012
16	0.7467	.0033	0.4967	.0033	0.2495	.0005
32	0.7483	.0017	0.4983	.0017	0.2498	.0002
improved estimate	0.7499		0.4999		0.2501	

The results in Table 16 suggest that the numerical solution is converging at a rate of n^{-1}.

For the finite region the behaviour of the method in each of the four problems is likely to be similar. Unlike the situation in Section 5.2 where Problem III was different, for the finite region where $t > t_0$ the method should perform equally well on each problem. That is the rate of convergence of the results ought to be similar to that observed in Table 16. If we assume this to be true then we can obtain improved estimates by extrapolation. For example, if the true position of the temperature r/4, r = 1,2 or 3, is $\delta(r/4)$ and the sequence of estimates is denoted by $\delta^{n}_{\frac{nr}{4}}$ then

$$\delta(r/4) \simeq \delta^{n}_{\frac{nr}{4}} + \frac{A}{n}$$

and

$$\delta(r/4) \simeq \delta^{2n}_{\frac{nr}{2}} + \frac{A}{2n} ..$$

Therefore

$$\delta(r/4) \simeq 2\delta^{2n}_{\frac{nr}{2}} - \delta^{n}_{\frac{nr}{4}} .$$

Applying this to the results in Tables 12, 13, 14 and 15 provides improved estimates. These are given in those tables. The results obtained in this way in Table 15 are used to provide estimates of T, as described earlier, for Table 16. As may be seen the improved values in Table 16 are very close to the exact solution.

5.4 Results for the Steady-State Solution

As mentioned in Section 2.3 of Chapter 2 the steady-state solution can often be obtained by integration. For the four problems in Section 5.1 the steady-state is given by

Problem I : $T + \frac{1}{4} T^2 = \frac{5}{4}(1 - x)$

Problem II : $\log(1 + \frac{1}{2}T) = (1 - x)\log(1.5)$

Problem III : $T^2 = 1 - x$

Problem IV : $T = 1 - x$.

We saw in Section 2.3 of Chapter 2 that the integral method described in that section will give the correct solution for Problem IV as might be expected as the solution is a straight line. In this section we compare values obtained from the correct steady-state solution with those produced by the integral method with equal sub-division of the temperature range. In Tables 17, 18 and 19 the position of three values of temperature are given for different numbers of sub-intervals. Also an estimate of the rate of flow at $x = 1$ is given, see equation (2.3.7).

Table 17 Problem I

n \ Temp	0.75	error	0.5	error	0.25	error	f	error
4	0.2857	.0018	0.5476	.0024	0.7857	.0018	1.3125	.0625
8	0.2866	.0009	0.5488	.0012	0.7866	.0009	1.2812	.0312
16	0.2870	.0005	0.5494	.0006	0.7870	.0005	1.2656	.0156
32	0.2872	.0003	0.5497	.0003	0.7873	.0002	1.2578	.0078
64	0.2874	.0001	0.5498	.0002	0.7874	.0001	1.2539	.0039
exact solution	0.2875		0.5500		0.7875		1.2500	

Table 18 Problem II

n \ Temp	0.75	error	0.5	error	0.25	error	f	error
4	0.2162	.0017	0.4521	.0025	0.7116	.0021	0.9752	.1643
8	0.2154	.0009	0.4509	.0013	0.7106	.0011	0.8919	.0810
16	0.2150	.0005	0.4502	.0006	0.7100	.0005	0.8503	.0394
32	0.2148	.0002	0.4499	.0003	0.7097	.0002	0.8308	.0199
64	0.2146	.0001	0.4498	.0002	0.7096	.0001	0.8201	.0092
exact solution	0.2145		0.4496		0.7095		0.8109	

Table 19   Problem III

Temp / n	0.75	error	0.5	error	0.25	error	f	error
4	0.4000	.0375	0.7000	.0500	0.9000	.0375	0.625	.1250
8	0.4167	.0208	0.7222	.0278	0.9167	.0208	0.5625	.0625
16	0.4265	.0110	0.7353	.0147	0.9265	.0110	0.5312	.0312
32	0.4318	.0056	0.7424	.0076	0.9318	.0057	0.5156	.0156
64	0.4346	.0029	0.7462	.0038	0.9346	.0029	0.5076	.0076
128	0.4361	.0014	0.7480	.0020	0.9360	.0015	0.5044	.0044
exact solution	0.4375		0.7500		0.9375		0.5000	

The results are consistent with those given in Section 5.3. The rate of convergence seems to be proportional to n^{-1} again. This provides some justification for the method of improving the solution given in the previous section.

