ANALYSIS OF NUMERICAL SOLUTION OF THE STEFAN PROBLEM

by

Ole Østerby

DAIMI PB-24

February 1974

Institute of Mathematics University of Aarhus

DEPARTMENT OF COMPUTER SCIENCE

Ny Munkegade - 8000 Aarhus C - Denmark

Phone 06-12 83 55

The following is the author's dissertation, written in partial satisfaction of the requirements for a Ph. D. in Mathematics at the University of California, Berkeley, and under the supervision and guidance of professor René DeVogelaere. The research has been done while the author has been appointed at the Computer Center, University of California, Berkeley, at the ACME Facility, Stanford University Computer Center, and at Aarhus University Computer Center, and computer time has been generously supplied at all three installations.

My sincere thanks to the dissertation committee: Professor René DeVogelaere and professor Edmund Pinney of the Department of Mathematics and professor Frederick Sherman of the Department of Aeronautical Engineering for reading the dissertation and giving valuable advice and criticism, and also to my colleagues at the above-mentioned institutions. In particular I wish to thank dr. Robert M. Baer, Berkeley, for his friendship, his help and encouragement during various stages of this work.

Aarhus, February 1974

Ole Østerby

Analysis of Numerical Solution of the Stefan Problem.

by

Ole Østerby

Abstract

A Stefan problem is a problem involving a parabolic differential equation with a moving boundary. We study one particular one-dimensional, one-phase Stefan problem and two numerical methods for solving it. The first method which has been published by J. Douglas and T. M. Gallie is a finite difference method with variable step size in the t-direction. We supply a convergence proof for the iteration which, at each time step, is needed to determine the size of the step. We also derive certain estimates which we use subsequently to obtain bounds for the solution functions of the original problem. We also discuss stability of the method showing partial results but without being able to prove stability.

We prove that the boundary curve of the particular Stefan problem in question is monotone increasing with a derivative that tends to zero as t tends to infinity. Furthermore, we show that the temperature at the t-axis, $u(0,t)$, goes asymptoticly like $2\pi^{-\frac{1}{2}}t^{\frac{1}{2}}$.

Returning to the numerical method we go into a thorough investigation of the discretization error. Without being able

to arrive at a definite proof our conjecture is that the discretization error is of the form $h w_1 + h^2 w_2 + \dots$ where w_1 and w_2 are continuous functions and h is the step size.

The second numerical method, which is due to A. Wragg, is a Chebyshev-series method for which we conjecture a similar form of the discretization error but also here without a proof.

In an appendix we discuss a particular parabolic boundary value problem with a boundary condition containing a combination of normal and tangential derivatives. We give a uniqueness proof for solutions to this type of problem subject to certain conditions on the coefficients involved in the boundary condition.

We include a listing of an ALGOL program for the Douglas-Gallie method and we give numerical tables of the solution functions of the Stefan problem.

Contents.

Chapter 1.

Introduction.

This thesis is devoted to a close study of one particular Stefan problem and two numerical methods for solving it. The work has essentially followed two paths: 1, a study of the analytic properties of the solution functions, and 2, a detailed analysis of the discretization error when an approximate solution is sought using one of two numerical methods for solving the problem.

The aim was to prove that the discretization error in the large could be expressed in the form: $h w_1 + h^2 w_2 + \ldots$ where h is the step size used and w_1 and w_2 are continuous functions. One is particularly interested in results of this type because they open the possibility of using Richardson extrapolation on the results that are obtained from the numerical method using several different step sizes in the difference schemes. In this way it is possible to combine, say, three runs of a first-order method into one third-order method.

Several difficulties have arisen along the way, however, making it impossible at the present time to complete the analysis in the manner desired. Still we hope that this thesis will be valuable in posing problems - although it provides incomplete answers to these - in pointing to possible directions of research, and in partially paving the way for future investigations on this problem.

In chapter 2 we state the general Stefan problem, as well as define the particular (one-dimensional, one-phase) problem with which we shall deal. In addition, we give a brief survey of literature pertaining to this subject, such as papers on existence and uniqueness theorems and various numerical methods for approximate solution of parabolic boundary value problems of this type.

One particular numerical scheme, due to J. Douglas and T. M. Gallie [7] is discussed thoroughly in chapter 3. The method is an implicit difference method and is particularly interesting because it avoids interpolation at the moving boundary by introducing a variable step size in the t-direction. In the original, and most efficient, form of the algorithm which is discussed in the paper, an iteration is necessary at each time step in order to determine the size of the step. The authors supplied a convergence proof for this iteration only for the interval $0 \leq t < t_1$, where $y(t_1) = 1$, y being the boundary curve. Jim Douglas has later mentioned that this restriction can be waived, but without supplying a proof [6]. In Theorem 4 of chapter 3 we give a proof which is valid for arbitrarily large t. Certain estimates for the t-step which we derive in this chapter are useful in the succeeding chapters and this is the reason for discussing the numerical method before deriving analytical results for the solution functions of the Stefan problem (chapter 4).

The above-mentioned iteration will exhibit an extremely slow convergence for large t, but, as we point out in section 3.4, a very effective acceleration is at hand, and that is what makes this method one of the most effective ones for the Stefan problem.

The last section (3.6) of this chapter is a discussion of stability of the method against small errors. Although computer results has shown no indication of the contrary, it has not been possible for us to present a satisfactory proof of stability. Douglas and Gallie claims that they have given a stability proof, but it is not completely clear what their result (Theorem 5 of [7]) actually implies. In this section we present the results which we have derived in the hope that they may be of use for future investigations.

Chapter 4 is devoted to theoretical results on the solution functions and their derivatives. Based on results of Trench [22], DeVogelaere [24], and Cannon and Douglas [2] we derive a number of results, stated as Lemmas 5 - 8 and Theorem 9. The last result is probably the most interesting one. It points at asymptotic results for the boundary curve, $y(t)$, although the $\sqrt{t}$ -behaviour of $u(0,t)$ places it between the two cases in Theorem 7 of [25]. Various results indicate that the boundary curve, $y(t)$, increases faster than $t^{\frac{1}{2}}$, i.e. that $t^{-\frac{1}{2}} \cdot y(t)$ tends to infinity, although probably very slowly.

The discretization error of the Douglas-Gallie scheme is the subject of chapter 5. Assuming that the numerical method yields mesh functions which can be expanded in powers of h: $W = u + h w_1 + h^2 w_2 + \dots$ and $Y = y + h \eta_1 + h^2 \eta_2 + \dots$ we derive the equations to be satisfied by the functions w_1, η_1, w_2, and η_2. These functions satisfy parabolic boundary value problems of a special type which we discuss in Appendix A. In section 5.4 we focus our attention on the ...-term in the expansions for W and Y, defining functions V and X by $h^2 V = W - u - h w_1 - h^2 w_2$ and $h^2 X = Y - y - h \eta_1 - h^2 \eta_2$. From the equations which we have obtained we have not been able to show boundedness of the functions V and X.

In chapter 6 we study a Chebyshev approximation method, due to A. Wragg [23], with main emphasis on a study of the discretization error. Just as before, we divide the study into two steps. Firstly, guessing at the form of the error term (which we assume to be similar to the one for the Douglas-Gallie method), we obtain equations which the auxiliary functions w_1, η_1, w_2, and η_2 must necessarily fulfil. The resulting equations are very similar to the corresponding ones of the preceding chapter and they are also covered by the considerations of Appendix A. With these functions given we then seek estimates of the remainder terms of the expansions. Just as for the Douglas-Gallie method, our results do not match our intentions. It is hoped, nevertheless, that the present work will prove valuable as a starting point for future investigations.

As already mentioned, Appendix A contains a brief discussion of the existence and uniqueness of solutions of one particular type of parabolic boundary value problem where the condition on the moving boundary involves a combination of normal and tangential derivatives. We give a uniqueness proof for solutions to one such system.

In Appendix B we give a listing of an ALGOL program for the author's modification of the Douglas-Gallie method and in Appendix C we give numerical tables of the solution functions.

The list of references contain certain papers which are not essential to this work. They have been included, partly because of their contents, partly because of their bibliography, as an aid to the reader in tracing back to other papers on the Stefan problem or related problems.

One such paper is the one by Ruoff [18] whose main contribution is an exact solution to the problem which we have called Stefan problem B (sec 2.2). This result, however is a rediscovery of a result by Stefan [21].

Chapter 2.

Definition of the Stefan Problem.

2.1 The general problem.

The name Stefan is used in connection with a wide variety of free boundary problems of parabolic type. These problems appear in the mathematical treatment of various diffusion problems, for example in the description of systems involving heat conduction together with a phase change, such as the melting of a solid. The original paper by J. Stefan [21] was a study of the formation of ice in the arctic seas. It should be mentioned here, however, that free boundary problems have been mentioned in the litterature before Stefan. We refer to Brillouin [1] for further information.

To illustrate the one-dimensional Stefan problem consider the following system: A horizontal rod of ice is kept initially at the freezing point, $0^{\circ}C$. If the rod was of finite length, all the ice might eventually melt, and the resulting system could be described by a boundary value problem with known boundaries. We shall therefore assume the length of the rod to be infinite. It is enclosed in a tube with non-conducting walls, and we shall not take into consideration the change of volume, occurring during melting. Now supply heat to one end of the rod (or keep this end at a specified temperature which may vary in time). The problem is to determine the position of the ice-water interface as a function of time and to find the temperature distribution of the water as a function of time and the distance from the heat-source.

Mathematically this can be formulated as

(1) $$\alpha^2 u_{xx} = u_t , \qquad t > 0,\ 0 < x < y(t),$$

(2) $$u(x,0) = \varphi(x) , \qquad 0 \leq x \leq b ,$$

(3) $$u_x(0,t) = -g(t) , \qquad t > 0 ,$$

(4) $$u(y(t),t) = 0 , \qquad t \geq 0 ,$$

(5) $$\frac{dy(t)}{dt} = -k\, u_x(y(t),t) , \qquad t > 0 ,$$

(6) $$y(0) = b \geq 0 .$$

α^2 and k are positive constants and b is a non-negative constant.

In case of the alternate formulation, where one end of the ice is kept at a prescribed temperature $f(t)$, equation (3) should be replaced by

(3a) $$u(0,t) = f(t) , \qquad t \geq 0 .$$

In this formulation we have made provision for there being initially some water to the left of the ice with a temperature distribution $\varphi(x)$ (to be assumed non-negative). $u(x,t)$ is the temperature of the water at time t and distance x from the end of the rod, and $y(t)$ is the distance to the ice-water interface at time t.

A solution of (1) - (6) is a pair of functions $u(x,t), y(t)$, where $y(t)$ is defined for $t \geq 0$ and $u(x,t)$ is defined for $t \geq 0$, $0 \leq x \leq y(t)$, and such that:

a. $\frac{dy}{dt}$ exists and is continuous for $t > 0$, and y is continuous at $t = 0$;

b. u_x exists and is continuous for $t > 0$, $0 \leq x \leq y(t)$;

c. u_{xx} and u_t exist and are continuous for $t > 0$, $0 < x < y(t)$;

d. the equations (1) - (6) are satisfied.

Since there is no heat diffusion in the ice, this problem is referred to as a one-phase Stefan problem. If the temperature of the ice was initially less than $0^\circ C$, say given by

$$(7) \qquad v(x,0) = \psi(x), \qquad b \leq x < \infty,$$

then heat diffusion would occur in both phases and we would have a two-phase Stefan problem. In this case equation (5) should be replaced by

$$(5a) \qquad \frac{dy(t)}{dt} = -k_1 u_x(y(t),t) + k_2 v_x(y(t),t),$$

and we would have additional equations for v, the temperature distribution in the ice, similar to (1), (3), and (4).

We shall not discuss two-phase problems here, but just mention, that they have been treated by Li-Shang [14].

Problems involving more than two phases have been discussed by Oleinik [16].

2.2 Stefan problem A.

We shall in the following restrict ourselves to a simplified version of problem (1) - (6) in which

a. The heat supplied is assumed constant;

b. There is initially no water in the system, i. e. $b = 0$;

c. By suitable transformations all constants involved are equal to 1, i. e. $\alpha^2 = k = 1$, $g(t) \equiv 1$.

The resulting equations are

$$(8) \qquad u_{xx} - u_t = 0, \qquad t > 0,\ 0 < x < y(t),$$

$$(9) \qquad u_x(0,t) = -1, \qquad t > 0,$$

$$(10) \qquad u(y(t),t) = 0, \qquad t \geq 0,$$

$$(11) \qquad u_x(y(t),t) = -\frac{dy(t)}{dt}, \qquad t > 0,$$

$$(12) \qquad y(0) = 0.$$

Instead of equation (11) we shall often use the relation

$$(13) \qquad y(t) = t - \int_0^{y(t)} u(x,t)\, dx$$

which is equivalent to (11) given (8) - (10).

In the following we shall refer to the problem defined in (8) - (12) as Stefan problem A. Similarly, the problem defined by (8) - (12), replacing (9) by $u(0,t) = C$, where C is a constant will be referred to as Stefan problem B.

2.3 A short review of earlier work.

Although the Stefan problem is a fairly old problem, not much work seems to have been devoted to it until 1947. Since then it has been attacked by several mathematicians, and many papers have been published. Numerical methods have been proposed by Crank [3], Douglas & Gallie [7], Trench [22], and Wragg [23] among others. Existence and uniqueness proofs, other than those that are derived from the numerical methods above, have been published by Sestini [19], Douglas [5], Evans [9], Friedman [10], and Li-Shang [14] among others.

It can be mentioned here, that an existence proof, valid for all t, is a consequence of the results of section 3.3 together with arguments given in [7], but we shall not pursue this further. We shall assume the existence, uniqueness and differentiability (as proved in above-mentioned papers) of the solution functions $u(x,t)$ and $y(t)$ for the Stefan problem A, and on this basis begin the study of the properties of these functions.

2.4 Properties of u and y.

For the system which is described mathematically by Stefan problem A it is intuitively clear that, as time passes, more and more ice will melt and that the temperature of the water at any particular point will increase. We should like to give the exact mathematical results corresponding to some of these intuitive feelings and in addition give answers to some other questions, for which we may not have ready answers, such as: what is the rate of melting or the rate of increase of temperature for large t.

We shall here just state some of the most elementary consequences of equations (8) - (12) and postpone a more detailed analysis to chapter 4.

From (11) and (9) we get

$$y'(0) = 1 . \tag{14}$$

Equations (8) - (10) together with the maximum principle [15] yield

$$u(x,t) > 0 , \qquad t > 0,\ 0 \leq x < y(t) , \tag{15}$$

and

$$u_x(y(t),t) \leq 0 , \qquad t > 0 , \tag{16}$$

and (11) immediately gives

$$y'(t) \geq 0 , \qquad t > 0 . \tag{17}$$

(13) together with (15) implies that

$$y(t) < t , \qquad t > 0 . \tag{18}$$

From equation (17) we see that the distance to the ice-water interface is a non-decreasing function of t.

This result is not the best possible since it is true that the distance is a strictly increasing function of t, but in order to show this we shall first study a difference scheme for the numerical solution of Stefan problem A.

Chapter 3.

The difference scheme of Douglas and Gallie.

3.1 Description of the method.

Several finite-difference methods have been proposed for the approximate solution of the one-dimensional Stefan problem. Among these the most efficient one seems to be the method described by J. Douglas and T. M. Gallie [7]. Being an implicit method it is not subject to the condition $\Delta t \leq \frac{1}{2}\Delta x^2$, and furthermore the equations are simplified considerably by letting Δt vary as the computations proceed.

If fixed step sizes $h = \Delta x$ and Δt are chosen, and a corresponding grid constructed, interpolation is necessary to determine the position of the moving boundary. If, on the other hand, only the step size in one direction is fixed, then the other one can be determined such that the boundary curve will pass through one grid point on each grid line, and interpolation is avoided. It seems most practical to keep the step size in the x-direction, h, fixed and compute the successive t-steps Δt_1, Δt_2, ...

A drawback of this approach is, of course, that the calculated function values correspond to non-equidistant values of the independent variable, t, such that a final interpolation is necessary if a table with equidistant entries is desired for presentation or comparison of results. It is our opinion, that this is a minor inconvenience compared to the effectiveness of the method.

Notation.

(1) $$x_i = i \cdot h\ , \qquad t_n = \sum_{k=1}^{n} \Delta t_k\ ,$$

(2) $$w_{in} = w(x_i, t_n), \quad i = 0, 1, \ldots, n; \quad n = 0, 1, \ldots$$

w denotes the solution of the difference equations and is a function of two variables, defined on the grid points. The boundary curve, as computed using this scheme is determined by the points (x_n, t_n), $n = 0, 1, 2, \ldots$

Equations.

(3) $$w_{oo} = 0\ .$$

(4) $$\Delta t_1 = h\ , \quad w_{o1} = h\ , \quad w_{11} = 0\ .$$

At the n-th step an iteration (on r) is performed to find Δt_n and $w_{i,n}$, $i = 0, 1, \ldots, n$. $\Delta t_n^{(o)}$ can be chosen arbitrarily but positive, and $w_{i,n}^{(r)}$ are the solutions of

(5) $$\Delta_x^2\, w_{i,n}^{(r)} \equiv \frac{w_{i+1,n}^{(r)} - 2\, w_{i,n}^{(r)} + w_{i-1,n}^{(r)}}{h^2} = \frac{w_{i,n}^{(r)} - w_{i,n-1}}{\Delta t_n^{(r)}}\ ,$$

$$i = 1, 2, \ldots, n-1; \quad r = 0, 1, \ldots,$$

(6) $$w_{o,n}^{(r)} - w_{1,n}^{(r)} = h\ , \qquad r = 0, 1, \ldots,$$

(7) $$w_{n,n}^{(r)} = 0\ , \qquad r = 0, 1, \ldots,$$

The next approximation to Δt_n can now be found from

(8) $$\Delta t_n^{(r+1)} = \left(n + \sum_{i=1}^{n} w_{i,n}^{(r)} \right) \cdot h - t_{n-1}\ .$$

The iteration is continued to a certain point, say $r = q$, when we presumably are close to the limit value. We then delete the superscript (r) and the replace n by $n+1$.

Remark. A discretization variant is discussed in Appendix D.

Remark. The Δt_n in [7] corresponds to our Δt_{n+1}.

Remark. Equation (8) is the discretization of (2.13).

Another possibility is to discretize (2.11) to

$$(9) \qquad \Delta t_n^{(r+1)} = h^2 / w_{n-1,n}^{(r)} .$$

This leads to a scheme which, if the iteration on r is convergent, will give almost identical results, since equations (9) and (18) (see section 3.2) become identical in the limit $r \to \infty$.

The solution of equations (6) - (8) for $n = 1$ is given in (4). The solution of equations (5) - (7) for $n = 2$ can also be written explicitly:

$$(10) \qquad \frac{w_{2,2}^{(r)} - 2\,w_{1,2}^{(r)} + w_{0,2}^{(r)}}{h^2} = \frac{w_{1,2}^{(r)} - w_{1,1}}{\Delta t_2^{(r)}} ,$$

$$(11) \qquad w_{0,2}^{(r)} - w_{1,2}^{(r)} = h , \qquad w_{2,2}^{(r)} = 0 ,$$

$$(12) \qquad w_{1,2}^{(r)} = \frac{h}{1 + h^2/\Delta t_2^{(r)}} , \qquad w_{0,2}^{(r)} = w_{1,2}^{(r)} + h .$$

From equation (8) we now have

$$(13) \qquad \Delta t_2^{(r+1)} = (2 + w_{1,2}^{(r)}) \cdot h - t_1 = (1 + w_{1,2}^{(r)}) \cdot h .$$

We can solve (12) - (13) by iteration starting with

$\Delta t_2^{(0)} = h$ or use directly

(14) $$w_{1,2} = -\tfrac{1}{2} + \sqrt{h + 1/4}\,.$$

Remark. Calculations show that the sequence $\Delta t_1, \Delta t_2, \ldots$ is increasing, and hence a reasonable starting value for $\Delta t_n^{(0)}$ is Δt_{n-1}. An even better value is $\Delta t_n^{(0)} = 2\Delta t_{n-1} - \Delta t_{n-2}$ as indicated by Lemma 7, for if the bound (49) is reasonably good, then $t(x)$ behaves somewhat like a quadratic function, and the third difference of t, which is equal to the second difference of Δt, will be close to 0.

3.2 Elementary properties of solutions.

Introducing the notation

(15) $$s_n^{(r)} = \frac{\Delta t_n^{(r)}}{h}\,,$$

(16) $$v_{i,n}^{(r)} = w_{i,n}^{(r)} - w_{i,n-1}\,,$$

(17) $$m_{i,n}^{(r)} = \frac{w_{i,n}^{(r)} - w_{i+1,n}^{(r)}}{h}\,,$$

Douglas and Gallie proved (for $n = 2, 3, \ldots$)

(18) $$s_n^{(r)} = 1 + s_n^{(r-1)}\cdot(1 - m_{n-1,n}^{(r-1)})\,, \qquad r \geq 1\,,$$

(19) $$0 < m_{i,n}^{(r)} < 1\,, \qquad r \geq 0,\ i = 1, 2, \ldots, n-1\,,$$

(20) $$0 < w_{i,n}^{(r)} < (n-i)\cdot h\,, \qquad r \geq 0,\ i = 0, 1, \ldots, n-1\,,$$

(21) $$s_n^{(r)} > 1\,, \qquad r \geq 1\,,$$

$$0 < \min\left\{ \frac{m_{12}}{s_2^{(q)}}, \ldots, \frac{m_{n-1,n}}{s_n^{(q)}}, \frac{m_{n,n+1}^{(r)}}{s_{n+1}^{(r)}} \right\} \leq \Delta_x^2 w_{i,n+1}^{(r)}$$

$$(22) \qquad \leq \max\left\{ \frac{m_{12}}{s_2^{(q)}}, \ldots, \frac{m_{n-1,n}}{s_n^{(q)}}, \frac{m_{n,n+1}^{(r)}}{s_{n+1}^{(r)}} \right\} < 1,$$

$$r \geq 0, \; i = 1, 2, \ldots, n,$$

$$(23) \qquad w_{i,n}^{(r)} > w_{i,n-1}, \qquad r \geq 0, \; i = 1, 2, \ldots, n-1.$$

3.3 Further properties.

The result in (19) can be improved somewhat, and this is important for the proof of convergence of the iteration on r. First we shall need a few preliminary results.

