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# Mathematics of moving boundary problems in diffusion

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# MATHEMATICS OF MOVING BOUNDARY PROBLEMS
# IN DIFFUSION

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## DEPARTMENT OF MATHEMATICS

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# DEDICATION

**To my parents, sister and her family**

# ACKNOWLEDGEMENTS

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# ABSTRACT

This thesis is concerned with the development, generalization and application of a formal series technique for classical one-dimensional moving boundary diffusion problems. The solution procedure consists of two major steps. Firstly, the introduction of a boundary fixing transformation, which fixes the moving boundary and simplifies the transformed equations. Secondly, the assumption of a formal series solution which leads to a system of ordinary differential equations for the unknown coefficients in the series. The method generalizes to multi-phase and heterogeneous moving boundary problems for both constant temperature and Newton's radiation conditions and yields simple and highly accurate estimates for both the temperature and boundary motion.

The first chapter provides a survey of the applications and a literature review for moving boundary diffusion problems. In Chapter 2 the classical idealized problem of melting single phase planes, cylinders and spheres are considered. For the planar problem the method yields the exact Neumann solution, while for the cylinder and sphere the method generates accurate boundary motions. The effect of changing the surface conditions is also investigated. An alternative solution for the spherical problem is presented, which yields the same approximate boundary motion predicted by previous authors. In Chapter 3 the problem of the planar solidification of a semi-infinite half-space, initially at its freezing temperature with Newton's cooling at the surface is considered. Two series solutions are obtained, the first valid for small times and the second for large times. In the limit of no Newton's cooling at the surface the large time solution is shown to give Neumann's solution. In Chapters 4, 5 and 6 the method is applied to full two-phase, heterogeneous and internal heat loss problems respectively. In all cases the method is shown to yield accurate temperature profiles and boundary motion. In Chapter 7 the classical

problem of heat transfer controlled growth and collapse of an isolated spherical bubble in a fluid of infinite extent is investigated. Two series solutions are obtained, the first for the collapsing case and the second for the expanding case.

The success of the method hinges on selecting the appropriate boundary fixing transformation. In general one can construct a large number of transformations which fix the moving boundary. However, many transformations do not give meaningful numerical results. A procedure is noted which appears to produce the optimal transformation for the particular problem at hand. The application and accuracy of the method is not entirely understood since the complexity of the terms in the series makes it difficult to gauge series convergence rate. Furthermore, the accuracy of the method appears also to depend on the nature of the boundary conditions imposed.

# CHAPTER ONE

# Literature Review, Applications and Formulation

## 1.1 General introduction

The study of boundary-initial value problems is a classical branch of analysis dating back to the early 1750's (for a historical account see Engelsman, 1984). Today, there are many important applications of the subject in the physical sciences and engineering. Moreover, it continues to be an active field of modern mathematical research. There exists a vast amount of literature pertaining to the development and practical applications (see Bateman, 1944; Sommerfeld, 1949; Duff, 1956; Sneddon, 1957; Greenspan, 1961; Epstein, 1962; Friedman, 1964; Garabedian, 1964; Greenberg, 1971).

In classical boundary-initial value problems the domains of the governing equations are fixed in space and are known along with the boundary and initial conditions. Such problems lend themselves to standard analytical and numerical solution techniques. In contrast, for diffusion controlled moving boundary problems the domains of the equations are separated by boundaries which are neither fixed in space nor known *a priori* but which must be determined together with the solution of the equations.

The inherent difficulty in the analysis of these problems lies in the nonlinear nature of the moving boundary which, in general, precludes superpositioning and necessitates the development of special approximation techniques. The other major

difficulty arises in finite domain problems where similarity solutions cannot be constructed.

## 1.2 Review

Despite their practical importance, only the simplest moving boundary problems have known exact solutions, the most important being the freezing of a semi-infinite region $x > 0$, initially at a constant temperature $V$ above the freezing point, and with the surface $x = 0$ subsequently maintained at zero temperature. The problem is believed to have been originally posed in connection with determining the thickness of polar ice (Lamé and Clapeyron, 1831). The problem was first fully solved by F. Neumann (hence, Neumann solution) and presented in a series of lectures at Konigsberg, in the early 1860's (Neumann, 1912; Weber, 1919; Rubinstein, 1971). However, the solution did not appear, in text, until some thirty years later, as part of a series of articles by J. Stefan in his work on the freezing of ground-water (Stefan, 1889a,b), diffusion controlled reactions (Stefan, 1889c), and evaporation and condensation processes (Stefan, 1889d).