5.5 Finite-Difference Solutions

In an attempt to judge the performance of the integral methods described we solve the problems given in Section 5.1 using finite-difference methods. The methods to be used are described in Section 4.2, Chapter 4. The first is the simple explicit method and in order to guarantee stability we require

$$r = \frac{k}{h^2} \leqslant \frac{1}{2\max\limits_{T}[K(T)]} .$$

The second method is a three level implicit method requiring starting values at $t = 0$ and $t = k$. We consider two possible starting procedures. The first is simply to take the values at $t = 0$ and $t = k$ to be the same. The second is to use the Boltzmann transformation results obtained earlier for $t = k$.

In order to produce results at the same times as those given in Tables 12, 13 and 14, it is necessary to select k so that mk, where m is an integer, is the required time. For example, in Table 12 the results are given at time $t = 0.15$ so $mk = 0.15$ and $r = k/h^2$ where h is taken to be a power of two. Therefore to ensure that m is an integer we take $r = 0.3$ which gives $m = 2^{2s-1}$ where $h = 2^{-s}$, $s \geqslant 3$. The value of k is $0.3/2^{2s}$. Note that for Problem I the explicit method is stable for $r \leqslant 1/3$. A similar procedure for choosing r and k was used when solving Problems II and III. Since the implicit method is a three level scheme the number of time steps is m-1.

The results obtained for the explicit method and the implicit method with the two different starting procedures are given for each problem in Tables 20, 21, 22 and 23.

Table 20   Problem I

(time = 0.15, r = 0.3, h = 1/n), value of x = i/8

n	method	1	2	3	4	5	6	7
8	explicit	.8583	.7141	.5721	.4368	.3122	.1997	.0975
	implicit 1	.8600	.7158	.5721	.4347	.3086	.1960	.0952
	implicit 2	.8578	.7128	.5698	.4339	.3091	.1971	.0960
16	explicit	.8575	.7127	.5702	.4348	.3103	.1983	.0968
	implicit 1	.8577	.7127	.5698	.4340	.3093	.1973	.0962
	implicit 2	.8574	.7123	.5696	.4340	.3096	.1977	.0964
32	explicit	.8574	.7124	.5698	.4344	.3099	.1980	.0967
	implicit 1	.8574	.7123	.5696	.4341	.3097	.1978	.0965
	implicit 2	.8573	.7123	.5696	.4342	.3098	.1979	.0966
64	explicit	.8573	.7123	.5697	.4343	.3099	.1979	.0966
	implicit 1	.8573	.7123	.5696	.4342	.3098	.1979	.0966
	implicit 2	.8573	.7123	.5696	.4342	.3098	.1979	.0966

Note : implicit 1 is the implicit method with the first starting procedure which assume values at t = k to be the same as at t = 0.

Table 21 Problem II

(time = 0.2, r = 0.4, h = 1/n)

n	method	1	2	3	4	5	6	7
8	explicit	.8025	.6264	.4745	.3465	.2396	.1494	.0712
	implicit 1	.8071	.6341	.4823	.3520	.2422	.1501	.0712
	implicit 2	.8006	.6232	.4707	.3424	.2358	.1466	.0697
16	explicit	.8008	.6234	.4709	.3429	.2364	.1471	.0700
	implicit 1	.8025	.6263	.4740	.3453	.2378	.1477	.0702
	implicit 2	.8004	.6227	.4701	.3420	.2355	.1464	.0696
32	explicit	.8004	.6226	.4699	.3419	.2355	.1465	.0697
	implicit 1	.8010	.6237	.4711	.3428	.2361	.1468	.0698
	implicit 2	.8003	.6225	.4698	.3417	.2354	.1463	.0696
64	explicit	.8002	.6224	.4697	.3416	.2353	.1463	.0696
	implicit 1	.8005	.6228	.4701	.3420	.2356	.1465	.0697
	implicit 2	.8002	.6224	.4697	.3416	.2353	.1463	.0696

Table 22   Problem III

(time = 0.4, r = 0.4, h = 1/n)

n	method	1	2	3	4	5	6	7
8	explicit	.9041	.7992	.6847	.5599	.4235	.2724	.0822
	implicit 1	.9081	.8081	.6996	.5825	.4564	.3208	.1750
	implicit 2	.9081	.8082	.6998	.5828	.4568	.3214	.1757
16	explicit	.9059	.8034	.6919	.5709	.4397	.2968	.1387
	implicit 1	.9083	.8086	.7006	.5840	.4585	.3239	.1798
	implicit 2	.9083	.8086	.7007	.5841	.4586	.3241	.1800
32	explicit	.9071	.8059	.6961	.5773	.4490	.3105	.1600
	implicit 1	.9084	.8088	.7008	.5844	.4591	.3247	.1809
	implicit 2	.9084	.8088	.7009	.5844	.4591	.3247	.1810
64	explicit	.9077	.8073	.6985	.5808	.4540	.3176	.1707
	implicit 1	.9084	.8088	.7009	.5845	.4592	.3248	.1812
	implicit 2	.9084	.8088	.7009	.5845	.4592	.3248	.1812