From (16), (19), and (23) it follows that

$$(24) \qquad 0 < v_{i,n}^{(r)} < h, \qquad r \geq 0, \; i = 0, 1, \ldots, n-1.$$

1. Lemma. If $\Delta t_n^{(0)} = \Delta t_{n-1}$ then

$$(25) \qquad w_{i,n}^{(0)} - w_{i-1,n-1} \leq 0, \qquad i = 1, 2, \ldots, n-1$$

and

$$(26) \qquad \Delta t_n^{(r+1)} > \Delta t_n^{(r)}, \qquad r \geq 0.$$

Proof: Introduce the function $z_{i,n}^{(r)} \equiv w_{i,n}^{(r)} - w_{i-1,n-1}$.

We have $z_{n,n}^{(r)} = 0$ and

$$(27) \qquad z_{1,n}^{(r)} = v_{1,n}^{(r)} - h < 0.$$

Furthermore

$$(28)\qquad \Delta_x^2 z_{i,n}^{(r)} = \frac{w_{i,n}^{(r)} - w_{i,n-1}}{\Delta t_n^{(r)}} - \frac{w_{i-1,n-1} - w_{i-1,n-2}}{\Delta t_{n-1}}$$

$$= \frac{z_{i,n}^{(r)} - z_{i,n-1}}{\Delta t_n^{(r)}} + (w_{i-1,n-1} - w_{i-1,n-2})\left(\frac{1}{\Delta t_n^{(r)}} - \frac{1}{\Delta t_{n-1}}\right).$$

For $r = 0$ the last term vanishes, and we can use the maximum principle of Theorem 1 of [7] such that

$$(29)\qquad z_{i,n}^{(0)} = w_{i,n}^{(0)} - w_{i-1,n-1} \leq 0, \quad i = 1, 2, \ldots, n-1.$$

Now

$$\Delta t_n^{(r+1)} - \Delta t_{n-1}$$

$$(30)\qquad = h\left\{1 + \sum_{i=1}^{n-1}(w_{i,n}^{(r)} - w_{i,n-1}) - 1 - \sum_{i=1}^{n-2}(w_{i,n-1} - w_{i,n-2})\right\}$$

$$= \Delta t_n^{(r)}(1 - m_{n-1,n}^{(r)}) - \Delta t_{n-1}(1 - m_{n-2,n-1}),$$

$$(31)\qquad \Delta t_n^{(r+1)} - \Delta t_n^{(r)} = \Delta t_{n-1} \cdot m_{n-2,n-1} - \Delta t_n^{(r)} \cdot m_{n-1,n}^{(r)}.$$

Set $r = 0$ and use (29) to get $\Delta t_n^{(1)} \geq \Delta t_n^{(0)}$, and (26) now follows immediately from section 5 of [7].

<u>2. Lemma.</u> $m_{n,n+1}^{(r)} \geq (2 + h)^{-n}, \qquad r, n \geq 0.$

<u>Proof:</u> For $n = 0$ we have from (4) and (17) that $m_{o1} = 1$. By induction on n we now wish to find positive numbers $\delta_n = \delta_n(h)$ such that $m_{n,n+1}^{(r)} \geq \delta_n$, for $r, n \geq 0$. We already have $\delta_o = 1$. Now assume that $m_{n-1,n} \geq \delta_{n-1} > 0$. From (5), (15), and (17) we derive

$$(32)\qquad \Delta_x^2 w_{n,n+1}^{(r)} = \frac{m_{n,n+1}^{(r)}}{s_{n+1}^{(r)}}$$

and

$$(33)\qquad m_{n-1,n+1}^{(r)} = m_{n,n+1}^{(r)} + h\cdot\Delta_x^2 w_{n,n+1}^{(r)} = m_{n,n+1}^{(r)}\left(1 + \frac{h}{s_{n+1}^{(r)}}\right).$$

Furthermore

$$(34)\qquad \begin{aligned} s_{n+1}^{(r)}\Delta_x^2 w_{n-1,n+1}^{(r)} &= s_{n+1}^{(r)}\Delta_x^2 w_{n,n+1}^{(r)} + m_{n-1,n+1}^{(r)} - m_{n-1,n} \\ &= m_{n,n+1}^{(r)}\left(2 + \frac{h}{s_{n+1}^{(r)}}\right) - m_{n-1,n} \end{aligned}$$

or

$$(35)\qquad m_{n,n+1}^{(r)} = \frac{m_{n-1,n} + s_{n+1}^{(r)}\Delta_x^2 w_{n-1,n+1}^{(r)}}{2 + \frac{h}{s_{n+1}^{(r)}}} \geq \frac{m_{n-1,n}}{2+h} \geq \frac{\delta_{n-1}}{2+h},$$

such that by induction

$$(36)\qquad m_{n,n+1}^{(r)} \geq \delta_n = (2+h)^{-n}, \qquad r,\ n \geq 0.$$

<u>3. Lemma.</u> If $\Delta t_n^{(1)} \geq \Delta t_n^{(0)}$ then for $r,\ n \geq 1$

$$(37)\qquad 0 \leq \Delta t_n^{(r+1)} - \Delta t_n^{(r)} \leq (1 - m_{n-1,n}^{(r)})(\Delta t_n^{(r)} - \Delta t_n^{(r-1)}).$$

If $\Delta t_n^{(1)} \leq \Delta t_n^{(0)}$ then for $r,\ n \geq 1$

$$(38)\qquad 0 \geq \Delta t_n^{(r+1)} - \Delta t_n^{(r)} \geq (1 - m_{n-1,n}^{(r)})(\Delta t_n^{(r)} - \Delta t_n^{(r-1)}).$$

<u>Remark.</u> A similar but somewhat weaker result was proved by Douglas and Gallie [7, Theorem 2].

<u>Proof:</u> From (18) we get

$$s_n^{(r+1)} - s_n^{(r)} = (s_n^{(r)} - s_n^{(r-1)})(1 - m_{n-1,n}^{(r)}) \tag{39}$$
$$- s_n^{(r-1)}(m_{n-1,n}^{(r)} - m_{n-1,n}^{(r-1)}) .$$

Douglas and Gallie showed, that $\Delta t_n^{(1)} \geq \Delta t_n^{(0)}$ implies $\Delta t_n^{(r+1)} \geq \Delta t_n^{(r)}$, $r \geq 1$, and furthermore that under this condition

$$z_{n-1,n} \equiv h\cdot(m_{n-1,n}^{(r)} - m_{n-1,n}^{(r-1)}) \geq 0, \qquad r \geq 1, \tag{40}$$

which together with (39) gives (37). (38) is proved similarly.

4. Theorem. For arbitrary n we have: $\lim_{r\to\infty} \Delta t_n^{(r)}$ and $\lim_{r\to\infty} w_{i,n}^{(r)}$, $i = 0, 1, \ldots, n$ exist and are finite.

Remark. This theorem is an extension of Theorem 2 of [7], which only holds for $n\cdot h < 1$.

Proof:

$$\lim_{r\to\infty} \Delta t_n^{(r)} = \Delta t_n^{(0)} + (\Delta t_n^{(1)} - \Delta t_n^{(0)}) + \ldots \tag{41}$$
$$+ (\Delta t_n^{(r+1)} - \Delta t_n^{(r)}) + \ldots$$

Using Lemmas 2 and 3 the above series is majorized by a geometric series with quotient $q = 1 - (2 + h)^{-n} < 1$ and is therefore convergent. Similarly

$$\lim_{r\to\infty} w_{i,n}^{(r)} = w_{i,n}^{(0)} + (w_{i,n}^{(1)} - w_{i,n}^{(0)}) + \ldots \tag{42}$$
$$+ (w_{i,n}^{(r+1)} - w_{i,n}^{(r)}) + \ldots$$

and this series is majorized by the series for $\lim_{r \to \infty} \Delta t_n^{(r)}$

We shall, from now on, assume that the limit of the iterations have been reached for each n, and Δt_n, $w_{i,n}$, etc. will denote the limit values.

5. Lemma.

$$0 < \frac{m_{n-1,n}}{s_n} \leq \Delta_x^2 w_{i,n} \leq \frac{m_{12}}{s_2} < 1 . \tag{43}$$

Proof: It follows from Lemma 1 that

$$\Delta t_1 < \Delta t_2 < \dots < \Delta t_{n-1} < \Delta t_n \tag{44}$$

under the condition $\Delta t_j^{(0)} = \Delta t_{j-1}$, $j = 1, 2, \dots, n$. Since the limit value does not depend on the starting guess, once convergence is established, we can leave this condition out.

In the limit $(r \to \infty)$, equation (18) reduces to

$$s_n \cdot m_{n-1,n} = 1 , \tag{45}$$

such that by (44)

$$m_{1,2} > m_{2,3} > \dots > m_{n-1,n} > m_{n,n+1} \tag{46}$$

and (43) now follows from (22).

6. Lemma. $m_{n,n+1} > (1 + h)^{-n}$, $n = 1, 2, \dots$

Proof: Use Lemma 5 on the left hand side of equation (34) (for $r \to \infty$):

(47) $$m_{n,n+1} \geq \frac{m_{n-1,n}}{1 + \frac{h}{s_n}} > \frac{m_{n-1,n}}{1 + h}$$

and the result is immediate.

The following estimate which we shall use later in chapters 4 and 5 is derived from Lemma 6 together with (21) and (45)

(48) $$1 < s_n < (1 + h)^{n-1}.$$

Another result which has several applications is given in Lemma 6 of [7] and is stated slightly more generally as

7. Lemma.

(49) $$n \cdot h < t_n < n \cdot h + \tfrac{1}{2}(n \cdot h)^2, \qquad n \geq 2.$$

Proof: The left inequality follows from (21) and the right inequality follows from (8) and (20) which in the limit give

$$\begin{aligned} t_n &= \left(n + \sum_{i=1}^{n} w_{i,n} \right) \cdot h \\ &< n \cdot h + \sum_{i=1}^{n} (n - i) \cdot h^2 \\ &< n \cdot h + \tfrac{1}{2}(n \cdot h)^2 . \end{aligned}$$

As a consequence of Theorem 4, the results of sections 6 and 7 of [7] now extend to any interval $0 \leq x \leq X$, where X is arbitrarily large. In particular, a pair of functions $(t(x), u(x,t))$ exists for $0 \leq x \leq X$,

$t(x) \leq t \leq t(X) = T$. The function $t(x)$ is continuous and monotonicly increasing and therefore has an inverse function $y(t)$, and the pair $(y(t), u(x,t))$, $0 \leq t \leq T$, $0 \leq x \leq y(t)$ is the solution to the Stefan problem A. Furthermore the solution functions of the difference scheme will converge uniformly to that solution as $h \to 0$.

3.4 Accelerating the convergence.

The result of Theorem 4 indicates, that the convergence of $\Delta t_n^{(r)}$ may be rather slow, but the comparison with a geometric series also suggests a possible way of accelerating it. We could expect, that an acceleration of the form

$$\Delta t_n^{acc} = \frac{\Delta t_n^{(1)} - \Delta t_n^{(0)}}{1 - q} + \Delta t_n^{(0)} \tag{50}$$

where

$$q = \frac{\Delta t_n^{(2)} - \Delta t_n^{(1)}}{\Delta t_n^{(1)} - \Delta t_n^{(0)}} \tag{51}$$

would be efficient, and empirical evidence supports this strongly. Actual computations have been performed with $h = .1$ and using as initial guess $\Delta t_n^{(0)} = 2\Delta t_{n-1} - \Delta t_{n-2}$. At $n = 20$ the values of $\Delta t_n^{(r)}$ for $r = 0, 1, 2$ gave a value of $q = .71$ corresponding to a rather slow convergence. Since the value for $\Delta t_n^{(0)}$ was a fairly good guess there was an agreement between $\Delta t_n^{(2)}$ and the limit value Δt_n to 4 significant figures. Δt_n^{acc} and Δt_n, however, agreed to 6 significant figures. It would take more than 5 iterations to reach a comparable agreement without acceleration. For larger n the iteration exhibits a slower convergence, (q approaches 1), whereas the acceleration is equally effective and therefore reduces the computation time by considerably more than the 60 % indicated here.

3.5 Space and time requirements.

The space needed for storage of data arrays is proportional to n, and because of the estimate (49) the size of these arrays is proportional to 1/h. The number of arithmetic operations is at each step proportional to the current n, such that the time required for a full run is proportional to h^{-2}. These are estimates of the space and time requirements for computations up to a fixed T as functions of h.

It might also be of interest to know how space and time depends on T for fixed h. Actual calculations show that the upper bound for t_n in (49) is the more realistic one, i. e. that t(x) for large x behaves like a quadratic function. With this assumption we see that the space needed for calculations up to time T increases like $T^{\frac{1}{2}}$ and that the computation time increases linearly with T for large T.

3.6 Stability.

We have seen that the difference scheme (5) - (8) converges in r, and that it for small h gives a solution which is close to the solution of Stefan problem A. In order for the method to be useful, however, it must be stable against round-off (or other small) errors.

We shall now consider the effect of errors, introduced at one particular time step, say $t = t_p$, upon t_n, Δt_n, and $w_{i,n}$ for $n > p$, assuming that no more errors are introduced in the calculations. Let t_n^*, Δt_n^*, and $w_{i,n}^*$ denote the perturbed values and set

(52) $$\delta_{i,n} = w_{i,n}^* - w_{i,n} ,$$

(53) $$\delta_n = \max_i |\delta_{i,n}| .$$

We shall use the notation $\delta_{\cdot,n}$ to denote the column vector with components $\delta_{i,n}$, $i = 0, 1, \ldots, n$.

Douglas and Gallie showed that

(54) $$\delta_{i,n} = \delta_{i,n-1} + (\Delta t_n^* - \Delta t_n)\Delta_x^2 w_{i,n} + \Delta t_n^* \Delta_x^2 \delta_{i,n} ,$$

(55) $$\Delta t_n^* - \Delta t_n = h \sum_{i=1}^{n-1} \delta_{i,n} - (t_{n-1}^* - t_{n-1}) ,$$

(56) $$t_n^* - t_n = h \sum_{i=1}^{n-1} \delta_{i,n} ,$$

and using this they were able to prove stability, for fixed h and provided $n \cdot h < 1$.

Although actual calculations have shown no sign of instability even for large t and x (we have data up to $t \doteq 64$, $y(t) \doteq 16$, with $h = .1$), we have not been able to arrive at a proof of stability. We shall here just give some results on the effect of small errors.

From (54), (55), and (56) we get

$$\Delta t_n^* - \Delta t_n = h(\Delta t_n^* - \Delta t_n) \sum_{i=1}^{n-1} \Delta_x^2 w_{i,n}$$

(57)
$$+ h \Delta t_n^* \sum_{i=1}^{n-1} \Delta_x^2 \delta_{i,n}$$

$$= (\Delta t_n^* - \Delta t_n)(1 - m_{n-1,n}) - \frac{\Delta t_n^*}{h} \delta_{n-1,n}$$

or

(58)
$$\Delta t_n^* - \Delta t_n = - \frac{\Delta t_n^*}{h} \frac{\delta_{n-1,n}}{m_{n-1,n}} = - s_n^2 \frac{\Delta t_n^*}{\Delta t_n} \delta_{n-1,n}$$

or

(59)
$$\Delta t_n^* = \frac{\Delta t_n}{1 + s_n \delta_{n-1,n}/h} .$$

Let us take a closer look at (54) writing $\Delta_x^2 \delta_{i,n}$ in full, divide by $\delta_{i,n}$ and multiply by $h^2/\Delta t_n^*$.

(60)
$$\frac{h^2}{\Delta t_n^*} \left(1 - \frac{\delta_{i,n-1}}{\delta_{i,n}}\right) = - \Delta t_n \frac{\delta_{n-1,n}}{\delta_{i,n}} \Delta_x^2 w_{i,n}$$

$$+ \frac{\delta_{i-1,n}}{\delta_{i,n}} - 2 + \frac{\delta_{i+1,n}}{\delta_{i,n}} .$$

Set $i = n-1$ and rearrange

(61)
$$\frac{\delta_{n-2,n}}{\delta_{n-1,n}} = 2 + w_{n-1,n} + \frac{h^2}{\Delta t_n^*} > 2 .$$

$i = n-2$ gives

(62)
$$\frac{\delta_{n-3,n}}{\delta_{n-2,n}} = 2 - \frac{\delta_{n-1,n}}{\delta_{n-2,n}} + \Delta t_n \frac{\delta_{n-1,n}}{\delta_{n-2,n}} \Delta_x^2 w_{n-2,n}$$

$$+ \frac{h^2}{\Delta t_n^*} \left(1 - \frac{\delta_{n-2,n-1}}{\delta_{n-2,n}} \right)$$

which is $> 3/2$ if the last parenthesis is non-negative. In any case $|\delta_{n-2,n}| < \max(|\delta_{n-2,n-1}|, \frac{2}{3}|\delta_{n-3,n}|)$.

Continuing along these lines we conclude, that $\delta_{i,n}$ for i close to $n-2$ has the same sign as $\delta_{n-1,n}$ and is of larger absolute value.

The first relative maximum for $|\delta_{i,n}|$ as i decreases from $n-1$, is accompanied by a decrease in absolute value as compared to $\delta_{i,n-1}$, as is easily seen from equation (60). This is also the case for all other relative maxima for $|\delta_{i,n}|$, for which $\text{sign}(\delta_{i,n}) = \text{sign}(\delta_{n-1,n})$.

From equations (55) and (56) it would appear, that the most unfortunate case would be the one where all δ's were of the same sign. Ironically enough, in this case a stability proof follows directly from the considerations above. At $t = t_p$ we shall of course expect errors that are randomly distributed with respect to sign (and magnitude), but it appears from experiments that the operator that maps $\delta_{\cdot,n-1}$ onto $\delta_{\cdot,n}$ has certain smoothing properties, such that after a few steps all δ's will have the same sign. We have already seen indications of this for i close to $n-2$.

When considering the effect of small errors on the computations one should keep in mind that our grid-points change with t_n. Therefore $\delta_{i,n}$ as defined in (52) is a difference of values of two functions at two different points. In order to compare function values at the same point, let us introduce $\bar{w}_{i,n} = w(i \cdot h, t_n^*)$ and study

$$w^*_{i,n} - \overline{w}_{i,n} = \delta_{i,n} + w_{i,n} - \overline{w}_{i,n}$$

(63)
$$\doteq \delta_{i,n} + (t_n - t^*_n)\frac{w_{i,n} - w_{i,n-1}}{\Delta t_n}$$

$$= \delta_{i,n} - h\sum_{i=1}^{n-1}\delta_{i,n}\cdot\Delta_x^2 w_{i,n}$$

where we have used a truncated Taylor expansion and approximated a derivative by a first difference. We notice a built-in compensation in the case where all δ's are of the same sign since a (partial) cancellation will occur, and thus the effect of round-off errors on $w_{\cdot,n}$ is to some extent counteracted by the effect of the same errors on t_n.

It is possible to express explicitly the operator that maps $\delta_{\cdot,n-1}$ onto $\delta_{\cdot,n}$ and in order to do this let us turn to the systems of equations for $w_{i,n}$ and $w^*_{i,n}$.

Set

(64)
$$\varepsilon = \frac{h^2}{\Delta t_n}\ , \quad \varepsilon^* = \frac{h^2}{\Delta t^*_n}\ ,$$

(65)
$$A_n = \begin{bmatrix} 1 & -1 & & & & \\ -1 & 2+\varepsilon & -1 & & & \\ & -1 & 2+\varepsilon & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & -1 \\ & & & & -1 & 2+\varepsilon \end{bmatrix}, \quad b_n = \begin{bmatrix} h \\ \varepsilon w_{1,n} \\ \varepsilon w_{2,n} \\ \vdots \\ \varepsilon w_{n-1,n} \\ \varepsilon w_{n,n} \end{bmatrix},$$

and similarly for A^*_n and b^*_n.