The Neumann solution has been generalized to include substances which have $n$ transformation temperatures (Wiener, 1955; Moog and Rubinsky, 1985), different phase densities (Wilson, 1982), temperature dependent thermal properties (Hamill and Bankoff, 1964b; Cho and Sunderland, 1974), prescribed boundary motions (Langford, 1967a,b), vapour bubble dynamics (Zener, 1949; Shestakov and Tkachev, 1975), and non-Fourier governing equations (Sadd and Didlake, 1977). These solutions are all expressible in terms of a single similarity variable $x/t^{1/2}$. That is to say, the partial differential equations are reducible to a set of ordinary differential equations (for a detailed discussion see Bluman and Cole, 1969). Such reductions are only possible for infinite and semi-infinite regions with very restricted

boundary conditions. Unfortunately there are no such closed form solutions for other important boundary conditions such as constant flux or Newton's cooling condition at $x = 0$. For problems with radial flow, the only exact solutions are those corresponding to a constant line source and a linearly increasing point source (Carslaw and Jaeger, 1959). For regions bounded internally or externally by circular cylinders or spheres with isothermal boundaries, there are no known exact solutions.

There also exists a small number of solutions, for some very special problems, which can not be expressed in terms of a single similarity variable (Furzeland, 1980; Elliott and Ockendon, 1982). These solutions seem to have somewhat limited physical use and therefore have not received a great deal of attention. Nevertheless, such solutions can be very useful in checking the convergence and accuracy of numerical methods.

Various approximations have been developed for problems which have no known exact solutions. The simplest, and therefore probably the most important, being the pseudo steady state approximation. The approximation involves making the assumption that the rate of movement of the boundary is very much slower than the rate of diffusion. Under such an assumption, the boundary is taken to be stationary at any one time, and within each phase, a steady state problem solved. The heat flux is then equated to the rate of latent heat absorbed (or liberated) in order to determine the boundary motion as a function of time (Hill, 1928; Pekeris and Slichter, 1939; Yagi and Kunii, 1961; Narsimhan, 1961; Levenspiel, 1962; Zhang *et al.*, 1983, 1985). However, it has been shown that such pseudo steady state approximations are only valid when the ratio of the latent heat to the sensible heat of the substance is large (Bischoff, 1963, 1965a,b; Bowen, 1965; Hill, 1984). Furthermore, it has also been shown that pseudo steady state approximations are

not applicable to all planar problems (Kirkaldy, 1958), nor to problems which do not admit steady state solutions (e.g. inner phases of cylinders and spheres).

A large number of perturbation (or asymptotic) procedures have been developed for moving boundary problems. Regular perturbation techniques have been applied to problems concerned with the melting and freezing of idealized single phase planes (Lock, 1971; Pedroso and Domoto, 1973a; Huang and Shih, 1975a), cylinders (Lock and Nyven, 1971; Huang and Shih, 1975b), and spheres (Pedroso and Domoto, 1973b,c). However, for the radially symmetric problems, the analysis breaks down in a small region just before the moving boundary reaches the center. The breakdown occurs because of the relatively fast change in the nature of the process, despite the fact that the time-scale, on the whole, might be large. As a result, a singularity appears in the final temperature profile estimate. The sharp change in the temperature profile has been partially accommodated by a two-region boundary layer analysis (see Riley *et al.*, 1974), considerably improving the boundary motion estimate. However, it has been pointed out that the inner solution of the boundary layer analysis itself breaks down leaving the final temperature profile estimate still singular (Stewartson and Waechter, 1976; Soward, 1980). Similar perturbation expansions have also been used on full two phase problems (Weinbaum and Jiji, 1977; Jiji and Weinbaum, 1978) the growth and dissolution of vapour bubbles (Duda and Vrentas, 1969a,b; Vrentas and Shih, 1980a,b; Chahine and Liu, 1984), and certain two dimensional problems (Rasmussen and Christiansen, 1976a,b).

Useful though such perturbation techniques are, their applications to practical problems can present difficulties. Firstly, the numerical evaluations of the solutions are usually by no means trivial. Secondly, the methods are for the most part restricted to highly idealized problems. Lastly, all the expansions are strictly

asymptotic in nature. That is to say, the approximations are only valid when the ratios of the latent heat to the sensible heat of the substance in question is large. If the ratio is much smaller than unity, the expansion breaks down.