Table 23 Problem III

(time = 0.1, r = 0.4, h = 1/n)

n	method	1	2	3	4	5	6	7
8	explicit	.7957	.5458	.2026	.0056	.0000	.0000	.0000
	implicit 1	.8086	.5750	.3078	.0537	.0007	-	-
	implicit 2	.8087	.5764	.3100	.0552	.0007	-	-
16	explicit	.7992	.5599	.2724	.0018	.0000	-	-
	implicit 1	.8081	.5825	.3209	.0378	-	-	-
	implicit 2	.8082	.5828	.3214	.0383	-	-	-
32	explicit	.8034	.5709	.2968	.0010	-	-	-
	implicit 1	.8086	.5840	.3239	.0294	-	-	-
	implicit 2	.8086	.5841	.3241	.0296	-	-	-
64	explicit	.8059	.5773	.3105	.0015	-	-	-
	implicit 1	.8088	.5844	.3247	.0274	-	-	-
	implicit 2	.8088	.5844	.3247	.0274	-	-	-
Boltzmann Result		.8087	.5844	.3247	.0282	.0000		

As might be expected the implicit method with the Boltzmann starting solution appears to be the best in each of the three problems. The results obtained are good even when h is fairly large ($n = 8$) except for Problem III when t is small. It is not surprising that the finite-difference methods for this situation, Table 23, do poorly since the solution is discontinuous at $x = 0.511$.

All three approaches appear to converge as h becomes small. The explicit method and the first implicit approach both do reasonably well for Problems I and II. The implicit method with the same starting values at $t = 0$ and $t = k$ seems to be worst. For Problem III however this implicit approach seems better than the explicit and less affected by the discontinuity in the early stages.

To assess the performance of the integral method we now compare results of the best finite difference method with the best of the integral methods considered. These results are presented in Tables 24 and 25 for Problems I and II. The results representing the integral method are based on the results obtained from equal sub-division of the temperature range and have been obtained by interpolation. As we saw earlier interpolation can upset the solution when n is small and the comparison may not be doing the integral method justice. Such aspects will be discussed in the last Chapter.

Table 24 Problem I

A comparison of finite-difference methods with integral methods, t = 0.15

n	x = 1/4	x = 1/2	x = 3/4	$-\left.\frac{\partial T}{\partial x}\right\|_{x=0}$
8	.7213	.4447	.2020	1.1236
	.7218	.4339	.1971	1.1264
16	.7170	.4393	.1992	1.1208
	.7123	.4340	.1977	1.1216
32	.7150	.4371	.1986	1.1216
	.7123	.4342	.1979	1.1200

Table 25 Problem II

A comparison of finite-difference methods with integral methods, t = 0.2

n	x = 1/4	x = 1/2	x = 3/4	$-\left.\frac{\partial T}{\partial x}\right\|_{x=0}$
8	.6602	.3768	.1250	1.6656
	.6232	.3424	.1466	1.6832
16	.6357	.3544	.1517	1.6672
	.6227	.3420	.1464	1.6736
32	.6277	.3463	.1479	1.6672
	.6225	.3417	.1463	1.6672

Note the lower entry is the finite-difference value.

CHAPTER 6

CONCLUSIONS

In this thesis we have considered two types of refinement of Goodman's integral method. Instead of constructing polynomial profiles for the entire region under investigation we have sub-divided the region and used piece-wise linear temperature profiles. Two forms of sub-division have been used and the results suggest that one is better than the other. We have shown that both forms of sub-division produce results that converge as the number of sub-divisions is increased and a mathematical analysis of one of them has been presented. The integral methods discussed overcome some of the limitations of Goodman's original technique. For example in Goodman's article he shows that for problems with temperature dependent thermal parameters that his approach does not necessarily give sensible results for the steady-state situation. With the method of sub-dividing the temperature range equally we have shown that the results obtained converge to the exact solution for the steady-state problem.

However, the results given in Chapter 5 suggest that the integral method described in Chapter 2 are not as good, or as versatile as standard finite-difference methods.

The accuracy of the integral methods could be improved by using a piece-wise quadratic profile rather than a linear one but this would increase the complexity of the numerical techniques.

There seems to be little advantage in using integral techniques for problems like Problem I and II given in Chapter 5. The results suggest that the integral method is perhaps more suited to problems like Problem III where the solution may either be discontinuous or have a steep gradient. For such problems standard finite-difference methods do poorly as seen earlier (Table 23). This observation perhaps explains why integral methods have been so successful for problems involving melting or freezing.

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