We now have

(66) $$A_n w_{\cdot,n} = b_{n-1} \quad \text{and} \quad A_n^* w^*_{\cdot,n} = b^*_{n-1} .$$

Subtraction gives

(67) $$A_n^* \delta_{\cdot,n} + (A_n^* - A_n) w_{\cdot,n} = b^*_{n-1} - b_{n-1} .$$

Application of (58) gives the following

(68) $$\varepsilon^* - \varepsilon = \frac{h^2}{\Delta t_n^*} - \frac{h^2}{\Delta t_n} = h^2 \frac{\Delta t_n - \Delta t_n^*}{\Delta t_n^* \cdot \Delta t_n} = \delta_{n-1,n}$$

such that

(69) $$A_n^* - A_n = \operatorname{diag}\left\{ 0, \delta_{n-1,n}, \delta_{n-1,n}, \ldots, \delta_{n-1,n} \right\} .$$

The first component of both b_{n-1} and b^*_{n-1} is h. The i-th component $(i \geq 1)$ of $b^*_{n-1} - b_{n-1}$ is

(70) $$\begin{aligned} \varepsilon^* w^*_{i,n-1} - \varepsilon w_{i,n-1} &= \varepsilon^* \delta_{i,n-1} + (\varepsilon^* - \varepsilon) w_{i,n-1} \\ &= \varepsilon^* \delta_{i,n-1} + w_{i,n-1} \delta_{n-1,n} . \end{aligned}$$

We shall add equation number 0 in (67)

(71) $$\delta_{0,n} - \delta_{1,n} = 0$$

to equation number 1

(72) $$\begin{aligned} - \delta_{0,n} + (2 + \varepsilon^*) \delta_{1,n} - \delta_{2,n} + (w_{1,n} - w_{1,n-1}) \delta_{n-1,n} \\ = \varepsilon^* \delta_{1,n-1} \end{aligned}$$

and end up with the following system of $n-1$ equations for the $n-1$ unknowns $\delta_{1,n}, \delta_{2,n}, \ldots, \delta_{n-1,n}$:
(For typographical reasons we shall write e for ε^*.)

$$(73)\quad \begin{bmatrix} 1+e & -1 & & & & v_{1,n} \\ -1 & 2+e & -1 & & & v_{2,n} \\ & -1 & 2+e & -1 & & v_{3,n} \\ & & & & & \vdots \\ & & & -1 & 2+e & -1+v_{n-2,n} \\ & & & & -1 & 2+e+v_{n-1,n} \end{bmatrix} \begin{bmatrix} \delta_{1,n} \\ \delta_{2,n} \\ \delta_{3,n} \\ \vdots \\ \delta_{n-2,n} \\ \delta_{n-1,n} \end{bmatrix} = e \begin{bmatrix} \delta_{1,n-1} \\ \delta_{2,n-1} \\ \delta_{3,n-1} \\ \vdots \\ \delta_{n-2,n-1} \\ \delta_{n-1,n-1} \end{bmatrix}$$

or in short

$$(74)\qquad \hat{A}\,\delta_{\cdot,n} = e\,\delta_{\cdot,n-1}\,.$$

Set $B = \hat{A}^{-1}$ and compute the elements of B using Gaussian elimination on the $n-1$ sets of equations with the right hand sides equal to the $n-1$ unit vectors :

$$(75)\qquad \hat{A}\cdot B = I\,.$$

Introduce

$$(76)\qquad d_1 = v_{1,n}\,,\quad d_i = v_{i,n} + \frac{d_{i-1}}{\eta_{i-1}}\,,\qquad i = 2, 3, \ldots, n-1;$$

$$(77)\qquad \begin{aligned} \eta_1 &= 1+e\,,\quad \eta_i = 2+e-\frac{1}{\eta_{i-1}}\,,\qquad i = 2, 3, \ldots, n-2, \\ \eta_{n-1} &= 2+e-\frac{1}{\eta_{n-2}} + d_{n-1}\,; \end{aligned}$$

$$(78)\qquad H_{ik} = \begin{cases} 1 & \text{if } i > k\,, \\ \prod_{j=i}^{k} \eta_j & \text{otherwise}\,; \end{cases}$$

$$(79)\qquad \nu_{jk} = \begin{cases} 1 & \text{if } j \le k\,, \\ 0 & \text{if } j > k\,. \end{cases}$$

After triangularization the coefficient matrix A has the following appearance:

$$(80) \quad \begin{bmatrix} \eta_1 & -1 & 0 & \cdots & & d_1 \\ 0 & \eta_2 & -1 & & & d_2 \\ \vdots & & & & & \vdots \\ & & & \eta_{n-3} & -1 & d_{n-3} \\ & & & & \eta_{n-2} & -1+d_{n-2} \\ & & \cdots & & 0 & \eta_{n-1} \end{bmatrix}$$

and the unit matrix on the right hand side has been transformed into a matrix C the elements of which are given by

$$(81) \qquad c_{ij} = \frac{\nu_{ji}}{H_{j,i-1}} .$$

<u>8. Lemma.</u> The elements b_{ij} of B are given by the formula

$$(82) \qquad H_{j,n-1} b_{ij} = \sum_{k=i}^{n-1} \frac{\nu_{jk} H_{k+1,n-1}}{H_{i,k-1}} - \sum_{k=i}^{n-2} \frac{d_k}{H_{ik}} .$$

<u>Remark.</u> The lower summation index in the first sum can be changed to $k = \max(i,j)$ and the factor ν_{jk} can then be omitted.

<u>Proof:</u> (by induction on i). For $i = n-1$ we have

$$(83) \qquad b_{n-1,j} = \frac{c_{n-1,j}}{\eta_{n-1}} = \frac{\nu_{j,n-1}}{H_{j,n-1}} \quad \text{or} \quad H_{j,n-1} b_{n-1,j} = \nu_{j,n-1} = 1$$

in agreement with (82).

Suppose (82) is true for $b_{i+1,j}$ $(1 \leq i \leq n-2)$, then

$$H_{j,n-1} b_{ij} = \frac{H_{j,n-1}}{\eta_i} \left\{ c_{ij} + b_{i+1,j} - b_{n-1,j} d_i \right\}$$

$$(84) \qquad = \frac{1}{\eta_i} \left\{ \frac{\nu_{ji} H_{j,n-1}}{H_{j,i-1}} + \sum_{k=i+1}^{n-1} \frac{\nu_{jk} H_{k+1,n-1}}{H_{i+1,k-1}} - \sum_{k=i+1}^{n-2} \frac{d_k}{H_{i+1,k}} - d_i \right\}$$

$$= \sum_{k=i}^{n-1} \frac{\nu_{jk} H_{k+1,n-1}}{H_{i,k-1}} - \sum_{k=i}^{n-2} \frac{d_k}{H_{ik}} \qquad \text{Q.E.D.}$$

With available bounds for the quantities in (82) it has not been possible to arrive at useful estimates for $\delta_{i,n}$. For the quantities η_i of (77) we have the following

9. Lemma.

(85) If $\eta_i \geq 1 + \alpha$ then $\eta_{i+1} > 1 + e + \alpha - \alpha^2$,

$\alpha > 0, \quad i = 1, 2, \ldots, n-3.$

(86) $\eta_1 < \eta_2 < \cdots < \eta_{n-2} \leq 1 + \frac{e}{2} + \sqrt{e}\sqrt{1 + \frac{e}{4}}$.

Proof: If $\eta_i \geq 1 + \alpha$ then

(87) $$\eta_{i+1} = 2 + e - \frac{1}{\eta_i} > 2 + e - (1 - \alpha + \alpha^2) .$$

In particular $\eta_{i+1} > 1 + e$ if $0 < \alpha < 1$.
If the η_i approach a limit η as i increases, then we must have $\eta = 2 + e - \frac{1}{\eta}$ or

(88) $$\eta = 1 + \frac{e}{2} + \sqrt{e}\sqrt{1 + \frac{e}{4}} \leq 1 + \sqrt{e} + \frac{e}{2} + \frac{e\sqrt{e}}{8} .$$

Since we are only interested in roots that are greater than 1 we have discarded the negative square root. Observe that (since $e > 0$) $1 < \eta_1 < \eta$ and furthermore

(89) $$\eta - \eta_{i+1} = 2 + e - \frac{1}{\eta} - (2 + e - \frac{1}{\eta_i}) = \frac{\eta - \eta_i}{\eta\,\eta_i}$$

and (86) follows.

As $h \to 0$ the matrix $\hat{A}$ will tend to the tri-diagonal matrix which has 2's on the diagonal and -1's on the side diagonals. This matrix has all its eigenvalues between 0 and 4. For $\hat{A}$ it can be shown that the eigenvalues lie between ε^* and $4 + \varepsilon^*$. This gives rise to finite bounds for $\delta_{i,n}$ for any finite region although it does not prove that the method is stable.

Chapter 4.

Theoretical results.

4.1 Some bounds for u and y.

We are now ready to continue the investigations which we began in chapter 2. We shall consider two problems both related to Stefan problem A.

First let $y(t)$ be a function satisfying

(1) $$y(0) = 0, \qquad y(t) > 0, \qquad t > 0,$$

(2) $$0 \leq y(t_2) - y(t_1) \leq t_2 - t_1, \qquad 0 \leq t_1 \leq t_2.$$

With $y(t)$ satisfying (1) - (2) there exists a unique function, $u(x,t)$, satisfying

(3) $$u_{xx}(x,t) = u_t(x,t), \qquad 0 < x < y(t),\ t > 0,$$

(4) $$u_x(0,t) = -1, \qquad t > 0,$$

(5) $$u(y(t),t) = 0, \qquad t \geq 0.$$

With $y(t)$ as above there is also a unique function, $v(x,t)$, satisfying

(6) $$v_{xx}(x,t) = v_t(x,t), \qquad -y(t) < x < y(t),\ t > 0,$$

(7) $$v(\pm y(t),t) = y(t), \qquad t \geq 0.$$

<u>1. Lemma.</u> (Trench [22]) The solution of (6) - (7) is given by

$$(8) \qquad v(x,t) = u(x,t) + x\,, \qquad 0 \le x \le y(t),\ t \ge 0,$$

$$(9) \qquad v(-x,t) = v(x,t)\,, \qquad 0 \le x \le y(t),\ t \ge 0.$$

<u>Proof:</u> $v(-x,t)$ also satisfies (6) and (7) so we have (9) by uniqueness. Therefore $v_x(0,t) = 0$, such that $v(x,t) - x$ satisfies (3) - (5). By uniqueness (8) follows.

Using the maximum principle [15] on v, remembering that y is non-decreasing, we get

$$(10) \qquad 0 \le v(x,t) \le y(t)\,, \qquad |x| \le y(t),\ t > 0;$$

and from (8) and (2.15) (which holds for the solution of (3) - (5)) we have

$$(11) \qquad 0 < u(x,t) \le y(t) - x\,, \qquad 0 \le x < y(t),\ t > 0.$$

<u>2. Lemma.</u> If $u(x,t)$ is the solution of (3) - (5), then

$$(12) \qquad 0 \le u_t(x,t) \le 1\,, \qquad 0 \le x < y(t),\ t > 0.$$

<u>Proof:</u> Let $\Delta t > 0$ and define

$$(13) \qquad Q(x,t) = \frac{v(x,t+\Delta t) - v(x,t)}{\Delta t}\,, \quad -y(t) \le x \le y(t),\ t \ge 0,$$

where $v(x,t)$ is the solution of (6) - (7). $Q(x,t)$ is continuous for $-y(t) \le x \le y(t)$, $t \ge 0$, and satisfies the heat equation in the interior of this domain. By (8), (9), and (5)

(14) $$Q(\pm y(t),t) = \frac{u(y(t),t+\Delta t)}{\Delta t}, \qquad t \geq 0,$$

and by (2) and (11)

(15) $$0 < Q(\pm y(t),t) \leq \frac{y(t+\Delta t) - y(t)}{\Delta t} \leq 1, \qquad t \geq 0.$$

From the maximum principle it now follows that

(16) $$0 < Q(x,t) \leq 1, \qquad t \geq 0.$$

From the definition of $Q(x,t)$, and the fact that $v_t(x,t) = u_t(x,t)$, (12) now follows by letting Δt tend to 0.

Remark. The results of chapter 4 up to this point are due to W. Trench [22].

3. Lemma. The boundary curve, $y(t)$, of Stefan problem A satisfies (1) and (2).

Proof: Formula (1) and the left inequality of (2) follow immediately from equations (12), (14), and (17) of chapter 2. As a consequence of the considerations of the last part of section 3.3, we have that the boundary curve, considered as a function of x, $t(x)$, is differentiable. The inverse function, $y(t)$, is therefore also differentiable, and because of (3.21) we have $\frac{h}{\Delta t_n} < 1$ which implies

(17) $$y'(t) < 1, \qquad t > 0,$$

and in turn the right inequality of (2).

As a corollary we have that (11) and (12) hold for the solution of Stefan problem A. Since $u_{xx} = u_t$ we also have that $u_x(x,t)$ is an increasing function of x and since $u_x(y(t),t) = -y'(t)$ we have

$$(18) \qquad y'(t)\cdot(y(t) - x) \le u(x,t), \quad 0 \le x \le y(t),\ t > 0.$$

Consider the estimate (3.49):

$$t_n < n\cdot h + \tfrac{1}{2}(n\cdot h)^2.$$

Letting h tend to 0 we get an estimate for the boundary curve $t(x) = \lim_{h\to 0} t(x,h)$:

$$(19) \qquad t(x) \le x + \tfrac{1}{2}x^2, \qquad x > 0,$$

or

$$(20) \qquad t \le y(t) + \tfrac{1}{2}(y(t))^2, \qquad t > 0,$$

or

$$(21) \qquad y(t) \ge \sqrt{2\cdot t + 1} - 1, \qquad t > 0.$$

Summarizing, we now have the following bounds :

$$(22) \qquad \sqrt{2\cdot t + 1} - 1 \le y(t) < t, \qquad t > 0,$$

$$(23) \qquad y'(t)\cdot(y(t) - x) \le u(x,t) \le y(t) - x,$$

$$0 \le x \le y(t),\ t > 0.$$

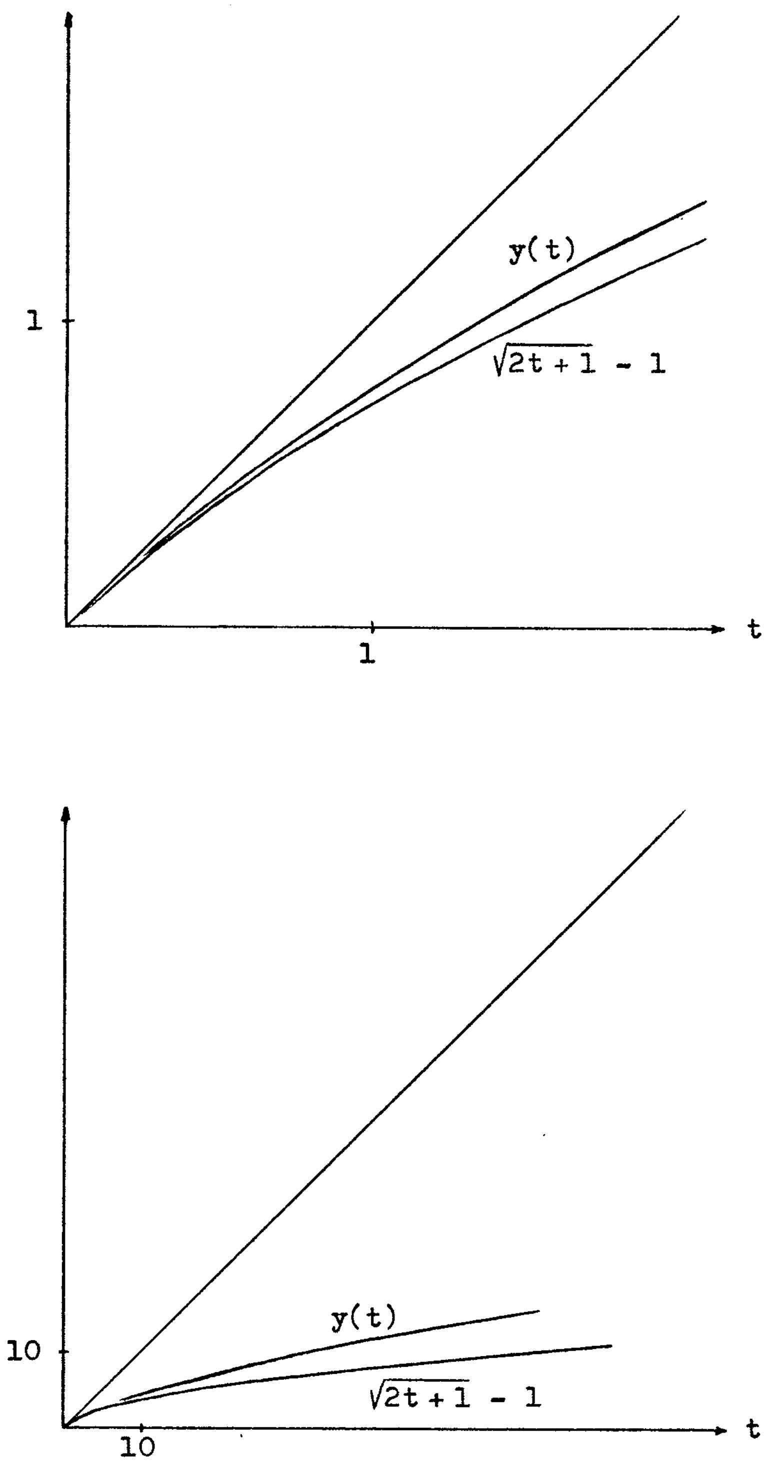

Fig. 1. The boundary curve y(t).

4.2 On the derivatives.

Notation. We shall to some extent use operator notation in the following. D shall denote the differentiation operator, and we shall indicate partial derivatives by subscripts :

$$Dy = \frac{dy}{dt} = y' ,$$

$$D_o u = \frac{\partial u}{\partial x} , \qquad D_o^i u = \frac{\partial^i u}{\partial x^i},$$

$$D_1 u = \frac{\partial u}{\partial t} , \qquad \text{etc.}$$

I denotes the identity operator such that for instance

$$u(y,I)(t) = u(y(t),t) .$$

The following result is due to R. deVogelaere [24] :

4. Lemma. Let $z = Dy$ and $g_i = D_o^i u(y,I)$.

The g_i can be obtained by the recurrence relations :

$$g_o = 0 , \qquad g_1 = -z , \tag{24}$$

$$g_{n+1} = D g_{n-1} - g_n \cdot z , \qquad n = 1, 2, \ldots \tag{25}$$

Proof: (24) follows from (10) and (11) of chapter 2.

Let $f_{ij} = D_o^i D_1^j u(y,I)$. Then $f_{ij} = f_{i+2j,o} = g_{i+2j}$ and

$$D f_{ij} = f_{i+1,j} \cdot z + f_{i,j+1} ,$$

$$\Downarrow$$

$$D g_{i+2j} = g_{i+2j+1} \cdot z + g_{i+2j+2} , \qquad i+2j = 0, 1, \ldots$$

$$\Downarrow$$

$$g_{n+1} = D g_{n-1} - g_n \cdot z , \qquad n = 1, 2, \ldots$$

In particular we have

(26) $$u_{xx}(y,I) = g_2 = z^2 ,$$

(27) $$u_{xxx}(y,I) = g_3 = -(Dz + z^3) ,$$

(28) $$u_{xxxx}(y,I) = g_4 = 3\,z\,Dz + z^4 ,$$

As a corollary we can determine the behaviour of the boundary curve, $y(t)$, near the origin from the Taylor expansion of u_x applied from the boundary curve down to the line $x = 0$:

(29) $$-1 = u_x(0,I) = \sum_{i=o} \frac{(-y)^i}{i!} g_{i+1} = g_1 - y\,g_2 + \tfrac{1}{2} y^2 g_3 - \cdots$$

Take derivatives and evaluate at 0 :

(30) $$1 = -g_1(0) = z(0) ,$$

(31) $$0 = (D\,g_1 - D\,y\cdot g_2)(0) = -(Dz + z^3)(0) ,$$

(32) $$0 = (D^2 g_1 - 2\,D\,y\cdot D\,g_2 - D^2 y\cdot g_2 + (D\,y)^2\cdot g_3)(0)$$
$$= -(D^2 z + 6\,z^2\,Dz + z^5)(0) ,$$

such that

(33) $$y'(0) = 1, \quad y''(0) = -1, \quad y'''(0) = 5 ; \quad \ldots$$

These results have also been found by Evans, Isaacson, and McDonald [8].

5. Lemma. $y'(t) > 0, \qquad t \geq 0.$

Proof: From (3.48) we have

(34) $$s_{n+1} \leq (1 + h)^n = (1 + \frac{nh}{n})^n < e^{n \cdot h}.$$

Since $n \cdot h = x$ we see that the derivative of $t(x)$ is bounded away from infinity for finite x. The derivative of the inverse function is therefore bounded away from 0.

6. Lemma. $u_{tx}(x,t) < 0, \qquad 0 < x \leq y(t),\ t > 0.$

Proof: $u_{tx}(y,I) = g_3$; $g_3(0) = 0$; $D g_3(0) = -2 < 0$; implies $u_{tx}(y(t),t) < 0$ close to the origin. Suppose u_{tx} becomes positive eventually. Because of the maximum principle and the fact that $u_{tx}(0,I) = 0$ $u_{tx}(y,I)$ must then change sign. Let T be the smallest value of t such that $u_{tx}(y(t),t) = 0$.
Since $u_{tx}(x,T) \leq 0$, $0 \leq x \leq y(T)$, we have $u_{txx}(y(T),T) \geq 0$, but then

$$D g_2(T) = (2 z Dz)(T) = (u_{tx}(y,I) \cdot z + u_{tt}(y,I))(T) \geq 0$$
$$\Downarrow$$
$$D z(T) \geq 0;$$

but then by Lemma 5

$$-u_{tx}(y(T),T) = +(Dz + z^3)(T) > 0,$$

contradicting the existence of T.

7. Lemma. If $0 < t_1 < t_2$ and $0 \leq x_1 < x_2 \leq y(t_1)$, then for t_2 sufficiently close to t_1 we have

$$(35)\qquad u(x_1,t_2) - u(x_1,t_1) > u(x_2,t_2) - u(x_2,t_1) .$$

Proof: Let t_1 be arbitrary, positive, and let x_1 and x_2 be arbitrary but fixed such that $0 \leq x_1 < x_2 \leq y(t_1)$. By Lemma 6 we have

$$(36)\qquad u_t(x_1,t_1) > u_t(x_2,t_1) .$$

Furthermore, since the function $\varphi(\tau) = u_t(x_1,\tau) - u_t(x_2,\tau)$ is continuous for $\tau > t_1$, and $\varphi(t_1) = \delta > 0$, it is true that for sufficiently small ε'

$$(37)\qquad u_t(x_1,\tau) - u_t(x_2,\tau) > \frac{\delta}{2}, \qquad t_1 \leq \tau \leq t_1 + \varepsilon' .$$

u_t satisfies a Lipschitz condition in the t-direction near (x_2,t_1):

$$(38)\qquad |u_t(x_2,\tau_1) - u_t(x_2,\tau_2)| \leq |\tau_2 - \tau_1|\cdot K, \quad t_1 \leq \tau_1, \tau_2 \leq t_1 + \varepsilon'' .$$

Now choose $\varepsilon = \min\left\{\varepsilon', \varepsilon'', \frac{\delta}{4K}\right\}$, and we have for arbitrary t_2 such that $t_1 < t_2 < t_1 + \varepsilon$:

$$u(x_1,t_2) - u(x_1,t_1) - u(x_2,t_2) + u(x_2,t_1)$$

$$(39)\qquad = (t_2 - t_1)\cdot\left\{u_t(x_1,\tau_1) - u_t(x_2,\tau_1) + u_t(x_2,\tau_1) - u_t(x_2,\tau_2)\right\}$$

$$\geq (t_2 - t_1)\cdot\left(\frac{\delta}{2} - \frac{\delta}{4}\right) = (t_2 - t_1)\cdot\frac{\delta}{4} > 0.$$

The existence of τ_1 and τ_2 between t_1 and t_2

follows from the mean value theorem, and (37) and (38) give the estimate.