Adapting the "momentum and energy integral method" of fluid dynamics (see Pohlhausen, 1921; Goldstein, 1938; Schlichting, 1956), the so-called "Heat Balance Method" was developed. In its simplest form, the method consists of assuming a suitable temperature profile, usually a low order polynomial or an exponential, which is then made to satisfy all the boundary and initial conditions. The complete solution thus obtained does not satisfy the governing equation exactly but rather an integrated "average" of the equation. As a result, the position of the moving boundary emerges as the solution of an ordinary nonlinear differential equation with time as the independent variable. The method, as described, has provided reasonable estimates for various planar problems (see Goodman, 1958; Veinik, 1959; Altman, 1961; Hrycak, 1963; Vallerani, 1974; Zien, 1977, 1978; Chung *et al..*, 1983). Additional boundary conditions can be generated, for higher order approximations, by successively differentiating the "natural" boundary conditions (Goodman, 1964; Crank and Gupta, 1972a). However, it becomes extremely tedious to determine the unknown coefficients, with no real assurance of generating a better estimate. Furthermore, the algebraic manipulations required become considerably more cumbersome, and less accurate for radially symmetric problems (Theofanous *et al..*, 1969; Biasi *et al.* , 1971). Generally speaking, extreme care must be taken in choosing the appropriate form of the required temperature profiles (for a discussion see Lardner and Pohle, 1961; Poots, 1962a).

From numerical comparisons, it would appear that the heat balance method is best suited to single phase problems. Although it has been applied successfully to two phase planar problems without too many difficulties (see Kumar and Gupta, 1971;

Gupta, 1974), in treating radially symmetric two-phase problems, the resulting set of simultaneous equations for the boundary motion are initially singular requiring special starting solutions (Lunardini, 1981). Such computational complexities tend to negate the basic simplicity of the method.

Isolated attempts have been made to extend the basic heat balance method to two dimensional problems (Poots, 1962b). Again, the extreme difficulties in determining the unknown coefficients and the increased numerical work required makes the method unattractive. Some refinements of the basic method have been put forward which increase the accuracy of the approximations (Bell, 1978, 1979; El-Genk and Cronenberg, 1979), with only a small increase in numerical work.

Another method in the heat balance category is based on Biot's variational principal (see Biot, 1956, 1957), where a Lagrangian formulation leads to a system of ordinary differential equations. The solution then proceeds by assuming a suitable temperature profile (Biot and Agrawal, 1964; Prasad and Agrawal, 1972; Dharma *et al.*, 1985). The method also permits one to account for the heating history prior to melting.

Several semi-analytic series techniques have been developed and used on a number of problems. These usually involve expanding the temperature profiles in Fourier series (Melamed, 1958; Frjazinov, 1962), in terms of heat polynomials (Tao, 1978, 1981, 1982), or the application of appropriate finite integral transforms (Selim and Seagrave, 1973a,b,c). The major disadvantage of such methods lies in the enormous numerical complexity required in determining the unknown coefficients, which often require special starting solutions (Lederman and Boley, 1970). Furthermore, the results are usually restricted to very specific problems and to a limited range of the parameters. Alternatively, a much simpler series can be obtained by applying a boundary fixing transformation and expanding the temperature in powers of the

moving boundary (Davis and Hill, 1982a,b). The leading terms are determined analytically and are sufficient for very accurate temperature and boundary motion estimates. The approach is readily applicable to problems in various geometries and a variety of boundary conditions (Hill and Dewynne, 1986). Moreover, the solutions may be used in other circumstances, such as problems of mass transfer with rapid chemical reactions or diffusion controlled problems.

It has been argued that the application of integral techniques circumvent some of the mathematical difficulties associated with moving boundary problems. The most common of the reformulations involve the introduction of appropriate Green's functions (Rubinstein, 1971: Chuang and Szekely, 1971, 1972; Chuang and Ehrich, 1974). In such reformulations the moving boundaries are shown to satisfy either integral or integro-differential equations, which naturally lend themselves to pre-existing numerical and asymptotic solution techniques (Hansen and Hougaard, 1974). The primary advantage of such integral formulation techniques appears to lie in their rather uniform approach to both one and higher dimensional problems. While it is true that one dimensional problems have been successfully treated by a number of other semi-analytic methods, integral techniques appear to be superior in their treatment of higher dimensional problems (Jiji and Rathjen, 1970; Rathjen and Jiji, 1971; Budhia and Kreith, 1973). However, in most cases the reformulation is by no means unique and a large number of different equations can be written down for any one particular problem (Miranker, 1958; Griffin and Coughanowr, 1965a,b,c). The difficulty then appears to be in choosing the appropriate formulation for the particular problem at hand.

Frequently analytic iteration techniques have been employed in generating both temperature and boundary motion estimates (see Kreith and Romie, 1955; Hamill and Bankoff, 1964a; Savino and Siegel, 1969; Shih and Tsay, 1971; Theofanous

and Lim, 1971; Shih and Chou, 1971; Krishnamurthy and Shah, 1979), each successive iteration being used to generate a new approximation until convergence is obtained or the equations become too unwieldy to manipulate. Unfortunately, the convergence of such analytic iteration methods is not entirely understood, and therefore the estimates generated must be compared to numerical solutions in order to gauge their performance.

Even if the exact solution of a governing equation, together with its boundary and initial conditions, can not be found, establishing tight bounds can have great practical importance. One of the most successful techniques for obtaining such bounds involves casting the system into an integral equation form. The required reformulation is usually accomplished by integrating the governing equation twice with respect to $x$ and once with respect to $t$. Substituting physically apparent inequalities into the new equations generates the desired bounds. The technique has been applied to problems involving such situations as growth of vapour films (Hamill and Bankoff, 1963b), solidification of slabs (Kern, 1977; Glasser and Kern, 1978), and time dependent boundary conditions (Hamill and Bankoff, 1963a; Dewynne and Hill, 1984). Extensions and improvements of the basic technique have been developed to generate tighter bounds (Hill and Dewynne, 1984) and to incorporate diffusion-controlled problems with two chemical reactions (Dewynne and Hill, 1985), and multiphase problems (Dewynne and Hill, 1986a,b). Alternatively, in the construction of existence and uniqueness theorems, the theorems themselves construct bounds (Boley, 1963; Wu and Boley, 1966; Wu, 1966). In aerodynamic surface heating, by carefully treating the evaporation and mechanical effects as separate independent mechanisms, tight bounds on the melting rates can be established (see Masters, 1956).

Results concerning the existence, uniqueness, stability and asymptotic behaviour have been obtained by various methods under certain hypotheses on the data. Using both integral formulations and variational inequalities, it has been shown that single phase moving boundary problems, under various assumptions on data, have unique solutions in the "classical" sense (Evans, 1951; Kyner, 1959a,b; Cannon and Hill, 1967; Cannon and Primicerio, 1971a: Rubinstein, 1971). Many of the results were quickly and easily extended to accommodate full two- and multi-phase problems (Rubinstein, 1971: Chan, 1971; Cannon and Primicerio, 1971b,c,d, 1973; Fasano and Primicerio, 1977a,b,c, 1979, 1981; White, 1985). Furthermore, the nonlinear nature of the moving boundary itself suggested the use of weak (or generalized) formulations. The theoretical properties of such "weak" formulations are useful in cases where the existence and uniqueness of "classical" solutions cannot be determined (e.g., multi-dimensional problems: Oleinik , 1960; Friedman, 1968a, mush regions: Atthey, 1974, and disappearing phases: Friedman, 1968b). It is also of interest to note here that if existence is assumed, uniqueness can be established for certain single phase radially symmetric problems (Morrison and Frisch, 1960).

Several straightforward numerical methods based on finite-difference replacements of the governing equations have been proposed. In general, with constant time steps and a fixed grid, the moving boundary will not coincide with a mesh point in successive time steps. To overcome the difficulty, a number of fixed grid variable time step methods have been devised for single dimensional problems (see Douglas and Gallie, 1955; Crank, 1957; Ehrlich, 1958; Yuen and Kleinman, 1980). In such methods, each time step is determined iteratively by requiring the moving boundary to be located at a mesh point, one grid space from its previous location. However, there seems to be no easy extension to more complicated and higher dimensional problems (Fox, 1974).