We have already learned, through the estimate (22), that $y(t) \to \infty$ as $t \to \infty$, a result that also can be proved directly, using (2.13) and (11). But $y(t)$ does not approach any straight line as follows from the following :

<u>8. Lemma.</u> $\lim_{t \to \infty} y'(t) = 0.$

<u>Proof:</u> Suppose $y'(t) > \alpha > 0$, $t \geq 0$. Let $t_2 > t_1 > 0$ with t_2 so close to t_1 that Lemma 7 holds, and let $\alpha' = y'(t_2) \geq \alpha$. Set $y_1 = y(t_1)$ and $y_2 = y(t_2)$,

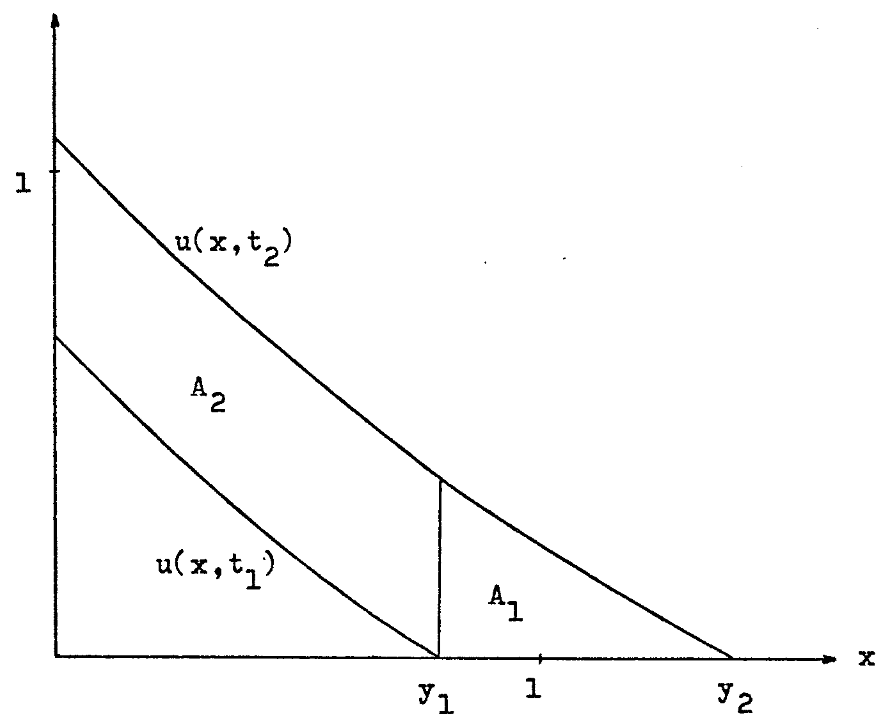

Fig. 2. $u(x,t)$ as a function of x. ($t_1 = 1$, $t_2 = 2$).

Let A_1 denote the area below the curve $u(x,t_2)$, $y_1 \le x \le y_2$, and let A_2 denote the area between $u(x,t_2)$ and $u(x,t_1)$, $0 \le x \le y_1$. (See Fig. 2) Using Lemma 7 and the fact, that u_x is an increasing function of x, we get

(40) $$u(0,t_2) - u(0,t_1) > u(y_1,t_2) - u(y_1,t_1) > \alpha'\cdot(y_2 - y_1).$$

Using this and equation (11) we get

(41) $$A_1 \ge \tfrac{1}{2}\alpha'(y_2 - y_1)^2$$

and

(42) $$A_2 \ge \alpha' y_1 (y_2 - y_1).$$

From (2.13) we have

(43) $$y_2 - y_1 = t_2 - t_1 - \int_0^{y_1}\{u(x,t_2) - u(x,t_1)\}\,dx - \int_{y_1}^{y_2} u(x,t_2)\,dx$$
$$= t_2 - t_1 - (A_2 + A_1).$$

Combining we get

(44) $$t_2 - t_1 = A_2 + A_1 + y_2 - y_1 \ge (y_2 - y_1)\cdot\{1 + \tfrac{1}{2}\alpha'(y_2 + y_1)\}$$

or

(45) $$\frac{y_2 - y_1}{t_2 - t_1} \le \frac{1}{1 + \frac{1}{2}\alpha'(y_2 + y_1)} \le \frac{1}{1 + \alpha' y_1} \le \frac{1}{1 + \alpha y_1}.$$

For any $\alpha > 0$ there exists a t_1, since $y(t) \to \infty$ as $t \to \infty$, such that $\frac{1}{1 + \alpha y_1} \le \frac{1}{2}\alpha$.

This contradicts the assumption.

4.3 An a priori estimate.

Cannon and Douglas [2] have discussed the following problem, which is related to the one we have defined in (2.1) - (2.6):

$$(46) \qquad u_{xx}(x,t) = u_t(x,t), \qquad 0 < t \leq T,\ 0 < x < y(t),$$

$$(47) \qquad u(x,0) = \varphi(x), \qquad 0 < x < y(0),$$

$$(48) \qquad u_x(0,t) = -g(t),\ |g(t)| \leq M,\ 0 < t \leq T, \quad M > 0,$$

$$(49) \qquad u(y(t),t) = f(t), \qquad 0 < t \leq T,\ f(0) = \varphi(y(0)),$$

$$(50) \qquad u_x(y(t),t) = \psi(t), \qquad 0 < t \leq T,\ \psi(0) = \varphi'(y(0)),$$

where y, φ, g, f, and ψ are given, differentiable functions. Introducing the Neumann function for the half plane $\{x > 0\}$

$$(51) \qquad N(x, t, \xi, \tau) = K(x, t, \xi, \tau) + K(-x, t, \xi, \tau),$$

where

$$(52) \qquad K(x, t, \xi, \tau) = \frac{1}{2\pi^{\frac{1}{2}}(t-\tau)^{\frac{1}{2}}} \cdot \exp\left\{\frac{-(x-\xi)^2}{4(t-\tau)}\right\}, \quad \tau < t,$$

it was shown that the solution, u, of (46) - (50) could be written as a sum of five integrals involving the functions K, y, φ, g, f, and ψ. If we restrict ourselves to a problem related to (2.8) - (2.12) by setting $y(0) = 0$, $g(t) \equiv 1$, $f(t) \equiv 0$, and $\psi(t) = -y'(t)$, only two integrals remain :

$$(53) \qquad \begin{aligned} u(x,t) &= \int_0^t N(x,t,0,\tau) \cdot g(\tau)\, d\tau \\ &\quad - \int_0^t N(x,t,y(\tau),\tau) \cdot y'(\tau)\, d\tau = I_1 - I_2, \end{aligned}$$

where

$$(54)\qquad \begin{aligned} I_1(x,t) &= \int_0^t N(x,\, t,\, 0,\tau)\, d\tau \\ &= \pi^{-\frac{1}{2}} \int_0^t (t-\tau)^{-\frac{1}{2}} \exp\left\{ \frac{-x^2}{4(t-\tau)} \right\} d\tau . \end{aligned}$$

In particular

$$(55)\qquad I_1(0,t) = 2\pi^{-\frac{1}{2}} t^{\frac{1}{2}}, \qquad t > 0,$$

and since $f = 0$:

$$(56)\qquad I_1(y(t),t) = I_2(y(t),t), \qquad t > 0.$$

Furthermore

$$(57)\qquad I_1(x,t) \leq I_1(0,t), \qquad 0 \leq x < y(t),\ t > 0,$$

and

$$(58)\qquad I_2(x,t) \geq 0, \qquad 0 \leq x < y(t),\ t > 0.$$

From (53), (55), and (58) we deduce

$$(59)\qquad u(0,t) \leq 2\pi^{-\frac{1}{2}} t^{\frac{1}{2}}, \qquad t > 0.$$

In order to get further information about the behaviour of $u(0,t)$ for large t, we shall first prove the following theorem.

9. Theorem. If $y(t)$ is a continuously differentiable function, defined for $t \geq 0$, such that $y(t) \geq 0$, $0 < y'(t) \leq 1$ for $t \geq 0$ and $\lim_{t \to \infty} t^{\alpha} y'(t) = 0$, where $0 \leq \alpha \leq \frac{1}{2}$, then $\lim_{t \to \infty} t^{\alpha - \frac{1}{2}} \cdot I_2(0,t) = 0$, where $I_2(x,t)$ is defined as in (53) using (51) and (52).

Proof: We shall prove, that to any $\varepsilon > 0$ there exists a t^* such that $t^{\alpha-\frac{1}{2}} I_2(0,t) < \varepsilon$ for $t > t^*$. So let $\varepsilon > 0$ be given. According to the assumption there exists a T such that $t^{\alpha} y'(t) < \varepsilon / 2\sqrt{\pi}$ for $t \geq T$. Introduce for convenience $a = (y(T))^2/4$ and consider only $t > T$.

$$(60) \qquad I_2(0,t) = \pi^{-\frac{1}{2}} \int_0^t y'(\tau) \cdot (t-\tau)^{-\frac{1}{2}} \exp\left\{ \frac{-y(\tau)^2}{4(t-\tau)} \right\} d\tau .$$

Divide the interval of integration into two: $[0,T]$ and $[T,t]$ and estimate the integrals:

$$(61) \qquad \begin{aligned} &\pi^{-\frac{1}{2}} \int_0^T y'(\tau) \cdot (t-\tau)^{-\frac{1}{2}} \exp\left\{ \frac{-y(\tau)^2}{4(t-\tau)} \right\} d\tau \\ &\leq \pi^{-\frac{1}{2}} \int_0^T (t-\tau)^{-\frac{1}{2}} d\tau \leq \pi^{-\frac{1}{2}} \cdot T \cdot (t-T)^{-\frac{1}{2}} , \end{aligned}$$

which is less than $\varepsilon/2$ for $t > t' = T + \frac{4}{\pi}\left(\frac{T}{\varepsilon}\right)^2$.

The second integral is estimated using the Beta function:

$$(62) \qquad B(m,n) = \int_0^1 x^{m-1} (1-x)^{n-1} dx = \frac{\Gamma(m) \cdot \Gamma(n)}{\Gamma(m+n)} ,$$

and we get

$$
(63)\quad
\begin{aligned}
&\pi^{-\frac{1}{2}} \int_T^t y'(\tau)\cdot(t-\tau)^{-\frac{1}{2}} \exp\left\{\frac{-y(\tau)^2}{4(t-\tau)}\right\} d\tau \\
&< \frac{\varepsilon}{2\pi} \int_T^t \tau^{-\alpha}(t-\tau)^{-\frac{1}{2}}\, d\tau = \frac{\varepsilon}{2\pi} \int_0^{t-T} (t-x)^{-\alpha} x^{-\frac{1}{2}}\, dx \\
&= \frac{\varepsilon}{2\pi}\, t^{-\alpha-\frac{1}{2}+1} \int_0^{1-T/t} (1-z)^{-\alpha} z^{-\frac{1}{2}}\, dz \\
&\leq \frac{\varepsilon}{2\pi}\cdot t^{\frac{1}{2}-\alpha}\cdot B(\tfrac{1}{2}, 1-\alpha).
\end{aligned}
$$

When α increases from 0 to $\frac{1}{2}$, the value of $B(\frac{1}{2}, 1-\alpha)$ will increase from 2 to π, and we have the bound $\frac{\varepsilon}{2}\cdot t^{\frac{1}{2}-\alpha}$ for this integral. We conclude that

$$
(64)\qquad t^{\alpha-\frac{1}{2}}\cdot I_2(0,t) < \frac{\varepsilon}{2}\cdot t^{\alpha-\frac{1}{2}} + \frac{\varepsilon}{2} \leq \varepsilon
$$

for $t > t^* = \max(t', 1)$.

<u>10. Corollary.</u> If $u(x,t)$ is the solution function for the Stefan problem A, then $\lim_{t\to\infty} t^{-\frac{1}{2}} u(0,t) = 2\pi^{-\frac{1}{2}}$.

<u>Proof:</u> follows from Lemma 8 and Theorem 9 (with $\alpha = 0$) together with equations (53) and (55).

Chapter 5.

The discretization error.

5.1 Expansions in powers of h.

We shall now return to the difference scheme of Douglas and Gallie. In order to study the discretization error connected with this scheme we introduce a function $W = W_h(x,t)$ which depends on the step size h and which by definition coincides with w, the solution function of the difference scheme, on all mesh points $(i \cdot h, t_n)$, $i = 0, 1, \ldots, n$; $n = 0, 1, \ldots$. Similarly we introduce the function $Y = Y_h(t)$ which satisfies $Y(t_n) = n \cdot h$, $n = 0, 1, \ldots$.

From a numerical point-of-view it is very useful to know whether the functions $W_h(x,t)$ and $Y_h(t)$ can be expanded in powers of h, for instance like

(1) $$W = u + h w_1 + h^2 w_2 + O(h^2) ,$$

(2) $$Y = y + h \eta_1 + h^2 \eta_2 + O(h^2) ,$$

where w_1, w_2, η_1, and η_2 are continuous functions, independent of h, with domains of definition identical to those of u and y, and where $O(h^p)$ denotes a function which after division by h^p is bounded as $h \to 0$. Equations (1) and (2) should be satisfied wherever W and Y are defined, i. e. on the mesh points.

A main reason for an analysis of the discretization error along these lines is that a proof of the validity of expansions such as (1) and (2) would imply corollaries of theoretical and practical interest. Firstly, the continuity of the functions involved implies the uniform convergence of the solution of the difference scheme to the solution of the Stefan problem for $h \to 0$ in any bounded region. Secondly Richardson's method of extrapolating to the limit [17] can be applied to the solution of the difference scheme in such a way that we can combine calculations performed with different stepsizes and obtain methods of higher order than the original method.

Suppose that (2) holds with remainder term $h^2 X(t,h)$:

$$Y = y + h\eta_1 + h^2\eta_2 + h^2 X$$

and that we have performed calculations with three values of h: h, h/2, and h/4. Using the formula

$$\bar{Y} = \frac{8}{3}Y_{h/4} - 2Y_{h/2} + \frac{1}{3}Y_h$$

we get

$$\bar{Y} = y + h^2\left\{\frac{1}{6}X(t,\tfrac{h}{4}) - \frac{1}{2}X(t,\tfrac{h}{2}) + \frac{1}{3}X(t,h)\right\}.$$

We can estimate the remainder term, $R = \bar{Y} - y$ either as

$$|R| \leq h^2 \max_I |X(t,.)| , \qquad I = \left[\frac{h}{4}, h\right]$$

or

$$|R| \leq \frac{5}{24} h^3 \max_I \left|\frac{\partial X}{\partial h}\right| , \qquad I = \left[\frac{h}{4}, h\right].$$

Unless the X-function behaves very wildly a considerable improvement is noted as the result of the Richardson extrapolation as compared to say $Y_{h/4}$. A similar result holds for W.

Since the time required for computing W_h and Y_h is proportional to h^{-2}, the time for $Y_{h/4}$ is $16\,h^{-2}$ compared to $21\,h^{-2}$ for acquiring the data for a Richardson extrapolation.

5.2 The equations for w_i and η_i.

In order to obtain information about the functions w_1, w_2, η_1, and η_2 we shall first assume that

$$W = u + h\,w_1 + h^2 w_2 + h^3 w_3 + h^4 w_4 + o(h^4)\,, \tag{3}$$

$$Y = y + h\,\eta_1 + h^2 \eta_2 + h^3 \eta_3 + o(h^3)\,, \tag{4}$$

where (u,y) denotes the solution of Stefan problem A, w_3, w_2, and w_1 are differentiable 1, 2, and 3 times respectively, and η_2 and η_1 are differentiable 1 and 2 times respectively. w_4 and η_3 are continuous and $o(h^p)$ denotes a function which, after division by h^p, tends to 0 as $h \to 0$. Under these assumptions we shall obtain equations for w_1, η_1 and w_2, η_2 and then, using that information, we shall return to the study of (1) and (2).

We shall assume that for each n we attain the limit in equations (3.5) - (3.8), and we shall not use equation (3.8) as it stands, but rather equation (3.9) which in the limit becomes

(5) $$\frac{w_{n-1,n}}{h} = \frac{h}{\Delta t_n} .$$

We shall use the notation

(6) $$W_{in} = W(ih, t_n), \qquad Y_n = Y(t_n),$$

and in cases where functions of one and two variables occur in an expression, such as for instance $y(t)\cdot u(x,t)$ we shall write in short $(y\cdot u)(x,t)$.

As in chapter 4 D shall denote the differentiation operator and partial derivatives are indicated by subscripts 0 and 1.

The equations we must satisfy are thus

(7) $$W_{i+1,n} - 2W_{i,n} + W_{i-1,n} = \frac{h^2}{\Delta t_n}(W_{i,n} - W_{i,n-1}),$$

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

(8) $$W_{o,n} - W_{1,n} = h ,$$

(9) $$W_{n,n} = 0 ,$$

(10) $$W_{n-1,n} = \frac{h^2}{\Delta t_n},$$

(11) $$Y_n = n\cdot h .$$

First note that, since $W_{oo} = w(0,0) = 0$ and $y(0) = 0$, we can take $w_1(0,0) = \eta_1(0) = w_2(0,0) = \eta_2(0) = 0$.

Using Taylor's formula on (3) and (4) we get

$$W_{i\pm1,n} = \Big(u \pm hD_o u + \tfrac{1}{2}h^2 D_o^2 u \pm \tfrac{1}{6}h^3 D_o^3 u + \tfrac{1}{24}h^4 D_o^4 u$$

(12)
$$+ h w_1 \pm h^2 D_o w_1 + \tfrac{1}{2}h^3 D_o^2 w_1 \pm \tfrac{1}{6}h^4 D_o^3 w_1$$
$$+ h^2 w_2 \pm h^3 D_o w_2 + \tfrac{1}{2}h^4 D_o^2 w_2 + h^3 w_3$$
$$\pm h^4 D_o w_3 + h^4 w_4 + o(h^4) \Big)(ih, t_n) ,$$

$$W_{i,n-1} = \Big(u - \Delta t_n D_1 u + \tfrac{1}{2}\Delta t_n^2 D_1^2 u - \tfrac{1}{6}\Delta t_n^3 D_1^3 u + h w_1$$

(13)
$$- h\Delta t_n D_1 w_1 + \tfrac{1}{2}h\Delta t_n^2 D_1^2 w_1 + h^2 w_2$$
$$- h^2 \Delta t_n D_1 w_2 + h^3 w_3 + o(h^3) \Big)(ih, t_n) ,$$

$$Y_{n-1} = \Big(y + h\eta_1 + h^2\eta_2 + h^3\eta_3 - \Delta t_n Dy - h\Delta t_n D\eta_1$$

(14)
$$+ \tfrac{1}{2}h\Delta t_n^2 D^2\eta_1 - h^2\Delta t_n D\eta_2 + \tfrac{1}{2}\Delta t_n^2 D^2 y$$
$$- \tfrac{1}{6}\Delta t_n^3 D^3 y + o(h^3) \Big)(t_n) .$$

We shall furthermore assume that Δt_n can be written on the form

(15) $$\Delta t_n = (c_1 h + c_2 h^2 + c_3 h^3 + o(h^3))(t_n) .$$

Since

(16) $$Y = (y + h\eta_1 + h^2\eta_2 + h^3\eta_3 + o(h^3))(t_n)$$

and $Y_n - Y_{n-1} = h$ we get by combining (14) - (16) and equate terms :

$$(17) \qquad 1 = (c_1 D y)(t_n) ,$$

$$(18) \qquad 0 = (c_2 D y + c_1 D \eta_1 - \tfrac{1}{2} c_1^2 D^2 y)(t_n) ,$$

$$(19) \qquad \begin{aligned} 0 = (& c_3 D y + c_2 D \eta_1 + c_1 D \eta_2 - c_1 c_2 D^2 y \\ & - \tfrac{1}{2} c_1^2 D^2 \eta_1 + \tfrac{1}{6} c_1^3 D^3 y)(t_n) , \end{aligned}$$

and from these equations c_1, c_2, and c_3 can be determined, (if we know η_1 and η_2) knowing that $D y > 0$.