An important reformulation involves a shuffling in the roles of the dependent and independent variables. Essentially the method consists of interchanging one of the space variables with temperature, making the former the dependent variable and the temperature one of the independent variables. In such a reformulation the migrating isothermals are followed by a finite-difference scheme on a fixed domain (Dix and Cizek, 1971; Crank and Phale, 1973; Crank and Gupta, 1975).

Immobilization techniques have been developed and widely employed in the analysis of both one- and two dimensional problems. The basic philosophy of the approach is to simplify the numerical analysis by transforming the moving boundary to a fixed boundary, of simple geometry, at the expense of complicating the governing equations, since standard techniques can readily handle complex equations but are difficult to adapt to moving boundaries. The transformation casts the problem into a form which utilizes the strength of finite-difference (Landau, 1950; Lotkin, 1960; Bankoff, 1964; Duda *et al.*, 1975; Rizza, 1981), finite-element (Ettouney and Brown, 1983), and orthogonal collocation (Dudukovic and Lamba, 1978) methods. Such transformations also permit flexible grid point distributions where large gradients exist in certain regions of the domain (Muehlbauer and Sunderland, 1965).

A commonly used constructive solution technique is the method of lines. In this method, the governing partial differential equation is reduced to a system of coupled ordinary differential equations by discretizing all but one of the independent variables (Sackett, 1971a,b; Meyer, 1971). Due to the recent advances in the numerical solutions of two point boundary problems (see Jones *et al.*, 1972) the method is receiving increasing attention (Meyer, 1977, 1981a,b). The appealing features of the method are that it's simple to understand, easy to program and

convenient to use. However, it has been noted that it may exact a high price in running time compared to other direct numerical methods (Meyer, 1978a).

The adaptation of classical finite-element methods has been proposed by a number of researchers. In such methods, at each time step the moving boundary is approximated by polygonal shapes whose vertices are required to coincide with triangulation nodes. Such conditions are easily achieved through the use of various space-time elements which allow a change in the position of the nodes at each time step (Bonnerot and Jamet, 1974, 1979; Miller *et al.*, 1978; Jamet, 1978, 1980; Lesaint and Raviart, 1979). So far, finite-element methods have been applied to contact problems in elasticity (Wellford and Oden, 1975; Oden and Kikuchi, 1978), compressible flows with moving boundaries (Jamet and Bonnerot, 1975) and multi-dimensional problems (Bonnerot and Jamet, 1979). However, it has been noted, as with most finite-element methods, computer implementation tends to be very time consuming and costly (Meyer, 1978b).

Recently interest has grown in applying boundary integral equation methods to heat conduction phase change problems (see Chuang and Szekely, 1971, 1972: Liggett, 1977: Liu *et al.*, 1981: Langerholc, 1981: Banerjee and Shaw, 1982). The method appears to be well suited for addressing multi-dimensional problems because it only requires the manipulation of a surface mesh. Furthermore, it has been pointed out that in some applications, coarse meshes and very large time steps may be used, relative to those required by other numerical methods (O'Neill, 1983). The method remains in a very active state of development, and may well make a major contribution to the understanding of moving boundaries in the next few years.

The theoretical properties of weak formulations have motivated a number of enthalpy based numerical methods. Following the same discretization procedures as for the classical formulations, efficient finite-difference schemes were easily obtained

for both implicit and explicit time discretizations (see Atthey, 1974: Meyer, 1973: Berger *et al.*, 1975; Shamsundar and Sparrow, 1976; Jerome, 1977; Rogers *et al.*, 1979; Morgan, 1981; Gartling, 1980; Voller and Cross, 1980, 1981, 1983a,b; Voller 1983, 1985; White, 1982a,b). Furthermore, finite-element equations have also been obtained with accompanying error estimates (Elliott, 1981). Similar schemes can also be obtained by posing the original problems in terms of variational inequalities (Duvaut, 1973; Fremond, 1974; Furzeland, 1977).

A relatively new nonlinear approximation technique has been proposed which follows a well known approach in the solution of operator equations. Namely, the solution of the desired equation is approximated by a member of a finite dimensional vector space for which the deficiency of the operator has a local minimum. The technique has been applied to a small number of problems with favourable results (Cheung, 1978; Lozano and Reemtsen, 1981). The existence of a solution to the approximation and global convergence of the method has been proven (Reemtsen, 1981; Reemtsen and Lozano, 1981).