Using (12) we get

$$(20) \qquad \begin{aligned} & \frac{1}{h^2}(W_{i+1,n} - 2 W_{i,n} + W_{i-1,n}) \\ & = (D_o^2 u + h D_o^2 w_1 + \tfrac{1}{12} h^2 D_o^4 u + h^2 D_o^2 w_2 + o(h^2))(ih, t_n) \end{aligned}$$

and using (13) we get

$$(21) \qquad \begin{aligned} \frac{1}{\Delta t_n}(W_{i,n} - W_{i,n-1}) = (& D_1 u - \tfrac{1}{2}\Delta t_n D_1^2 u + \tfrac{1}{6}\Delta t_n^2 D_1^3 u \\ & + h D_1 w_1 - \tfrac{1}{2} h \Delta t_n D_1^2 w_1 + h^2 D_1 w_2 + o(h^2))(ih, t_n) . \end{aligned}$$

Using (7) and (15) and equating terms we get the following relations

$$(22) \qquad 0 = (D_o^2 w_1 + \tfrac{1}{2} c_1 D_1^2 u - D_1 w_1)(ih, t_n) ,$$

$$(23) \qquad \begin{aligned} 0 = (& \tfrac{1}{12} D_o^4 u + D_o^2 w_2 + \tfrac{1}{2} c_2 D_1^2 u - \tfrac{1}{6} c_1^2 D_1^3 u \\ & + \tfrac{1}{2} c_1 D_1^2 w_1 - D_1 w_2)(ih, t_n) . \end{aligned}$$

We shall return to these equations after having treated the boundary conditions.

Equation (8) together with (12) leads to

$$h = W_{o,n} - W_{1,n} = h\cdot(-D_o u - \tfrac{1}{2} h D_o^2 u - \tfrac{1}{6} h^2 D_o^3 u \tag{24}$$
$$- h D_o w_1 - \tfrac{1}{2} h^2 D_o^2 w_1 - h^2 D_o w_2 + o(h^2))(0,t_n) .$$

Equating terms and remembering that $D_o u(0,t) = -1$ we get

$$0 = (\tfrac{1}{2} D_o^2 u + D_o w_1)(0,t_n) , \tag{25}$$

$$0 = (\tfrac{1}{6} D_o^3 u + \tfrac{1}{2} D_o^2 w_1 + D_o w_2)(0,t_n) . \tag{26}$$

The difference between the true boundary point and the one that results from our computations is

$$y_n - Y_n = y(t_n) - n\cdot h \tag{27}$$
$$= (-h\eta_1 - h^2\eta_2 - h^3\eta_3 + o(h^3))(t_n) .$$

Furthermore

$$u(nh,t_n) = (u + (h\eta_1 + h^2\eta_2 + h^3\eta_3)\cdot D_o u \tag{28}$$
$$+ \tfrac{1}{2} (h^2\eta_1^2 + 2h^3\eta_1\eta_2)\cdot D_o^2 u$$
$$+ \tfrac{1}{6} h^3 \eta_1^3 D_o^3 u + o(h^3))(y_n,t_n) .$$

Similar expressions hold for w_1, w_2, and w_3 and we shall use these in

$$0 = W_{n,n} = (u + h w_1 + h^2 w_2 + h^3 w_3 + o(h^3))(nh,t_n) . \tag{29}$$

We equate terms to get

$$(30) \qquad 0 = (w_1 + \eta_1 D_o u)(y_n, t_n) ,$$

$$(31) \qquad 0 = (w_2 + \eta_1 D_o w_1 + \eta_2 D_o u + \tfrac{1}{2}\eta_1^2 D_o^2 u)(y_n, t_n) .$$

<u>Remark.</u> In the derivation of equations (30) - (31) we have implicitly assumed that $n \cdot h \leq y_n$, such that u is defined at the point $(n \cdot h, t_n)$. In order to treat the case $n \cdot h > y_n$, i.e. the computed boundary point is above the true boundary point, we shall assume the function W to be extended between the mesh points as an (at least) three times differentiable function of x and t. Using (27) and (3) we then get

$$0 = W_{n,n} = (W + (Y - y) D_o W + \tfrac{1}{2}(Y - y)^2 D_o^2 W + \tfrac{1}{6}(Y - y)^3 D_o^3 W + o(h^3))(y_n, t_n)$$

$$(32) \qquad = (u + h w_1 + h^2 w_2 + h^3 w_3 + (h\eta_1 + h^2\eta_2)(D_o u + h D_o w_1 + h^2 D_o w_2) + (\tfrac{1}{2}h^2\eta_1^2 + h^3\eta_1\eta_2)(D_o^2 u + h D_o^2 w_1) + \tfrac{1}{6} h^3\eta_1^3 D_o^3 u + o(h^3))(y_n, t_n)$$

which leads to equations (30) - (31).

Finally, from equation (10) and equation (28) applied on W instead of u, we get

$$h^2 = \Delta t_n \cdot (W_{n-1,n} - W_{n,n})$$

$$= \Delta t_n \cdot (- h D_o W + \tfrac{1}{2} h^2 D_o^2 W - \tfrac{1}{6} h^3 D_o^3 W + o(h^3))(nh, t_n)$$

(33)

$$= \Delta t_n \cdot (- h D_o W - h (h \eta_1 + h^2 \eta_2) D_o^2 W - \tfrac{h}{2} h^2 \eta_1^2 D_o^3 W$$

$$+ \tfrac{1}{2} h^2 D_o^2 W + \tfrac{1}{2} h^2 h \eta_1 D_o^3 W - \tfrac{1}{6} h^3 D_o^3 W + o(h^3))(y_n, t_n).$$

Using formula (3) and equating terms we arrive at

$$(34) \qquad 1 = (- c_1 D_o u)(y_n, t_n) ,$$

$$(35) \qquad 0 = (- c_2 D_o u + c_1 \cdot (- D_o w_1 - \eta_1 D_o^2 u + \tfrac{1}{2} D_o^2 u))(y_n, t_n) ,$$

$$0 = (- c_3 D_o u + c_2 \cdot (- D_o w_1 - \eta_1 D_o^2 u + \tfrac{1}{2} D_o^2 u)$$

(36)

$$+ c_1 \cdot (- D_o w_2 - (\eta_1 - \tfrac{1}{2}) D_o^2 w_1 - \eta_2 D_o^2 u$$

$$- \tfrac{1}{2} (\eta_1^2 - \eta_1 + \tfrac{1}{3}) D_o^3 u))(y_n, t_n) .$$

Equation (34) contains no new information, but in (35) and (36) we use (17) - (19) to get, after division by c_1:

$$(37) \qquad D \eta_1 + \eta_1 D_o^2 u + D_o w_1 = \tfrac{1}{2} c_1 D^2 y + \tfrac{1}{2} D_o^2 u \quad \text{at } (y_n, t_n) ,$$

$$D \eta_2 + \eta_2 D_o^2 u + D_o w_2 = c_1 \cdot (\tfrac{1}{2} c_1 D^2 y - D \eta_1) \cdot$$

$$(- D \eta_1 + c_1 D^2 y - D_o w_1 - (\eta_1 - \tfrac{1}{2}) D_o^2 u)$$

(38)

$$+ \tfrac{1}{2} c_1 D^2 \eta_1 - \tfrac{1}{6} c_1^2 D^3 y - (\eta_1 - \tfrac{1}{2}) D_o^2 w_1$$

$$- \tfrac{1}{2} (\eta_1^2 - \eta_1 + \tfrac{1}{3}) D_o^3 u \qquad \text{at } (y_n, t_n) ,$$

The relationships which we have found for y, u, η_1, w_1, η_2, and w_2 hold only at grid points. We shall now, however, impose the extra conditions on the functions η_1, w_1, η_2, and w_2, that the relationships found also be satisfied in regions between the grid points. More precisely, with (u,y) the solution of Stefan problem A, the following are the equations for (w_1,η_1) (see (22), (25), (30), (37)):

(39) $$D_o^2 w_1 - D_1 w_1 = -\tfrac{1}{2} c_1 D_1^2 u, \quad 0 < x < y(t), \; t > 0,$$

(40) $$D_o w_1 = -\tfrac{1}{2} D_o^2 u, \quad x = 0, \quad t > 0,$$

(41) $$w_1 - \eta_1 D y = 0, \quad x = y(t), \; t > 0,$$

(42) $$D\eta_1 + \eta_1 D_o^2 u + D_o w_1 = \tfrac{1}{2}\frac{D^2 y}{Dy} + \tfrac{1}{2} D_o^2 u, \quad x = y(t), \; t > 0,$$

(43) $$w_1(0,0) = \eta_1(0) = 0.$$

η_1 can be eliminated from (42) using (41). We shall now prove a slightly more general result which we shall use several times in the following.

<u>1. Lemma.</u> Let y be a twice continuously differentiable function with $y'(t) > 0$, $t \geq 0$. Let $\eta(t)$ and $w(x,t)$ be continuously differentiable functions satisfying

(44) $$(w - \eta \cdot D y) \circ (y, I) = f,$$

(45) $$(D\eta + \eta \cdot \alpha + D_o w) \circ (y, I) = g,$$

where α, f, and g are continuous functions of t and in addition $\alpha > 0$ and f is continuously differentiable. Then η can be eliminated from (44) - (45) and the resulting equation for w is

$$((\alpha - \frac{D^2y}{Dy})w + 2\,Dy\,D_0 w + D_1 w)\circ(y,I) = g\cdot Dy + f\cdot\alpha + D\,f - f\cdot\frac{D^2y}{Dy}\,. \tag{46}$$

Proof: Differentiation of (44) gives

$$\begin{aligned} D\eta &= D\,\frac{w}{Dy}\circ(y,I) - D\,\frac{f}{Dy} \\ &= (\,D_0\,w + \frac{D_1 w}{Dy} - w\cdot\frac{D^2y}{(Dy)^2}\,)\circ(y,I) - D\,\frac{f}{Dy}\,. \end{aligned} \tag{47}$$

Insert this in (45), use (44), and multiply by Dy to get (46).

Lemma 1 can be used on (41) and (42) by setting $f = 0$, $g = \frac{1}{2}D^2y/Dy + \frac{1}{2}D_0^2\,u(y,I)$, and $\alpha = D_0^2\,u(y,I) = (Dy)^2 > 0$ by formula (26) and Lemma 5 of chapter 4:

$$(\,D_0^2 u - \frac{D^2y}{Dy}\,)\,w_1 + 2\,Dy\,D_0 w_1 + D_1 w_1 = \tfrac{1}{2}D^2y + \tfrac{1}{2}(Dy)^3\,, \quad x = y(t),\ t > 0. \tag{48}$$

Equations (39), (40), (43), and (48) define a boundary value problem (with known boundaries) for w_1. Since a combination of normal and tangential derivatives are present in the boundary condition (48), no general existence and uniqueness theorem for solutions to parabolic equations can be applied directly. We refer to Appendix A for a short discussion of this topic.

For the functions w_2 and η_2 we have a similar set of equations (see (23), (26), (31), (38)) :

$$D_o^2 w_2 - D_1 w_2 = -\frac{1}{12} D_o^4 u - \tfrac{1}{2} c_2 D_1^2 u + \frac{1}{6} c_1^2 D_1^3 u - \tfrac{1}{2} c_1 D_1^2 w_1 , \quad 0 < x < y(t), \ t > 0, \tag{49}$$

$$D_o w_2 = -\frac{1}{6} D_o^3 u - \tfrac{1}{2} D_o^2 w_1 , \quad x = 0, \quad t > 0, \tag{50}$$

$$w_2 - \eta_2 D y = -\eta_1 D_o w_1 - \tfrac{1}{2}\eta_1^2 D_o^2 u, \quad x = y(t), \ t > 0, \tag{51}$$

$$D \eta_2 + \eta_2 D_o^2 u + D_o w_2 = g(t) , \qquad x = y(t), \ t > 0, \tag{52}$$

$$w_2(0,0) = \eta_2(0) = 0 . \tag{53}$$

where c_1 and c_2 are given by (17) and (18), and where $g(t)$, as seen from (38), depends on u, y, w_1, and η_1 and, under the assumption that these are known functions, is a known function of t.

As before it is possible to eliminate η_2 from (51) and (52). Lemma 1 can be used with $\alpha = D_o^2 u(y,I)$ as before, $f = -\eta_1 D_o w_1 - \frac{1}{2}\eta_1^2 D_o^2 u(y,I)$, and g is given by the right hand side of (38).

We thus arrive at a boundary value problem for w_2 which is very similar to the one for w_1. The considerations in Appendix A apply to this problem, also.

5.3 The relation between n and h.

The significance of the independent variables x, t, and h is apparent from the previous sections. However, one extra variable, n, plays an important role. n is not independent of t and h, but coupled by

$$(54) \qquad t_n = t(n,h) = \sum_{k=1}^{n} \Delta t_k(h)$$

such that, for given h, we could choose either t or n as our time variable. Since we want to compare W and Y to u and y respectively it seems natural to keep t as the independent variable.

Formulae (1) and (2) will hold in a certain region of (x,t,h)-space and in order to be useful we should like this region to be of the form

$$0 < h < h_1, \quad 0 < t < t_1, \quad 0 < x < y(t),$$

with $h_1 > 0$ and $t_1 > 0$ and t_1 independent of h.

But when h decreases to zero n must increase like h^{-1} in order to keep t_1 independent of h, for we have from Lemma 7 of Chapter 3

$$(55) \qquad n\cdot h < t_n < n\cdot h + \tfrac{1}{2}(n\cdot h)^2 .$$

We should therefore consider $n\cdot h$ constant as $h \to 0$ in the considerations to follow.

5.4 The stepwise approach.

We shall not go directly to the proof of formula (1) by setting $W = u + h w_1 + h^2 w_2 + V$ and proving that $V = O(h^2)$, but rather divide the proof into three steps. For the first step we define functions $\gamma = \gamma_n$, $V = V_{in} = V(ih,t_n)$, and $X = X_n = X(t_n)$ by the relations

$$\Delta t = \gamma h, \qquad n = 1, 2, \dots;$$
$$W = u + V, \quad x = ih, \ t = t_n, \ n = 0, 1, \dots; \ i = 0, 1, \dots, n;$$
$$Y = y + X, \qquad t = t_n, \ n = 0, 1, \dots;$$

h is the step size in the x-direction, $\Delta t = \Delta t_n$ is the step size in the t-direction at time t_{n-1}, $(u(x,t), y(t))$ denotes the solution of Stefan problem A, and (W,Y) is the solution of the difference scheme (7) - (11).

For the second step of the proof we introduce three similar functions, and because of their profound similarity with the γ, V, and X above, we shall keep the same names, indicating their different origin with an occational superscript (2) which we shall usually omit, though, since it is most likely to be a source of confusion rather than a help.

The equations that define γ, V, and X of the second step are

$$\Delta t = h c_1 + h^2 \gamma, \qquad n = 1, 2, \dots;$$
$$W = u + h w_1 + h V, \qquad n = 0, 1, \dots; \ i = 0, 1, \dots, n;$$
$$Y = y + h \eta_1 + h X, \qquad n = 0, 1, \dots$$

Finally at the third step we are aiming at formulae (1) and (2). Again we introduce three functions γ, V, and X which can be given superscripts (3) to distinguish them from the ones above if there is a fear of confusion. In the next section we shall in a systematic way state the properties of these functions.

5.5 The equations for γ, V, and X.

The functions for each of the three steps are defined by

	Step 1.	Step 2.
(56.a.1-2)	$\Delta t = h\gamma$	$\Delta t = h\,c_1 + h^2\gamma$
(56.b.1-2)	$W = u + V$	$W = u + h\,w_1 + hV$
(56.c.1-2)	$Y = y + X$	$Y = y + h\,\eta_1 + hX$
	Step 3.	
(56.a.3)	$\Delta t = h\,c_1 + h^2 c_2 + h^3\gamma$	
(56.b.3)	$W = u + h\,w_1 + h^2 w_2 + h^2 V$	
(56.c.3)	$Y = y + h\,\eta_1 + h^2\eta_2 + h^2 X$	
(56.a)	$\gamma = \gamma_n$	$n = 1,2,\dots;$
(56.b)	$W = W_{in} = W(ih, t_n)$	$n = 0,1,\dots;\ i = 0,1,\dots,n;$
(56.c)	$Y = Y_n = Y(t_n)$	$n = 0,1,\dots;$

The equations for c_1, c_2, u, w_1, w_2, y, η_1, and η_2 are repeated on the next page for easier reference

	u, y	c_1, w_1, η_1
(57.a. 2)		$c_1 D y = 1$
(57.b.1-2)	$D_o^2 u - D_1 u = 0$	$D_o^2 w_1 - D_1 w_1 = -\frac{1}{2} c_1 D_1^2 u$
(57.c.1-2)	$D_o u = -1$	$D_o w_1 = -\frac{1}{2} D_o^2 u$
(57.d.1-2)	$u = 0$	$w_1 - \eta_1 D y = 0$
(57.e.1-2)	$D y + D_o u = 0$	$D \eta_1 + \eta_1 D_o^2 u + D_o w_1 = \frac{1}{2} c_1 D^2 y + \frac{1}{2} D_o^2 u$
(57.f.1-2)	$y(0) = u(0,0) = 0$	$\eta_1(0) = w_1(0,0) = 0$

	c_2, w_2, η_2
(57.a.3)	$c_2 D y = \frac{1}{2} c_1^2 D^2 y - c_1 D \eta_1$
(57.b.3)	$D_o^2 w_2 - D_1 w_2 = -\frac{1}{12} D_o^4 u - \frac{1}{2} c_2 D_1^2 u + \frac{1}{6} c_1^2 D_1^3 u - \frac{1}{2} c_1 D_1^2 w_1$
(57.c.3)	$D_o w_2 = -\frac{1}{6} D_o^3 u - \frac{1}{2} D_o^2 w_1$
(57.d.3)	$w_2 - \eta_2 D y = -\eta_1 D_o w_1 - \frac{1}{2} \eta_1^2 D_o^2 u$
(57.e.3)	$D_o w_2 + \eta_2 D_o^2 u + D \eta_2 = (-D\eta_1 + c_1 D^2 y - D_o w_1 - (\eta_1 - \frac{1}{2}) D_o^2 u) \cdot$
	$c_1 \cdot (\frac{1}{2} c_1 D^2 y - D\eta_1) + \frac{1}{2} c_1 D^2 \eta_1 - \frac{1}{6} c_1^2 D^3 y$
	$- (\eta_1 - \frac{1}{2}) D_o^2 w_1 - \frac{1}{2}(\eta_1^2 - \eta_1 + \frac{1}{3}) D_o^3 u$
(57.f.3)	$\eta_2(0) = w_2(0,0) = 0$

(57.a)	$t > 0,$
(57.b)	$0 < x < y(t), \quad t > 0,$
(57.c)	$x = 0, \quad t > 0,$
(57.d-e)	$x = y(t), \quad t > 0.$

We shall use equations (7) - (11) to derive the equations to be satisfied by γ, X, and V. First we shall find an equation for X corresponding to step 1 using (56.c.1) and (56.a.1) :

$$h = Y_n - Y_{n-1} = X_n - X_{n-1} + h\,\gamma_n D\,y_\xi \ .$$

The subscript ξ indicates that we shall take the derivative at some intermediate point (between t_{n-1} and t_n). For step 2 we get from (56.c.2) and (56.a.2) :

$$h = Y_n - Y_{n-1} = h\cdot(X_n - X_{n-1}) + (hc_1 + h^2\gamma)\,D\,y$$

$$- \tfrac{1}{2}(hc_1 + h^2\gamma)^2 D^2 y_\xi + h\cdot(hc_1 + h^2\gamma)\,D\,\eta_{1\xi} .$$

Again subscript ξ indicates that the derivative should be taken at some intermediate point, and not necessarily the same point for the two ξ's. $D\,y$ is to be evaluated at $t = t_n$ but since this is rather clear from the context we have not indicated the argument in the formula. Similarly γ should be evaluated at argument n. Note that the formula relates $X^{(2)}$ to $\gamma^{(2)}$.

For step 3 we get in a similar fashion, using (56.c.3) and (56.a.3) :

$$h = Y_n - Y_{n-1} = h^2(X_n - X_{n-1}) + (hc_1 + h^2c_2 + h^3\gamma)\,D\,y$$

$$- \tfrac{1}{2}(\ldots)^2 D^2 y + \tfrac{1}{6}(\ldots)^3 D^3 y_\xi + h(\ldots)\,D\,\eta_1$$

$$- \tfrac{1}{2}(\ldots)^2\, h\, D^2 \eta_{1\xi} + h^2(\ldots)\,D\,\eta_{2\xi} .$$

$(\ldots)$ indicates $(hc_1 + h^2c_2 + h^3\gamma)$ and the earlier remarks about arguments for the functions involved still apply.

For each of the three steps we can now solve for $X_n - X_{n-1}$ using equations (57.a.-) and we give the results in the following table

	$X_n - X_{n-1}$:
(58.1)	$- h\gamma D y_\xi + h$
(58.2)	$- h\gamma D y + \frac{1}{2} h (c_1 + h\gamma)^2 D^2 y_\xi - h (c_1 + h\gamma) D \eta_{1\xi}$
(58.3)	$- h\gamma D y \quad + \frac{1}{2}(E^2 - c_1^2)\, D^2 y - \frac{1}{6} h E^3 D^3 y_\xi$
	$- (E - c_1) D \eta_1 + \frac{1}{2} h E^2 D^2 \eta_{1\xi} - h E D \eta_{2\xi}$

with $E = c_1 + h\, c_2 + h^2\gamma$.

For the following equations we shall just state the results of the computations in tables similar to the one for equations (58.-) remembering that the numbers 1, 2, and 3 indicate the three steps in the process. This way of writing has been chosen, not only because it is compact, but also because it clearly exhibits the close similarity between corresponding equations.

We shall now in turn use equations (7) - (10) :

Step	$0 = (\Delta_x^2 - \Delta_t) W_{i,n}$:
1.	$(\Delta_x^2 - \Delta_t) V_{i,n} + \frac{1}{12} h^2 D_o^4 u_\xi + \frac{1}{2} h\gamma D_1^2 u_\xi$
2.	$h(\Delta_x^2 - \Delta_t) V_{i,n} + \frac{1}{12} h^2 D_o^4 u_\xi + \frac{1}{2} h(c_1 + h\gamma) D_1^2 u$ $- \frac{1}{6} h^2 (c_1 + h\gamma) D_1^3 u_\xi$ $+ h\{D_o^2 w_1 - D_1 w_1 + \frac{1}{12} h^2 D_o^4 w_{1\xi} + \frac{1}{2} h(c_1 + h\gamma) D_1^2 w_{1\xi}\}$
3.	$h^2(\Delta_x^2 - \Delta_t) V_{i,n} + \frac{1}{12} h^2 D_o^4 u + \frac{1}{360} h^4 D_o^6 u_\xi + \frac{1}{2} h E D_1^2 u$ $- \frac{1}{6} h^2 E^2 D_1^3 u + \frac{1}{24} h^3 E^3 D_1^4 u_\xi + h\{D_o^2 w_1 - D_1 w_1$ $+ \frac{1}{12} h^2 D_o^4 w_{1\xi} + \frac{1}{2} h E D_1^2 w_1 - \frac{1}{6} h^2 E^2 D_1^3 w_{1\xi}\}$ $+ h^2\{D_o^2 w_2 - D_1 w_2 + \frac{1}{12} h^2 D_o^4 w_{2\xi} + \frac{1}{2} h E D_1^2 w_{2\xi}\}$

Solving for V gives

	$-(\Delta_x^2 - \Delta_t) V_{i,n}$:
(59.1)	$\frac{1}{2} h\gamma D_1^2 u_\xi + \frac{1}{12} h^2 D_o^4 u_\xi$
(59.2)	$\frac{1}{2} h\gamma D_1^2 u + \frac{1}{12} h D_o^4 u_\xi - \frac{1}{6} h(c_1 + h\gamma) D_1^3 u_\xi$ $+ \frac{1}{2} h(c_1 + h\gamma) D_1^2 w_{1\xi} + \frac{1}{12} h^2 D_o^4 w_{1\xi}$
(59.3)	$\frac{1}{2} h\gamma D_1^2 u - \frac{1}{6}(E^2 - c_1^2) D_1^3 u + \frac{1}{24} h E^3 D_1^4 u_\xi + \frac{1}{12} h D_o^4 w_{1\xi}$ $+ \frac{1}{2}(E - c_1) D_1^2 w_1 - \frac{1}{6} h E^2 D_1^3 w_{1\xi} + \frac{1}{2} h E D_1^2 w_{2\xi}$ $+ \frac{1}{360} h^2 D_o^6 u_\xi + \frac{1}{12} h^2 D_o^4 w_{2\xi}$

Next consider the boundary condition on the t-axis :

Step	$-1 = \frac{1}{h}(W_{1,n} - W_{o,n})$:
1.	$\frac{1}{h}(V_{1,n} - V_{o,n}) + D_o u + \frac{1}{2} h D_o^2 u_\xi$
2.	$(V_{1,n} - V_{o,n}) + D_o u + \frac{1}{2} h D_o^2 u + \frac{1}{6} h^2 D_o^3 u_\xi + h D_o w_1 + \frac{1}{2} h^2 D_o^2 w_{1\xi}$
3.	$h(V_{1,n} - V_{o,n}) + D_o u + \frac{1}{2} h D_o^2 u + \frac{1}{6} h^2 D_o^3 u + \frac{1}{24} h^3 D_o^4 u_\xi$ $+ hD_o w_1 + \frac{1}{2} h^2 D_o^2 w_1 + \frac{1}{6} h^3 D_o^3 w_{1\xi} + h^2 D_o w_2 + \frac{1}{2} h^3 D_o^2 w_{2\xi}$

which gives

	$V_{o,n} - V_{1,n}$:
(60.1)	$\frac{1}{2} h^2 D_o^2 u_\xi$
(60.2)	$\frac{1}{6} h^2 D_o^3 u_\xi + \frac{1}{2} h^2 D_o^2 w_{1\xi}$
(60.3)	$\frac{1}{24} h^2 D_o^4 u_\xi + \frac{1}{6} h^2 D_o^3 w_{1\xi} + \frac{1}{2} h^2 D_o^2 w_{2\xi}$

The boundary condition on the moving boundary leads to

Step	$0 = W_{n,n}$:
1.	$V_{n,n} + X_n D_o u_\xi$
2.	$h V_{n,n} + h(\eta_1 + X) D_o u + \frac{1}{2} h^2 (\eta_1 + X)^2 D_o^2 u_\xi + h w_1$ $+ h(\eta_1 + X) D_o w_{1\xi}$
3.	$h^2 V_{n,n} + h F D_o u + \frac{1}{2} h^2 F^2 D_o^2 u + \frac{1}{6} h^3 F^3 D_o^3 u_\xi + h w_1$ $+ h^2 F D_o w_1 + \frac{1}{2} h^3 F^2 D_o^2 w_{1\xi} + h^2 w_2 + h^3 F D_o w_{2\xi}$

with $F = \eta_1 + h\eta_2 + hX$.

Solve for $V_{n,n}$:

$\underline{- V_{n,n}:}$

(61.1) $$X_n D_o u_\xi$$

(61.2) $$X_n D_o u + \tfrac{1}{2} h (\eta_1 + X)^2 D_o^2 u_\xi + h (\eta_1 + X) D_o w_{1\xi}$$

(61.3) $$X_n D_o u + \tfrac{1}{2} (F^2 - \eta_1^2) D_o^2 u + \tfrac{1}{6} h F^3 D_o^3 u_\xi + (F - \eta_1) D_o w_1 + \tfrac{1}{2} h F^2 D_o^2 w_{1\xi} + h F D_o w_{2\xi}$$

Furthermore we shall note that because of (57.f.-) our approximations are correct at the origin such that we can set

(62) $$X_o = V_{o,o} = 0$$

for all three steps.

5.6 Boundedness of X and V.

An inspection of equations (58.-) - (61.-) reveals common properties of the functions involved which we shall summarize below. Since the functions y, u, η_1, etc. are bounded and have bounded derivatives for t bounded we can state

2. Lemma. There exist bounded functions $f_1, f_2, \ldots, f_7$, where f_3 and f_4 are functions of x and t, the others only of t, and all are bounded for t bounded, such that

(58) $$X_n - X_{n-1} = h(f_1 + \gamma f_2),$$

(59) $$(\Delta_x^2 - \Delta_t) V_{i,n} = h(f_3 + \gamma f_4),$$

(60) $$V_{o,n} - V_{1,n} = h^2 f_5,$$

(61) $$V_{n,n} = X_n f_6 + h f_7,$$

(62) $$X_o = V_{o,o} = 0.$$

3. Lemma. If $\gamma = \gamma_n(x,t,h)$ is bounded in a region Ω of (x,t,h)-space for $n \to \infty$ then the solution functions X and V of (58) - (62) are bounded in $\Omega \cap \{t \leq T\}$ for any finite $T > 0$.

4. Corollary. The functions X and V of step 1 are bounded for t bounded.

Proof: For step 1 we have from formula (48) of chapter 3:

$$\gamma_n = \frac{\Delta t_n}{h} < (1 + h)^n = (1 + \frac{nh}{n})^n < e^{nh}$$

and nh is bounded by $\max\{Y(t)\} = Y(T) < T$ for $t \leq T$.

Proof of Lemma 3: is divided into four parts.

1. A bound for X.

If $\Gamma(n)$ is a bound for $|\gamma_i|$, $i = 1, 2, \ldots, n$ and $F_j(n)$ are corresponding bounds for $|f_j|$, $j = 1, 2, \ldots, 7$ we prove by induction

(63) $$|X_n| \leq n\,h(F_1 + \Gamma F_2)_n \,.$$

The assertion is clearly true for $n = 1$ and assuming that it holds for $n-1$ we get

$$X_n = X_{n-1} + h(f_1 + \gamma f_2)_n \,,$$

$$|X_n| \leq |X_{n-1}| + h(F_1 + \Gamma F_2)_n \leq n\,h(F_1 + \Gamma F_2)_n \,.$$

In order to arrive at a bound for V we shall use the principle of superposition and consider V as a sum of three components, each solving the system (59) - (62) with only one of the right-hand sides non-zero. We shall use superscripts (a) - (c) for these components.

2. $$(\Delta_x^2 - \Delta_t)V_{i,n}^{(a)} = h(f_3 + \gamma f_4)_n \,,$$

$$V_{o,n}^{(a)} - V_{1,n}^{(a)} = 0\,, \quad V_{n,n}^{(a)} = 0\,.$$

For $V^{(a)}$ we shall prove by induction

(64) $$|V_{i,n}^{(a)}| \leq n\,h^2 e^{nh}(F_3 + \Gamma F_4)_n \,.$$

We shall omit the superscript in what follows since we are only looking at $V^{(a)}$ for this part of the proof. First consider $n = 2$. We have $V_{11} = V_{22} = 0$, $V_{o2} = V_{12}$, and equation (59) is thus reduced to

$$-V_{12}\left(\frac{1}{h^2} + \frac{1}{\Delta t_2}\right) = h(f_3 + \gamma f_4)\,,$$

$$|V_{12}| \leq h(F_3 + \Gamma F_4)_2\, h^2 \frac{\Delta t_2}{h^2 + \Delta t_2} \leq 2h^2 e^{2h}(F_3 + \Gamma F_4)_2 \,.$$

Suppose the expression is true for $n-1$ and consider n. Since $V_{nn} = 0$ and $V_{on} = V_{1n}$ the maximum value for $|V_{in}|$ occurs for some i satisfying $1 \leq i \leq n-1$. Without loss of generality we can consider a (positive) maximum for V_{in}. In this case $\Delta_x^2 V_{in} \leq 0$ for this particular i and

$$\max_j V_{jn} = V_{in} \leq V_{i,n-1} + \Delta t_n h(f_3 + \gamma f_4)_n$$

$$\leq n h^2 e^{nh} (F_3 + \Gamma F_4)_n$$

since $\Delta t_n \leq h e^{nh}$.

3. $$V^{(b)}_{o,n} - V^{(b)}_{1,n} = h^2 f_5 ,$$

$$(\Delta_x^2 - \Delta_t) V^{(b)}_{i,n} = 0 , \quad V^{(b)}_{n,n} = 0 .$$

For this component we shall use a modified version of Lemma 2 in [7] which can be stated in the following way: If $(\Delta_x^2 - \Delta_t) w_{i,n} = 0$, $w_{o,n} - w_{1,n} = h$, $w_{n,n} = 0$, then $0 < w_{i,n} - w_{i+1,n} < h$, $i = 1, 2, \ldots, n-1$. In our case we shall replace the h in the second equation with $h^2 f_5$. The proof can still be carried through, word for word, and yields

$$|V^{(b)}_{i,n} - V^{(b)}_{i+1,n}| \leq h^2 F_5 , \qquad i = 0, 1, \ldots, n-1.$$

Using that $V^{(b)}_{n,n} = 0$ we get immediately

$$|V^{(b)}_{o,n}| \leq n h^2 F_5 .$$

Solutions of $(\Delta_x^2 - \Delta_t) V_{i,n} = 0$ satisfy a maximum principle (Theorem 1 in [7]), therefore the maximum value of $|V_{i,n}^{(b)}|$ is taken on the boundary, i.e. for $i = 0$ or $i = n$, and we have therefore

(65) $$|V_{i,n}^{(b)}| \leq n h^2 F_5 , \qquad i = 0, 1, \ldots, n-1.$$

4. $$V_{n,n}^{(c)} = X_n f_6 + h f_7 ,$$

$$(\Delta_x^2 - \Delta_t) V_{i,n}^{(c)} = 0 , \quad V_{o,n}^{(c)} - V_{1,n}^{(c)} = 0 .$$

$V^{(c)}$, too, satisfies a maximum principle, therefore $\max |V_{i,n}^{(c)}|$ is attained for $i = 0$ or $i = n$. But a maximum can not occur for $i = 0$ because from $V_{o,n} > V_{o,n-1}$ together with $V_{o,n-1} = V_{1,n-1}$, $V_{o,n} = V_{1,n}$, and $(\Delta_x^2 - \Delta_t) V_{1,n} = 0$ follows

$$- V_{1,n} + V_{2,n} = \frac{h^2}{\Delta t_n} (V_{1,n} - V_{1,n-1}) > 0$$

such that $V_{o,n}$ is not a maximum. (A similar argument holds for negative minima.) But then we have, using the bound for X from part 1:

(66) $$|V_{i,n}^{(c)}| \leq \max_{j \leq n} |V_{j,j}^{(c)}| \leq (h F_7 + n h (F_1 + \Gamma F_2) F_6)_n .$$

Summarizing the results of parts 2, 3 and 4 we have, for bounded functions F_8 and F_9,

(67) $$|V_{i,n}| \leq n h (F_8 + \Gamma F_9)$$

which together with (63) shows that X and V are bounded.

It is apparent that the estimates (63) and (67) are not the best possible, for from formulae (56.-) we read off the conjecture that V and X (of steps 1 and 2 at least) are O(h) and not just bounded. With the techniques used here it does not seem possible to arrive at better bounds and this is a reason for the failure of our attempts. The estimate for X is crucial here in the sense that if we could somehow prove that X were O(h), then a similar estimate for V would follow from the proof of Lemma 3, the estimates (64) and (65) being good enough already, and (66) being repaired by the better estimate for X.

Another 'missing link' is the transition from step 1 to step 2, and from step 2 to step 3. It is possible that the equation $h^2 = \Delta t_n W_{n-1,n}$ which we have not used in this section might be of value providing starting estimates for $\gamma^{(2)}$ and $\gamma^{(3)}$.

5.7 The heat equation in a rectangular strip.

The techniques which we have used in this chapter were not too succesful on the complicated problem of a moving boundary. For simpler problems, however, our method yields good results which we shall demonstrate now.

Consider the heat equation in a (semi-infinite) rectangular region of width 1.

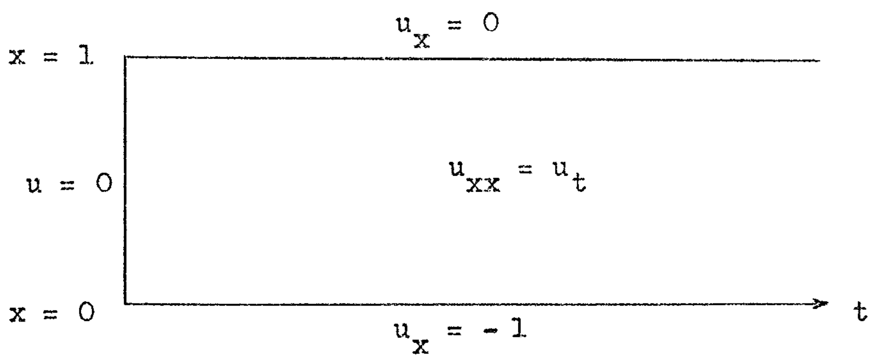

Fig. 3.

(68.a) $$D_o^2 u(x,t) = D_1 u(x,t) , \qquad 0 < x < 1,\ t > 0,$$

(68.b) $$u(x,0) = 0 , \qquad 0 < x < 1,$$

(68.c) $$D_o u(0,t) = -1 , \qquad t > 0,$$

(68.d) $$D_o u(1,t) = 0 , \qquad t > 0.$$

We shall use an implicit difference scheme similar to the one of chapter 3, and furthermore we shall choose $\Delta t = \Delta x = h = \frac{1}{p}$ where p is a positive integer, such that p steps in the x-direction will take us from 0 to 1.

The difference equations are

(69.a) $$(\Delta_x^2 - \Delta_t) W_{i,n} = 0, \qquad i = 1,2,\ldots, p-1;\ n = 1,2,\ldots$$

(69.b) $$W_{i,o} = 0, \qquad i = 0,1,\ldots, p;$$

(69.c) $$W_{o,n} - W_{1,n} = h, \qquad n = 1,2,\ldots$$

(69.d) $$W_{p,n} - W_{p-1,n} = 0, \qquad n = 1,2,\ldots$$

Assume the existence of an expansion similar to (3) :

$$(70) \qquad W = u + h\,w_1 + h^2 w_2 + h^3 w_3 + h^4 w_4 + o(h^4)$$

where w_3, w_2, and w_1 are differentiable 1, 2, and 3 times respectively and w_4 is continuous.

Application of equations (69.-) leads to the following equations for w_1 and w_2 :

$$(71.a) \qquad (D_o^2 - D_1)\,w_1 = \tfrac{1}{2} D_1^2 u\,, \qquad 0 < x < 1,\ t > 0,$$

$$(71.b) \qquad w_1 = 0\,, \qquad 0 < x < 1,$$

$$(71.c) \qquad D_o w_1 = -\tfrac{1}{2} D_o^2 u\,, \qquad x = 0,\ t > 0,$$

$$(71.d) \qquad D_o w_1 = \tfrac{1}{2} D_o^2 u\,, \qquad x = 1,\ t > 0,$$

$$(72.a) \qquad (D_o^2 - D_1)\,w_2 = -(\tfrac{1}{2}D_o^4 + D_1^3)\,\frac{u}{6} + \tfrac{1}{2} D_1^2 w_1, \quad 0 < x < 1,\ t > 0,$$

$$(72.b) \qquad w_2 = 0\,, \qquad 0 < x < 1,$$

$$(72.c) \qquad D_o w_2 = -\tfrac{1}{2} D_o^2 w_1 - \frac{1}{6} D_o^3 u\,, \qquad x = 0,\ t > 0,$$

$$(72.d) \qquad D_o w_2 = \tfrac{1}{2} D_o^2 w_1 - \frac{1}{6} D_o^3 u\,, \qquad x = 1,\ t > 0.$$

The derivation of these equations follows exactly the same lines as described in section 5.2 and we shall not go into the details.

Now define the function V by the following identity

$$(73) \qquad W = u + h\,w_1 + h^2 w_2 + h^2 V$$

where w_1 and w_2 satisfy (71.-) and (72.-) respectively.

In a similar way as in section 5.5 it is shown that V satisfies the difference equations :

(74.a) $$(\Delta_x^2 - \Delta_t) V_{i,n} = h f_1, \quad i = 1,2,..,p-1; \; n = 1,2, \,..$$

(74.b) $$V_{i,o} = 0, \quad i = 0,1,.., p;$$

(74.c) $$V_{o,n} - V_{1,n} = h^2 f_2, \quad n = 1,2, \,..$$

(74.d) $$V_{p,n} - V_{p-1,n} = h^2 f_3, \quad n = 1,2, \,..$$

where the functions f_1, f_2, and f_3 are bounded for t bounded.

<u>5. Theorem.</u> If V satisfies equations (74.-) then V is bounded as $h \to 0$ for $t \leq T$.

<u>Proof:</u> The proof is divided into three parts. We shall use the principle of superposition and consider V as a sum of three components, each solving the system (74.-) with only one of the right-hand sides non-zero. We shall use superscripts (a) - (d) for these components.

1. $$(\Delta_x^2 - \Delta_t) V_{i,n}^{(a)} = h f_1,$$

$$V_{o,n}^{(a)} - V_{1,n}^{(a)} = V_{p,n}^{(a)} - V_{p-1,n}^{(a)} = 0 .$$

A positive maximum for $V_{i,n}^{(a)}$ (n fixed) corresponds to

$$\Delta_x^2 V_{i,n}^{(a)} \leq 0 \iff \frac{V_{i,n}^{(a)} - V_{i,n-1}^{(a)}}{h} + h f_1 \leq 0$$

$$\Rightarrow V_{i,n}^{(a)} \leq V_{i,n-1}^{(a)} - h^2 f_1 \Rightarrow V_{i,n}^{(a)} \leq h \cdot nh \cdot F_1$$

where F_1 is a bound for $|(f_1)_i|$ for $i = 1,2, \ldots, n$.

2. $$V^{(c)}_{o,n} - V^{(c)}_{1,n} = h^2 f_2 ,$$

$$(\Delta_x^2 - \Delta_t) V^{(c)}_{i,n} = 0, \quad V^{(c)}_{p,n} - V^{(c)}_{p-1,n} = 0 .$$

Define

$$m_{i,n} = \frac{V^{(c)}_{i,n} - V^{(c)}_{i+1,n}}{h}, \qquad i = 0,1, \ldots, p-1$$

Since $(\Delta_x^2 - \Delta_t) m_{i,n} = 0$ we have a maximum principle for $m_{i,n}$ and from $m_{o,n} = h f_2$, $m_{p-1,n} = 0$ we have $|m_{i,n}| \leq h \cdot F_2$ where F_2 is a bound for $|(f_2)_i|$, $i = 1, 2, \ldots, n$. Now

$$V^{(c)}_{i,n} = V^{(c)}_{i,n-1} + h \Delta_x^2 V^{(c)}_{i,n}$$

$$\Longrightarrow \quad |V^{(c)}_{i,n}| \leq |V^{(c)}_{i,n-1}| + h \cdot 2 F_2$$

$$\Longrightarrow \quad |V^{(c)}_{i,n}| \leq n \cdot h \cdot 2 F_2 .$$

3. Identical to Part 2.

Conclusion: $\quad |V(x,t,h)| \leq t \cdot F(t)$,

where F is a bounded function.

Chapter 6.

The Chebyshev-series method of A. Wragg.

6.1 Definition of the method.

Besides the Douglas-Gallie scheme several other numerical methods have been devised for the approximate solution of the Stefan problem. We shall study one of these: The Chebyshev-series method of A. Wragg [23] and perform an analysis of this method similar to what we did for the Douglas-Gallie method.

We shall now outline the numerical method. We refer to [23] for further details.

Notation. Let $k = \Delta t$ be the step size in the t-direction, and assume that $U_o(x)$ and $U_1(x)$ are approximations to $u(x,t_o)$ and $u(x,t_1)$ where $t_1 = t_o + k$. Furthermore let (x_o,t_o) and (x_1,t_1) denote points on the computed boundary curve, i.e. x_o and x_1 are approximations to $y(t_o)$ and $y(t_1)$, respectively.
Discretization of equations (8) - (11) of chapter 2 now yields

(1) $$D^2U_1(x) - \frac{1}{k}(U_1(x) - U_o(x)) = 0 ,$$

(2) $$D\,U_1(0) = -1 ,$$

(3) $$U_1(x_1) = 0 ,$$

(4) $$D\,U_o(x_o) = -\frac{x_1 - x_o}{k} .$$

Instead of (4) a symmetric formula might be suggested:

(4a) $$\tfrac{1}{2}\{DU_o(x_o) + DU_1(x_1)\} = -\frac{x_1 - x_o}{k}.$$

One would expect a smaller truncation error when using (4a) instead of (4), the price for this being more complicated equations for x_1 and $U_1(x)$. We shall, however, not pursue this matter.