The need for an up-to-date survey is apparent from the large amount of research effort expended on these problems in recent years, especially with regard to the multi-dimensional case. Further references can be found in the texts: Rubinstein 1971, Ockendon and Hodgkins 1975, Wilson, Solomon and Boggs 1978 to which the interested reader is referred. There also exists a number of reviews: Ruddle 1957, Carslaw and Jaeger 1959, Bankoff 1964, Muehlbauer and Sunderland 1965, Mori and Araki 1976, Boley, 1978, and Crank 1981, which are of considerable value.

## 1.3 Applications

In the metal industry, moving boundaries occur in processes such as the solidification of metals and alloys (Lightfoot, 1929; Wagner, 1954; Crowley and Ockendon, 1979; Sinha and Gupta, 1982), solidification of interface shapes during continuous casting (Siegel, 1978a,b, 1983, 1984a,b, 1985 Sampson and Gibson, 1981, 1982) and the effects of shrinkage (Beckett and Hobson, 1980). Such phenomena play important roles in many processing operations. The melting of steel scrap in oxygen furnaces, ingot solidification, and continuous casting of steel, copper, and aluminium to mention only a few examples.

In extractive metallurgy, reactions involving moving boundaries occur frequently in material processing operations. The reduction of oxide ores (Turkdogan and coworkers, 1971a,b, 1972; Evans and Koo, 1979), the roasting of sulphides (Natesan and Philbrook, 1969; McCormick *et al.*, 1975; Khalafalla, 1979), thermal decomposition of calcium carbonates (Narsimhan, 1961), and calcination (Sohn and Turkdogan, 1979) may be quoted as examples. In these systems, after some reaction has occurred, the solid phase consists of an unreacted core surrounded by a reacted shell. In such cases the reaction occurs at the boundary separating the reacted and unreacted regions. Using such "shrinking core" models, experimental data have been made to fit very well (Szekely and Evans, 1970, 1971; Sohn and Szekely, 1972, 1973; Szekely, *et al.*, 1976; Olmstead, 1980).

One of the most exciting fields of research to which moving boundaries have been applied is that of biology. Important pioneering work centered on the study of simple one dimensional transportation consumption problems of oxygen in tissues (Hill, 1928; Chance *et al.*, 1964; Gonzalez-Fernandez and Atta, 1968; Rubinow, 1973). The main objective of such early work was simply to estimate the depth of

tissue containing oxygen for given surface concentrations. Following this, a number of diffusion reaction models were developed to study oxygen metabolism in tissues in the hope of estimating the effectiveness of irradiating tumor tissues which primarily dependson the presence or absence of oxygen (Crank and Gupta, 1972a,b; Evans and Gourlay, 1977; Miller *et al.*, 1978).

Other applications of practical interest include melting of polymers (Pearson, 1966, 1972, 1974, 1976), solidification of aqueous binary solutions (O'Callaghan *et al.*, 1982a,b), melting of reactor fuel elements (Lyons *et al.*, 1963; Lahoud and Boley, 1970), permafrost thermal design for pipelines (Wheeler, 1978), growth of crystals (Abrams and Viskanta, 1974), the growth and collapse of vapour bubbles (Zener, 1949; Skinner and Bankoff, 1964a,b; Hickling and Plesset, 1964; Readey and Cooper Jr, 1966; Cable and Evans, 1967) and melting induced by electric arcs (Blevin, 1952), and drying rates of wood particles (Dorri, *et al.*, 1985). Further references concerning applications in glass, oil and semiconductor industries, statistical decision theory, space vehicle design, preservation of foodstuff, astrophysics, geophysics, plasmaphysics and meteorology can be found in Turcotte and Schubert 1971, Wilson, Solomon and Boggs 1978, Furzeland 1977, Boley 1978, Wilson, *et al.*, 1978, Elliott and Ockendon, 1981, and Taylor 1982.

From the examples cited above, it is easy to see the important role played by moving boundaries in modelling many industrial and engineering processes. Moreover, there remains a potential for further development in similar areas, since each method incorporates a certain degree of flexibility. Further applications of moving boundaries to problems of high degree of difficulty can be expected in the very near future.