We shall assume that x_o and $U_o(x)$ are known and that $U_o(x)$ is a polynomial of the form

(5) $$U_o(x) = \sum_{m=0}^{n+1} a_m \left(\frac{x}{x_o}\right)^m .$$

In order to obtain a similar expression for $U_1(x)$:

(6) $$U_1(x) = \sum_{m=0}^{n+1} b_m \left(\frac{x}{x_1}\right)^m .$$

we shall replace (1) by the perturbed equation

(7) $$D^2 U_1(x) - \frac{1}{k}(U_1(x) - U_o(x)) = \tau_1' T_n^*\left(\frac{x}{x_1}\right) + \tau_2' T_{n+1}^*\left(\frac{x}{x_1}\right),$$

where T_n^* denotes the n-th Chebyshev polynomial of the first kind over the interval [0,1].

Equations (4) and (2) now give, using (5) and (6):

(8) $$x_1 = x_o - \frac{k}{x_o}\sum_{m=1}^{n+1} m\, a_m ; \qquad b_1 = -x_1 ;$$

and (7) and (3) now lead to a system of $n+3$ linear equations for $b_o, b_2, b_3, \ldots, b_{n+1}, \tau_1', \tau_2'$. We refer to [23] for the exact form of these equations which we shall not use here, since our further investigations are based directly on equations (2), (3), (4), and (7).

As mentioned by Wragg this numerical method might not be optimal near the origin, and therefore a special starting procedure might be useful for obtaining values up to a certain time T_o.

6.2 The discretization error.

We shall study the discretization error, connected with the numerical scheme outlined above, in a similar way as we did in chapter 5 for the Douglas-Gallie scheme. First let us introduce $W = W_k(x,t)$ as a function of k, x, and t, which coincides with $U_o(x)$ on each meshline $t = t_o = T_o + ik$,

$$(9) \qquad W(x, ik) = \sum_{j=0}^{n+1} c_j^{(i)} T_j^*\left(\frac{x}{x_i}\right), \qquad i = 0, 1, 2, \ldots$$

where $c_j^{(i)}$ denote the coefficients of the expansion (5) rewritten in terms of T_j^*, and x_i is the corresponding calculated boundary point, which was called x_o in (5). Similarly introduce $Y = Y_k(t)$ as a function of k and t, such that

$$(10) \qquad Y(i \cdot k) = x_i, \qquad i = 0, 1, 2, \ldots$$

The use of a special starting procedure up to time $t = T_o$ leads to an assignment of values for W and Y:

$$Y(T_o) = Y^*, \quad W(x,T_o) = \varphi(x), \qquad 0 < x < Y^*.$$

Considering formulae (11) and (12) below it appears to be desirable to let the starting procedure depend in some way of the chosen step size k. These considerations are somewhat similar to the ones put forward in [4] for an ordinary differential equation. To make the following analysis simpler we shall, however, from now on assume $T_o = 0$ and $W(0,0) = Y(0) = 0$.

Proceeding as in chapter 5 we shall now assume that W and Y can be expanded in terms of k:

$$(11) \qquad W = u + k w_1 + k^2 w_2 + k^3 w_3 + o(k^3) ,$$

$$(12) \qquad Y = y + k \eta_1 + k^2 \eta_2 + o(k^2) ,$$

where (u,y) is the solution of Stefan problem A, and where w_1, w_2, and w_3 are twice differentiable, η_1 is differentiable, and η_2 is continuous.

Remark. The functions W, Y, w_1, w_2, w_3, η_1, and η_2 are different from the ones of chapter 5.

The coefficients of the perturbation term in (7), τ_1' and τ_2' are now functions of t and k and we shall assume that they also can be expanded in powers of k:

$$(13) \qquad \tau_1' = \tau_1 + k \tau_3 + k^2 \tau_5 + o(k^2) ,$$

$$(14) \qquad \tau_2' = \tau_2 + k \tau_4 + k^2 \tau_6 + o(k^2) .$$

Now, let $t_o = i \cdot k$, $t_1 = (i+1) \cdot k$, and use equations (11) - (14) in (7):

$$\frac{U_1(x) - U_o(x)}{k} = \frac{W(x,t_1) - W(x,t_1-k)}{k} =$$

(15) $$(D_1 u + k (D_1 w_1 - \tfrac{1}{2} D_1^2 u) + k^2 (D_1 w_2 - \tfrac{1}{2} D_1^2 w_1 + \tfrac{1}{6} D_1^3 u) + o(k^2))(x,t_1) ,$$

(16) $$D^2 U_1(x) = D_o^2 W(x,t_1) = (D_o^2 u + k D_o^2 w_1 + k^2 D_o^2 w_2 + o(k^2)) (x,t_1) .$$

The perturbation term on the right hand side of (7) now becomes

(17) $$(\tau_1 + k\,\tau_3 + k^2 \tau_5)(t_1)\cdot T_n^*\left(\frac{x}{Y(t_1)}\right) + (\tau_2 + k\,\tau_4 + k^2 \tau_6)(t_1)\cdot T_{n+1}^*\left(\frac{x}{Y(t_1)}\right) + o(k^2) .$$

Combining (15), (16), and (17) and equating terms we get

(18) $$0 = (D_o^2 u - D_1 u)(x,t_1) = \tau_1(t_1)\, T_n^* + \tau_2(t_1)\, T_{n+1}^* ,$$

(19) $$(D_o^2 w_1 - D_1 w_1 + \tfrac{1}{2} D_1^2 u) (x,t_1) = \tau_3(t_1)\, T_n^* + \tau_4(t_1)\, T_{n+1}^* ,$$

(20) $$(D_o^2 w_2 - D_1 w_2 + \tfrac{1}{2} D_1^2 w_1 - \tfrac{1}{6} D_1^3 u)(x,t_1) = \tau_5\, T_n^* + \tau_6\, T_{n+1}^* ,$$

where we have omitted the argument $\left(\frac{x}{Y(t_1)}\right)$ of T_n^* and T_{n+1}^*.

Equation (18) gives $\tau_1 = \tau_2 = 0$.

Using (2) we get

(21) $$-1 = D\, U_1(0) = D_o W(0,t_1) = (D_o u + k D_o w_1 + k^2 D_o w_2 + o(k^2)) (0,t_1)$$

which yields

$$D_o w_1(0,t_1) = 0\,, \qquad D_o w_2(0,t_1) = 0\,. \tag{22}$$

In order to apply (3) we first note that

$$\begin{aligned} x_{i+1} - y((i+1)\cdot k) &= (Y - y)(t_1) = \\ &(k\eta_1 + k^2\eta_2 + o(k^2))(t_1)\,, \end{aligned} \tag{23}$$

and we now have

$$\begin{aligned} 0 &= W(x_{i+1}, (i+1)\cdot k) = \\ &(u + k w_1 + k^2 w_2 + o(k^2))(x_{i+1}, (i+1)\cdot k) = \\ &(u + (k\eta_1 + k^2\eta_2) D_o u + \tfrac{1}{2}k^2\eta_1^2 D_o^2 u + k w_1 \\ &\quad + k^2\eta_1 D_o w_1 + k^2 w_2 + o(k^2))(y(t_1),t_1)\,, \end{aligned} \tag{24}$$

which gives

$$0 = (\eta_1 D_o u + w_1)(y(t_1),t_1)\,, \tag{25}$$

$$0 = (\eta_2 D_o u + \tfrac{1}{2}\eta_1^2 D_o^2 u + \eta_1 D_o w_1 + w_2)(y(t_1),t_1)\,. \tag{26}$$

<u>Remark.</u> The derivation in (24) is valid only when $x_{i+1} \leq y(t_1)$, i.e. when the calculated boundary point lies on or below the true boundary curve. If, however, W is assumed twice differentiable, then we have

$$\begin{aligned} 0 = W(x_{i+1}, (i+1)\cdot k) &= (W + (k\eta_1 + k^2\eta_2) D_o W \\ &\quad + \tfrac{1}{2}k^2\eta_1^2 D_o^2 W + o(k^2))(y(t_1),t_1)\,. \end{aligned} \tag{24a}$$

Using (11) and equating terms we again arrive at equations (25) and (26) showing that these equations hold also when the calculated boundary lies above the true boundary.

Finally we shall consider equation (4) :

(27) $$\frac{x_1 - x_o}{k} = \frac{Y(t_o + k) - Y(t_o)}{k} = (Dy + k D\eta_1 + k^2 D\eta_2 + \tfrac{1}{2} k D^2 y + \tfrac{1}{2} k^2 D^2 \eta_1 + \tfrac{1}{6} k^2 D^3 y + o(k^2)) (t_o) ,$$

(28) $$D U_o(x_o) = D_o W(x_i, t_o) = (D_o u + (k\eta_1 + k^2\eta_2) D_o^2 u + \tfrac{1}{2} k^2 \eta_1^2 D_o^3 u + k D_o w_1 + k^2 \eta_1 D_o^2 w_1 + k^2 D_o w_2 + o(k^2)) (y(t_o), t_o) .$$

Combination of (27) and (28) using (4) yields

(29) $$0 = (D\eta_1 + \tfrac{1}{2} D^2 y + \eta_1 D_o^2 u + D_o w_1) (y(t_o), t_o) ,$$

(30) $$0 = (D\eta_2 + \tfrac{1}{2} D^2 \eta_1 + \tfrac{1}{6} D^3 y + \eta_2 D_o^2 u + \tfrac{1}{2} \eta_1^2 D_o^3 u + \eta_1 D_o^2 w_1 + D_o w_2) (y(t_o), t_o) .$$

According to the derivation the equations (19), (22), (25), and (29) are to be satisfied by (w_1, η_1) for $t = i \cdot k$, $i = 0, 1, 2, \ldots$; $0 < x < Y(t)$. We shall now impose the extra condition that they be satisfied for all $t > 0$, and at the same time we shall adjust the x-intervals to coincide with those for $u(x,t)$. In other words, given $u(x,t)$, $y(t)$, $\tau_3(t)$, and $\tau_4(t)$ we now define $w_1(x,t)$ and $\eta_1(t)$ by

$$D_o^2 w_1 - D_1 w_1 = -\tfrac{1}{2} D_1^2 u + \tau_3 T_n^*\left(\frac{x}{Y(t)}\right) + \tau_4 T_{n+1}^*\left(\frac{x}{Y(t)}\right), \tag{31}$$
$$0 < x < y(t),\ t > 0,$$

$$D_o w_1 = 0, \qquad x = 0, \quad t > 0, \tag{32}$$

$$w_1 - \eta_1 D y = 0, \qquad x = y(t),\ t > 0, \tag{33}$$

$$D\eta_1 + \eta_1 D_o^2 u + D_o w_1 = -\tfrac{1}{2} D^2 y, \qquad x = y(t),\ t > 0, \tag{34}$$

$$\eta_1(0) = w_1(0,0) = 0. \tag{35}$$

η_1 can be eliminated using (33) and (34), a result that follows directly from Lemma 1 of chapter 5. With $\alpha = D_o^2 u(y,I)$, $f = 0$, and $g = -\frac{1}{2} D^2 y$ we get

$$\left(\left(D_o^2 u - \frac{D^2 y}{Dy}\right) w_1 + 2\,Dy\,D_o w_1 + D_1 w_1\right)(y(t),t) = -\tfrac{1}{2}\,Dy\,D^2 y(t). \tag{36}$$

Equations (31), (32), (35), and (36) now define a boundary value problem for w_1. We refer to Appendix A for a discussion of existence and uniqueness of solutions to boundary value problems of this type where a combination of normal and tangential derivatives occur in the boundary condition.

Once w_1 is determined η_1 is easily found from equation (33).

It can be mentioned in passing that the effect of using (4a) instead of (4) is that the term containing $D^2 y$ disappears from the right hand sides of equations (34) and (36).

Based on equations (20), (22), (26), and (30) we shall now in a perfectly similar way define $w_2(x,t)$ and $\eta_2(t)$ by

$$D_o^2 w_2 - D_1 w_2 = \tfrac{1}{6} D_1^3 u - \tfrac{1}{2} D_1^2 w_1 + \tau_5 T_n^* + \tau_6 T_{n+1}^* ,$$

(37)

$$0 < x < y(t), \; t > 0,$$

(38) $$D_o w_2 = 0 , \qquad x = 0, \quad t > 0,$$

(39) $$w_2 - \eta_2 D y = -\tfrac{1}{2} \eta_1^2 D_o^2 u - \eta_1 D_o w_1 , \qquad x = y(t), \; t > 0,$$

$$D \eta_2 + \eta_2 D_o^2 u + D_o w_2 = -\tfrac{1}{2} D^2 \eta_1 - \tfrac{1}{2} \eta_1^2 D_o^3 u - \eta_1 D_o^2 w_1 - \tfrac{1}{6} D^3 y$$

(40)

$$x = y(t), \; t > 0,$$

(41) $$\eta_2(0) = w_2(0,0) = 0 .$$

Also here η_2 can be eliminated by Lemma 1 of chapter 5 and we can get a boundary value problem for w_2 similar to the one above and thereafter determine η_2 by means of (39).

6.3 The equations for V and X.

Now, with (u,y) given as the solution of Stefan problem A, with (W, Y, τ_1', τ_2') given as solutions to (2) - (4), (7), interpreted by means of (9) and (10) and extended between meshlines (resp. meshpoints) as twice differentiable functions of x and t, and with $(w_1, \eta_1, w_2, \eta_2)$ defined as the solutions to (31) - (41) we shall now define functions $V = V_k(x,t)$ and $X = X_k(t)$ by

(42) $$W = u + k w_1 + k^2 w_2 + k^2 V ,$$

(43) $$Y = y + k \eta_1 + k^2 \eta_2 + k^2 X .$$

The perturbation term of (7) causes considerable complications in the analysis so we shall for the moment assume that it is absent.

Let $t = i \cdot k$ for some i, and $0 < x < y(t)$:

(44) $$D_0^2 W = D_0^2 u + k D_0^2 w_1 + k^2 (D_0^2 w_2 + D_0^2 V) ,$$

(45) $$\begin{aligned} \frac{W(x,t) - W(x,t-k)}{k} = & (D_1 u + k (D_1 w_1 - \tfrac{1}{2} D_1^2 u) \\ & + k^2 (D_1 w_2 - \tfrac{1}{2} D_1^2 w_1 + \tfrac{1}{6} D_1^3 u) \\ & + k^3 (\tfrac{-1}{24} D_1^4 u_\xi + \tfrac{1}{6} D_1^3 w_{1\xi} - \tfrac{1}{2} D_1^2 w_{2\xi})) (x,t) \\ & + k (V(x,t) - V(x,t-k)) . \end{aligned}$$

Subtraction yields

(46) $$D_0^2 V(x,t) - \frac{V(x,t) - V(x,t-k)}{k} = O(k) ,$$

where we have used (31) and (37) and discarded the perturbation term.

Differentiating (42) with respect to x, setting $x = 0$, and using (2), (32), and (38) gives

(47) $$D_0 V(0,t) = 0 .$$

Now, setting $x = x_1 = Y(t)$:

$$0 = W(x_1,t) = k^2 V(x_1,t) + (u + kF D_o u + \tfrac{1}{2}k^2F^2 D_o^2 u$$

$$(48) \qquad + k w_1 + k^2 F D_o w_1 + k^2 w_2)(y(t),t)$$

$$+ k^3 (\tfrac{1}{6}F^3 D_o^3 u_\xi + \tfrac{1}{2}F^2 D_o^2 w_{1\xi} + F D_o w_{2\xi})$$

with $F = \eta_1 + k\eta_2 + kX$.

Formula (48) holds whether the true boundary is above or below the computed boundary.

Using (33) and (39) we get

$$-V(x_1,t) = (X D_o u + \tfrac{1}{2}(F^2 - \eta_1^2) D_o^2 u + (F - \eta_1) D_o w_1)(y(t),t)$$

$$(49) \qquad + k(\tfrac{1}{6}F^3 D_o^3 u_\xi + \tfrac{1}{2}F^2 D_o^2 w_{1\xi} + F D_o w_{2\xi}) .$$

Finally we shall use equation (4) and therefore compute

$$\frac{Y(t+k) - Y(t)}{k} = k(X(t+k) - X(t)) + (Dy + kD\eta_1$$

$$(50) \qquad + k^2 D\eta_2 + \tfrac{1}{2}kD^2y + \tfrac{1}{2}k^2D^2\eta_1 + \tfrac{1}{6}k^2D^3y)(t)$$

$$+ k^3(\tfrac{1}{24}D^4 y_\xi + \tfrac{1}{6}D^3\eta_{1\xi} + \tfrac{1}{2}D^2\eta_{2\xi}) ,$$

$$D_o W(Y(t),t) = k^2 D_o V(Y(t),t) + (D_o u + kF D_o^2 u + k D_o w_1$$

$$(51) \qquad + \tfrac{1}{2}k^2F^2 D_o^3 u + k^2 F D_o^2 w_1 + k^2 D_o w_2)(y(t),t)$$

$$+ k^3(\tfrac{1}{6}F^3 D_o^4 u_\xi + \tfrac{1}{2}F^2 D_o^3 w_{1\xi} + F D_o^2 w_{2\xi}) .$$

Combination and use of equations (34) and (40) gives

$$-D_o V(Y(t),t) - \frac{X(t+k) - X(t)}{k} =$$

(52) $$(X D_o^2 u + \tfrac{1}{2}(F^2 - \eta_1^2) D_o^3 u + (F - \eta_1) D_o^2 w_1)(y(t),t)$$
$$+ k(\tfrac{1}{6}F^3 D_o^4 u_{\xi} + \tfrac{1}{2}F^2 D_o^3 w_{1\xi} + F D_o^2 w_{2\xi}) + O(k) .$$

Finally we have from (35) and (41) that

(53) $$V(0,0) = X(0) = 0 .$$

The equations for V and X here are considerably more complicated than the similar ones in chapter 5. It is not clear whether we can prove boundedness of V and X as $h \to 0$, from equations (46), (47), (49), (52), and (53). Furthermore we must remember that these equations correspond to the simpler problem where the perturbation term of (7) is set equal to 0.

Appendix A.

On a special boundary value problem.

In chapters 5 and 6 we have encountered parabolic problems that are not covered by general existence and uniqueness theorems because of a special type of boundary condition (see (1.c) below). We shall in the following give a uniqueness proof for solutions to a certain class of such problems.

Consider a parabolic boundary value problem of the form

$$(1.a) \qquad (w_{xx} - w_t)(x,t) = f(x,t), \quad 0 < x < y(t), \quad t > 0,$$

$$(1.b) \qquad w_x(0,t) = -g(t), \qquad t > 0,$$

$$(1.c) \qquad (a\,w + b\,w_x + c\,w_t)(y(t),t) = d(t), \qquad t > 0,$$

$$(1.d) \qquad w(0,0) = 0,$$

where a, b, and c are positive functions of t, and y satisfies

$$(2) \qquad y(0) = 0, \quad y(t) > 0, \qquad t > 0,$$

$$(3) \qquad y'(0) = 1, \quad y'(t) > 0, \qquad t > 0,$$

and furthermore

$$(4) \qquad b(t) > y'(t)\cdot c(t), \qquad t \geq 0.$$

Suppose w_1 and w_2 are two functions satisfying (1.-). Then $w = w_1 - w_2$ satisfies

$$(5.a) \qquad (w_{xx} - w_t)(x,t) = 0, \quad 0 < x < y(t), \quad t > 0,$$

$$(5.b) \qquad w_x(0,t) = 0, \qquad t > 0,$$

$$(5.c) \qquad (a\,w + b\,w_x + c\,w_t)(y(t),t) = 0, \qquad t > 0,$$

$$(5.d) \qquad w(0,0) = 0 .$$

The function $w = 0$ is a solution of (5.-). We want to prove, by contradiction, that no other solution exists.

So assume that w solves (5.-) and that $\exists (x_o,t_o)$ such that $w(x_o,t_o) > 0$. (The case $w(x_o,t_o) < 0$ can be treated in a similar way.)

Because of the maximum principle and of the condition (5.b) a maximum must be attained on the upper boundary, i.e.

$$\exists t_1 > 0 \quad \text{such that} \quad w(y(t_1),t_1) > 0 .$$

Let t_1 be chosen such that $0 < t_1 \le t_o$ and

$$\max_{[0,t_o]} \{w(y(t),t)\} = w(y(t_1),t_1) .$$

At the point $(y(t_1),t_1)$ we must have either $w_x < 0$ or $w_t < 0$ because of (5.c).

<u>1.</u> But $w_x(y(t_1),t_1) < 0$ implies

$$w(y(t_1) - \delta, t_1) > w(y(t_1), t_1)$$

for δ positive and sufficiently small, contradicting the maximum principle.