## 1.4 Formulations

The classical two-phase melting problems in heat diffusion require the determination of the temperature field over some domain $D$ with prescribed boundary conditions on $\partial D$ of $D$. The domain $D$ consists of two regions $D_1$ and $D_2$ occupied by the two different phases respectively. The two regions are separated by a moving boundary $s(\underline{x}, t) = 0$. In each of the regions the temperature is assumed to satisfy the Fourier heat equation

$$\rho c_i \frac{\partial T_i}{\partial t} = \nabla.(k_i \nabla T_i) - f_i, \quad i = 1, 2 \tag{1.4.1}$$

where $c$ is the specific heat, $T$ the temperature, $k$ the thermal conductivity, and $f$ a piecewise differentiable source term which can be a function of all $\underline{x}$, $t$, and $T$. The density $\rho$ is assumed to be the same and constant for both phases avoiding complicated convection terms. For a one component system, the temperatures in the two phases must be equal at the phase interface, that is

$$T_1 = T_2 = T_m \quad \text{on} \quad s(\underline{x}, t) = 0, \tag{1.4.2}$$

where $T_m$ denotes the phase change temperature. The remaining boundary condition required is a relationship between the movement of the phase interface and the heat flow across it. Such a relationship is obtained by establishing a heat balance on the moving interface. Assuming that the transition from phase 2 to phase 1 is accomplished by an absorption of heat and the change of density under the phase change is neglected, we have

$$\nabla s.[k_2 \nabla T_2 - k_1 \nabla T_1] = \rho L \frac{\partial s}{\partial t}, \quad s(\underline{x}, t) = 0, \tag{1.4.3}$$

where L denotes the latent heat of fusion. In other words, the velocity of the moving boundary is proportional to the net heat flux in it. The formulation can be modified and generalized to include n phases and multi-dimensional systems

(Rubinstein, 1971; Sohn and Wadsworth, 1979), the instantaneous removal of melt "ablation problems" (Vallerani, 1974; Zien, 1977, 1978; Chung *et al.*, 1983), incorporating density changes (Chambre, 1956; Sutton, 1958), prescribed boundary motions "inverse problems" (Martynov, 1960; Redozubov, 1962; Langford, 1966a,b; Bluman, 1974), or put in the context of chemical reactions "shrinking core model" (Evans, 1979). A comprehensive survey of the different formulations can be found in Furzeland 1977.

## 1.5 The scope of the thesis

This thesis is concerned with the development, generalization and application of a formal series technique for classical, one-dimensional, moving boundary problems.

The solution procedure consists of two steps. Firstly, the introduction of a boundary fixing transformation, which not only fixes the boundary but also simplifies the transformed equations. Secondly, assuming a formal series solution which yields a system of ordinary linear differential equations for the unknown coefficients.

The method naturally generalizes to multiphase and heterogeneous moving boundary problems and can cope with both constant temperature and Newton cooling boundary conditions.

The results of this thesis expand, unify and generalize the results of Davis and Hill (1982) and Hill and Dewynne (1986), who applied the method to the spherical and cylindrical problems respectively.

In Chapter 2, the classical Stefan problem of melting idealized single phase planes is considered. The analysis is presented in terms of melting, however the results are applicable to freezing problems, with only minor changes, in the non-dimensionalization of the equations. For comparison purposes, an extra term in the series expansion for the spherical problem of Davis and Hill (1982), is found and presented. The effect of changing the fixed boundary condition is also investigated. An alternate solution for the spherical problem is also presented, which surprisingly, yields the same boundary motion estimates as obtained by Davis and Hill (1982).

In Chapter 3, the classical problem of the planar solidification of a semi-infinite half-space, initially at its freezing temperature, with Newton cooling at the surface is considered. By fixing the boundary, two iterative analytic series solutions are obtained, the first valid for small times the, second valid for large times. In the limit of no Newton cooling at the surface, the initial time interval over which the short time solution is applicable shrinks to zero and the large time solution yields precisely the well known Neumann solution.

In Chapter 4, the boundary fixing series technique is applied to full two phase problems. For such problems, the technique involves introducing a transformation which fixes three points: the origin, the moving boundary and the outer surface of the cylinder or sphere. Thus the original two phase moving boundary problem is transformed into a fixed boundary problem. For the case of the two phase semi-infinite plane the method is shown to yield the exact similarity solution.

Chapter 5 is concerned with the application, evaluation and comparison between the boundary fixing series technique and a new polynomial type approximation technique. The analysis is presented in terms of melting heterogeneous idealized single-phase planes, cylinders and spheres. Both methods are used to generate approximations for temperature profiles and boundary motions for a large range of

parameters. For completeness, asymptotic properties and extensions to higher order approximations are presented at the end of the chapter.