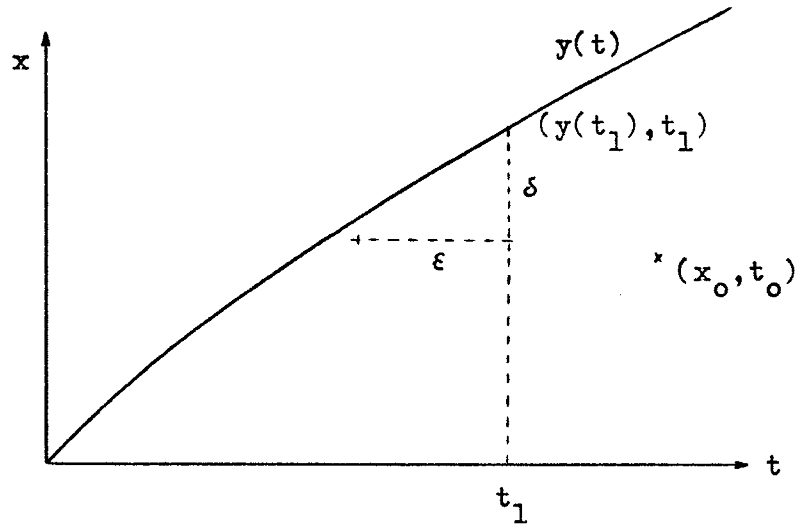

Fig. 4.

2. Now, assume $w_t(y(t_1),t_1) < 0$. Let $\varepsilon, \delta > 0$ such that

(6) $$0 < y(t_1) - \delta < y(t_1 - \varepsilon).$$

$$w(\,y(t_1) - \delta,\ t_1 - \varepsilon\,) - w(\,y(t_1),\ t_1\,)$$

(7)
$$= (-\varepsilon w_t - \delta w_x)(y(t_1),t_1) + \text{second order terms}$$

$$\doteq (-\varepsilon w_t + \frac{\delta}{b}(\,a w + c w_t\,)(y(t_1),t_1)$$

$$=(\delta \frac{a}{b} w - (\,\varepsilon - \delta \frac{c}{b}\,) w_t\,)(y(t_1),t_1)\,.$$

If δ and ε are sufficiently small and satisfy

(8) $$\varepsilon > \delta \frac{c}{b}$$

then (7) will be positive which is another contradiction. Now the condition (6) is identical to

(9) $$\delta > y(t_1) - y(t_1 - \varepsilon) = \varepsilon \cdot y'(t_1) - \tfrac{1}{2}\varepsilon^2 y''(\tau)$$

and (8) and (9) can be satisfied at the same time, provided

$$\varepsilon \cdot y'(t_1) < \varepsilon \cdot \frac{b}{c}$$

which is the condition (4).

In chapters 5 and 6 we had

$$a = u_{xx}(y, I) - \frac{y''}{y'} ,$$

$$b = 2y' ,$$

$$c = 1 ,$$

such that $\frac{b}{c} = 2y' > y' \quad (t > 0)$.

Furthermore, by (4.26)

$$a = z^2 - \frac{Dz}{z} > 0 \iff Dz < z^3 .$$

But from (3.44) $\Delta t_i < \Delta t_{i+1}$, $i = 1, 2, \ldots$ which implies that the boundary function, $y(t)$, has a non-positive second derivative, and since $z = D y > 0$ we therefore have $a > 0$.

The question of existence of solutions to the system (1.-) is open at the moment. We shall at this point only suggest a few techniques that might be used in the search for an existence proof:

1. A convergence proof for the solution of an approximating

difference scheme may imply existence of solutions to the original problem.

2. An a priori estimate for a problem together with duality theorems for Hilbert space may imply existence of solutions to a related problem.

Appendix B.

An ALGOL program for the Douglas-Gallie method.

Actual computations have been performed on the CDC 6400 computer at the University of California Computer Center, Berkeley and on the GIER computer at Aarhus University, Denmark. On the following pages is listed the ALGOL program which resulted from the experiments.

The number of iterations, q, is an input-variable. If acceleration, as mentioned in section 3.4, is used, a value of $q = 2$ is recommended for 7 decimals' accuracy in the computations.

We have used a number of step sizes ranging from $h = .1$ to $h = .06125$.

When preparing tables of the functions $w(x,t,h)$ with equidistant entries an interpolation in t is necessary. A standard 4 point method has proved satisfactory in many cases although not accurate enough near the origin.

Output statements have not been included since we have desired to give a description of the program as close to the reference language ALGOL 60 as possible. Furthermore we want to avoid here the practical considerations - concerning the width of the paper, the number of lines per page, printer control characters and special characters, and the general lay-out of the tables - which are largely irrelevant to the numerical problem.

Also, the specific form of the output statements often differ from one computer installation to the other such that an installation manual is needed to define the exact action of the statements.

The input statements have been included, however, since they are self-explanatory and clearly demonstrate what input is needed.

```
begin comment  Stefan problem;
    integer n, nn, i, i1, i2, q, r;
    real h, t, delt, d2, d3, diff, x, x1;
 QB: nn := readinteger; h := readreal; q := readinteger;
    comment  nn = number of time steps,  h = step size,
        q = number of iterations;
    if nn < 0 then go to QX;
    i1 := (nn + 2)×(nn + 1)/2 - 1;
  begin array A, C, D[0:nn], W[0:i1];
    comment a procedure for performing interpolation for use when
        preparing an output-table may be inserted here;
    D[0] := 0;
    for i := 0 step 1 until i1 do W[i] := 0;
     for i := 0 step 1 until nn do A[i] := C[i] := 0;
    W[1] := D[1] := t := d2 := delt := h;
    comment initialization of variables has just been performed,
        now comes the main loop;
    for n := 2 step 1 until nn do
    begin i2 := (n + 1)×n/2; i1 := i2 - n; r := 0;
        comment  r  counts the iterations,  i1  and  i2  are
            pointers in the  array W  which contains the
            values  w(i×h, t[n]),  arranged linearly;
  QF:   x := h×h/delt;
        comment the tri-diagonal system for  w(i,n)  has  A
            as diagonal and  C  as right-hand side
            and -1-s  in the side-diagonals;
        for i := 1 step 1 until n - 1 do
         begin A[i] := x + 2; C[i] := W[i1+i]×x end;
        A[0] := 1; C[0] := h;
```

```
        comment Gaussian reduction (backwards);
        for i := n - 2 step -1 until 0 do
         begin x := 1/A[i+1]; A[i] := A[i] - x;
            C[i] := C[i+1]×x + C[i]
        end;
        C[0] := C[0]/A[0];
        comment substitution;
        for i := 1 step 1 until n - 1 do
           C[i] := (C[i-1] + C[i])/A[i];
        comment equation (3.9) is used here instead of (3.8);
        d3 := h×h/C[n-1];
        if r = 1 then
        begin comment acceleration, see section 3.4;
            x := (d3 - delt)/diff;
            d3 := diff/(1.0 - x) - diff + delt
        end else diff := d3 - delt;
        delt := d3; r := r + 1; if r ≤ q then go to QF;
        comment D[n] contains t(n), delt is deltat[n],
            and d2 is deltat[n-1];
        D[n] := t := t + delt; x := delt;
         delt := delt×2 - d2; d2 := x;
        for i := 0 step 1 until n - 1 do W[i2+i] := C[i]
    end;
     comment output of tables of t(x,h) and W(x,t,h)
        can be performed here;
    go to QB
  end;
 QX:
end
```

Appendix C.

Numerical tables.

On the following pages are given tables of the solution functions of Stefan problem A. The numerical values of $t(x)$ and $u(x,t)$ have been obtained by the Douglas-Gallie method with Richardson extrapolation. We have used step sizes $h = .1, .05$, and $.025$ and for the region $0 \leq x \leq 1.0$, $0 \leq t \leq 1.3$ a check has been performed with step sizes $h = .05, .025$, and $.0125$.

The values have been checked against results obtained by the author using the method of W. Trench [22] and as far as possible with the power series expansions (see e.g. Evans, Isaacson, and MacDonald [8]). Coefficients for these have been calculated by the author on the CDC 6400 computer at the University of California Computer Center, Berkeley. The results indicate that the series have very small radii of convergence (possibly 0), but they can still be used to give results to 4 decimals or better in the interval $0 \leq t \leq .1$.

The values of $t(x)$ have also been compared with those given by A. Wragg [23]. When Richardson extrapolation is applied to his results (Table 2 of [23]) with $\Delta t = .04, .02$, and $.01$ the results agree with those given on the next page up to round-off.

The values for $y(t)$, which is the inverse function of $t(x)$, have been obtained using Newton-Raphson's method together with

4-point interpolation in the table of $t(x)$. For the interval $0 \leq t \leq .1$, though, the values have been obtained from the series expansion for $y(t)$.

All our computations have been performed to at least 7 decimals relative accuracy, such that round-off errors should be negligible compared to the discretization errors.

The computation time as a function of h is given in the following table. The values given are CP seconds on a CDC 6400 computer.

h	n	sec
.1	20	.36
.05	40	1.42
.025	80	5.62
.0125	160	22.25

Table of t(x), x = .00 (.05) 2.00

x	t(x)	x	t(x)
.00	.0000	1.00	1.3646
.05	.0512	1.05	1.4484
.10	.1047	1.10	1.5335
.15	.1604	1.15	1.6198
.20	.2180	1.20	1.7074
.25	.2776	1.25	1.7962
.30	.3390	1.30	1.8862
.35	.4022	1.35	1.9775
.40	.4671	1.40	2.0699
.45	.5337	1.45	2.1636
.50	.6019	1.50	2.2583
.55	.6716	1.55	2.3543
.60	.7429	1.60	2.4514
.65	.8157	1.65	2.5496
.70	.8899	1.70	2.6490
.75	.9656	1.75	2.7494
.80	1.0427	1.80	2.8510
.85	1.1211	1.85	2.9537
.90	1.2009	1.90	3.0574
.95	1.2821	1.95	3.1623
1.00	1.3646	2.00	3.2682

Table of u(x,t), t = .00 (.01) .30, x = .00 (.05) y(t),

Table of y(t), t = .00 (.01) .30.

t \ x	.00	.05	.10	.15	.20	.25	y(t)
.00	.0000						.00000
.01	.0099						.00995
.02	.0196						.01981
.03	.0292						.02957
.04	.0385						.03925
.05	.0478						.04884
.06	.0568	.0079					.05836
.07	.0658	.0169					.06779
.08	.0746	.0257					.07716
.09	.0832	.0343					.08645
.10	.0918	.0428					.09567
.11	.1002	.0513	.0044				.1048
.12	.1086	.0596	.0127				.1139
.13	.1168	.0678	.0209				.1229
.14	.1249	.0759	.0289				.1319
.15	.1329	.0839	.0369				.1408
.16	.1409	.0918	.0448				.1497
.17	.1487	.0997	.0526	.0075			.1585
.18	.1565	.1074	.0603	.0151			.1672
.19	.1641	.1151	.0679	.0227			.1759
.20	.1717	.1227	.0755	.0302			.1845
.21	.1792	.1302	.0830	.0376			.1931
.22	.1867	.1376	.0904	.0450	.0014		.2017
.23	.1940	.1450	.0977	.0523	.0087		.2102
.24	.2013	.1522	.1050	.0595	.0158		.2186
.25	.2086	.1595	.1122	.0666	.0229		.2270
.26	.2157	.1666	.1193	.0737	.0299		.2354
.27	.2228	.1737	.1263	.0807	.0369		.2437
.28	.2298	.1807	.1333	.0877	.0438	.0016	.2520
.29	.2368	.1877	.1403	.0946	.0507	.0084	.2602
.30	.2437	.1946	.1472	.1015	.0575	.0151	.2684

Table of u(x,t), t = .0 (.1) 3.0, x = .0 (.2) min{y(t),1},

Table of y(t), t = .0 (.1) 3.0.

t \ x	.0	.2	.4	.6	.8	1.0	y(t)
.0	.0000						.0000
.1	.0918						.0957
.2	.1717						.1845
.3	.2437	.0575					.2684
.4	.3099	.1226					.3483
.5	.3715	.1834	.0188				.4248
.6	.4294	.2407	.0741				.4986
.7	.4843	.2950	.1268				.5700
.8	.5365	.3467	.1771	.0272			.6393
.9	.5865	.3963	.2254	.0736			.7067
1.0	.6345	.4439	.2720	.1183			.7724
1.1	.6807	.4898	.3169	.1617	.0235		.8366
1.2	.7254	.5342	.3604	.2038	.0637		.8994
1.3	.7687	.5772	.4026	.2447	.1028		.9609
1.4	.8107	.6189	.4436	.2845	.1411	.0128	1.0212
1.5	.8515	.6595	.4835	.3233	.1784	.0483	1.0804
1.6	.8912	.6990	.5224	.3612	.2150	.0832	1.1386
1.7	.9299	.7375	.5604	.3983	.2508	.1174	1.1958
1.8	.9677	.7752	.5975	.4345	.2858	.1510	1.2521
1.9	1.0046	.8120	.6338	.4700	.3202	.1841	1.3076
2.0	1.0408	.8479	.6693	.5048	.3540	.2165	1.3622
2.1	1.0762	.8832	.7041	.5389	.3871	.2485	1.4161
2.2	1.1109	.9177	.7383	.5723	.4197	.2799	1.4693
2.3	1.1449	.9516	.7718	.6052	.4517	.3109	1.5218
2.4	1.1783	.9849	.8047	.6376	.4832	.3414	1.5736
2.5	1.2111	1.0176	.8371	.6693	.5142	.3714	1.6248
2.6	1.2433	1.0497	.8689	.7006	.5448	.4010	1.6754
2.7	1.2751	1.0813	.9002	.7314	.5749	.4303	1.7255
2.8	1.3063	1.1125	.9310	.7617	.6045	.4591	1.7750
2.9	1.3370	1.1431	.9613	.7916	.6338	.4875	1.8239
3.0	1.3672	1.1733	.9912	.8211	.6626	.5156	1.8724

Table of u(x,t), t = 1.4 (.1) 3.0, x = 1.0 (.2) y(t),

Table of y(t), t = 1.4 (.1) 3.0.

t \ x	1.0	1.2	1.4	1.6	1.8	y(t)
1.4	.0128					1.0212
1.5	.0483					1.0804
1.6	.0832					1.1386
1.7	.1174					1.1958
1.8	.1510	.0295				1.2521
1.9	.1841	.0610				1.3076
2.0	.2165	.0920				1.3622
2.1	.2485	.1225	.0087			1.4161
2.2	.2799	.1526	.0373			1.4693
2.3	.3109	.1823	.0656			1.5218
2.4	.3414	.2116	.0935			1.5736
2.5	.3714	.2405	.1211	.0126		1.6248
2.6	.4010	.2691	.1484	.0387		1.6754
2.7	.4303	.2973	.1755	.0644		1.7255
2.8	.4591	.3251	.2022	.0899		1.7750
2.9	.4875	.3526	.2286	.1151	.0117	1.8239
3.0	.5156	.3798	.2548	.1402	.0355	1.8724

Appendix D.

A discretization variant.

It is of interest to note, that instead of using the rectangular rule to approximate the integral (2.13), and a first order approximation for the boundary condition at the fixed boundary (2.9), we could use the trapezoidal rule for (2.13) and a second order approximation for (2.9), without changing in an essential way, the conclusions of the thesis.

In particular, the basic relation between the successive iterates for the time step $\Delta t_n^{(r)}$, namely (3.18), remains unchanged:

The approximations (3.8) and (3.6) being replaced by

$$(1) \qquad \Delta t_n^{(r+1)} = (n + \tfrac{1}{2} w_{o,n}^{(r)} + \sum_{i=1}^{n} w_{i,n}^{(r)}) \cdot h - t_{n-1}$$

and

$$(2) \qquad w_{-1,n}^{(r)} - w_{1,n}^{(r)} = 2\,h \ ,$$

we have, using (3.5), (3.15), and (3.17),

$$(3) \qquad s_n^{(r)}(m_{o,n}^{(r)} - 1) = \tfrac{1}{2}(w_{o,n-1} - w_{o,n}^{(r)}) \, .$$

If we sum the relations (3.5), for $i = 1, 2, \ldots, n-1$, and use (3.17) we obtain

$$(4) \qquad s_n^{(r)} (m_{o,n}^{(r)} - m_{n-1,n}^{(r)}) = \sum_{i=1}^{n-1} (w_{i,n}^{(r)} - w_{i,n-1}) \, .$$

Using (1) and (1) at the limit for the preceding step, namely

$$\Delta t_{n-1} = (n - 1 + \tfrac{1}{2} w_{o,n-1} + \sum_{i=1}^{n-1} w_{i,n-1})\,h - t_{n-2} ,$$

we obtain, because of (3)

$$s_n^{(r)}(m_{o,n}^{(r)} - m_{n-1,n}^{(r)}) = \frac{1}{h}(\Delta t_n^{(r+1)} - n\,h - \frac{h}{2} w_{o,n}^{(r)} + t_{n-1}$$

$$- \Delta t_{n-1} + (n-1)\,h + \frac{h}{2} w_{o,n-1} - t_{n-2})$$

$$= s_n^{(r+1)} - 1 + s_n^{(r)}(m_{o,n}^{(r)} - 1)$$

which gives (3.18) with r replaced by $r+1$.

The corresponding changes to be made in the ALGOL program are:

a) Replace the initialization statement (line 15 of page 98) by

```
W[1] := sqrt(2×h + 1) - 1;
D[1] := t := d2 := delt := (W[1]/2 + 1)×h;
```

b) Replace the last line of page 98 by

```
A[0] := x/2 + 1; C[0] := W[i1]×x/2 + h;
```

References.

[1] M. Brillouin, Sur quelques problèmes non résolus de la Physique Mathématique classique. Propagation de la fusion, Ann. Inst. H. Poincaré, 1 (1931) pp. 285 - 307.

[2] J. R. Cannon & J. Douglas, The Cauchy Problem for the Heat Equation, SIAM J. Numer. Anal. 4 (1967) pp. 317 - 336.

[3] J. Crank, Two Methods for the Numerical Solution of Moving-boundary problems in Diffusion and Heat Flow, Quart. J. Mech. Appl. Math. 10 (1957) pp. 220 - 231.

[4] R. DeVogelaere, On a Paper of Gaunt Concerned With the Start of Numerical Solutions of Differential Equations, Z. Angew. Math. Phys. 8 (1957) pp. 151 - 156.

[5] J. Douglas, A Uniqueness Theorem for the Solution of a Stefan Problem, Proc. Amer. Math. Soc. 8 (1957) pp. 402 - 408.

[6] J. Douglas, Numerical Methods for Parabolic Equations, sec 13, pp 46 - 48 in Advances in Computers (F. L. Alt, ed.) Vol 2, Academic Press, New York, 1961.

[7] J. Douglas & T. M. Gallie, On the Numerical Integration of a parabolic Differential Equation Subject to a Moving Boundary Condition, Duke Math. J. 22 (1955) pp. 557 - 571.

[8] G. W. Evans, E. Isaacson, J. K. L. MacDonald, Stefan-like Problems, Quart. Appl. Math. 8 (1950) pp. 312 - 319.

[9] G. W. Evans, A Note on the Existence of a Solution to a Problem of Stefan, Quart. Appl. Math. 9 (1951) pp. 185 - 193.

[10] A. Friedman, Free Boundary Problems for Parabolic Equations, I, J. Math. Mech. 8 (1959) pp. 499 - 518, II, same 9 (1960) pp. 19 - 66, III, same 9 (1960) pp. 327 - 345.

[11] A. Friedman, Partial Differential Equations of Parabolic Type, Prentice Hall, Englewood Cliffs, N. J. 1964.

[12] J. Lindley & A. Wragg, The numerical solution of sequential decision problems involving parabolic equations with moving boundaries, Comp. J. 9 (1966) pp. 294 - 297.

[13] C. Li-Shang, The proper posing of free boundary problems for non-linear parabolic differential equations, Chinese Math. 3 (1963) pp. 399 - 418. Translated from Acta Math. Sinica 12 (1962) pp. 369 - 388. (Russian translation in Sci. Sinica 13 (1964) pp. 193 - 212).

[14] C. Li-Shang, Existence and differentiability of the solution of a two-phase Stefan problem for quasilinear parabolic equations, Chinese Math. 7 (1965) pp. 481 - 496. Translated from Acta Math.Sinica 15 (1965) pp. 749 - 764.

[15] L. Nirenberg, A Strong Maximum Principle for Parabolic Equations, Comm. Pure Appl. Math. 6 (1953) pp. 167 - 177.

[16] O. A. Oleinik, A Method of Solution of the General Stefan Problem, Soviet Math. Dokl. 1 (1960) pp. 1350 - 1354. Translated from Dokl. Akad. Nauk SSSR 135 (1960) pp. 1054 - 1057.

[17] L. F. Richardson, The Deferred Approach to the Limit, Trans. Roy. Soc. London 226 (1927) pp. 299 - 349 (and pp. 350 - 361).

[18] A. L. Ruoff, An Alternate Solution of Stefan's Problem, Quart. Appl. Math. 16 (1958) pp. 197 - 201.

[19] G. Sestini, Esistenza di una soluzione in problemi analoghi a quello di Stefan, Riv. Mat. Univ. Parma 3 (1952) pp. 3 - 23 and 103 - 113.

[20] G. Sestini, Sul problema unidimensionale non lineare di Stefan, Ann. Mat. Pura Appl. Ser. 4, 51 (1960) pp. 203 - 224 and 56 (1961) pp. 193 - 207.

[21] J. Stefan, Über die Theorie der Eisbildung, insbesondere über die Eisbildung im Polarmeere, Sitz. Akad. Wiss. Wien, Mat.-Nat. Classe 98 2A (1889) pp. 965 - 983.

[22] W. Trench, On an explicit Method for the Solution of a Stefan Problem, J. SIAM 7 (1959) pp. 184 - 204.

[23] A. Wragg, The use of Lanczos τ-methods in the numerical solution of a Stefan problem, Comp. J. 9 (1966) pp. 106 - 109.

[24] R. Devogelaere, The Reduction of the Stefan Problem to the Solution of an Ordinary Differential Equation, pp. 101 - 107 in Proceedings of the Second International Conference on Numerical Methods in Fluid Dynamics, Lecture Notes in Physics, vol. 8, Springer, Berlin, 1971.

[25] J. R. Cannon & C. Denson Hill, Remarks on a Stefan Problem, J. Math. Mech. 17 (1967) pp. 433 - 441.