In Chapter 6, the boundary fixing series technique is applied to moving boundary problems which are accompanied by internal heat loss. That is to say, problems where, throughout the newly formed molten region, heat is being lost at a rate assumed to be proportional to its temperature. A short discussion is given, pertaining to the analogous shrinking core problem frequently used in chemical reaction modelling. In such problems it is usually hypothesized that a second reaction behind the moving front is taking place, assumed to be pseudo-first order.

In Chapter 7, the classical problem of heat transfer controlled growth and collapse of an isolated spherical bubble in a fluid of infinite extent is considered. The problem involves determining the time variation of the radius of the bubble immersed in an outer phase which is initially at a uniform temperature. By employing two different boundary fixing transformations, two iterative analytic series solutions are obtained. The first series is valid for the collapsing bubble, the second for the expanding bubble. The one known exact solution, being for the growth of a bubble of zero initial radius, is shown to be the leading term in the expanding bubble series approximation.

In all the following chapters, Chapter 2 - Chapter 7, the problems are stated in dimensionless form. Every attempt has been made to keep each chapter as self contained as possible, eliminating the need to flip between the chapters while reading. The only exception being Chapter 6 which has one of its calculations summarized in the Appendix. Each chapter also finishes with a numerical section. Both figures and tables have been included to present both the qualitative and quantitative behaviour of the results. Wherever possible, comparisons between the

derived analytic approximations, known theoretical bounds, existing perturbation and numerical solutions are given.

# CHAPTER TWO

# Melting of Idealized Single Phase Planes, Cylinders and Spheres

## 2.1 Introduction

In this chapter we investigate the classical single phase Stefan problem of melting idealized planes, cylinders and spheres. The problem involves determining the position of the time dependent moving boundary together with the appropriate temperature profiles. The analysis is presented in terms of melting, however the results are applicable to freezing problems with only minor changes in the non-dimensionalization of the equations. The approach adopted is the newly developed boundary fixing series technique recently introduced by Davis and Hill (1982). In Section 2.2, we describe the physical problems in detail and formulate the equations and boundary conditions in appropriate dimensionless variables. In Section 2.3 we present the classical Neumann solution for the plane and a summary of the work done by Davis and Hill (1982) and Hill and Dewynne (1986) is presented. For comparison purposes, an extra term in the series expansion for the spherical problem is given in Section 2.4. The effect of changing the boundary condition is investigated in Section 2.5. In Section 2.6 we outline an alternative solution for the spherical problem which surprisingly yields the same boundary estimate as obtained by Davis and Hill (1982). Numerical results and a discussion on the boundary fixing transformation are given in the final two sections respectively.

## 2.2 Governing equations

The first set of problems we consider $\check{v}$ the idealized melting of a plane of width $a^*$, and a cylinder and sphere of radius $a^*$, containing a solid initially at its fusion temperature $T_0^*$. At time zero, $t^* = 0$, the temperature, $T^*$, at the outer boundary, $r^* = a^*$, is raised to the value, $T_a^*$, above the melting point, $T_0^*$, and maintained at this constant value thereafter. To simplify the problem the volumetric expansion or contraction due to the phase change is neglected and the thermal properties of the system are assumed to be independent of temperature. Based on these simplifications the governing equation and boundary conditions (1.4.1)-(1.4.3) can be written in dimensionless form as

$$r^\lambda \frac{\partial T}{\partial t} = \frac{\partial}{\partial r}\left(r^\lambda \frac{\partial T}{\partial r}\right), \quad R(t) < r < 1, \tag{2.2.1}$$

subject to the boundary and initial conditions

$$T(1,t) = 1, \quad T(R,t) = 0, \quad T(r,0) = 0, \tag{2.2.2}$$

and the heat balance (Stefan) condition on the moving boundary

$$\frac{\partial T}{\partial r}(R,t) = -\alpha \frac{dR}{dt}, \quad R(0) = 1. \tag{2.2.3}$$

Here, $T(r,t)$ denotes the non-dimensional temperature, and the non-dimensional variables $r$, $t$ and $R(t)$ and constant $\alpha$ are given in terms of the starred physical quantities

$$r = \frac{r^*}{a^*}, \qquad t = \frac{k}{\rho c a^{*2}}t^*, \qquad R(t) = \frac{1}{a^*}R^*(t^*),$$

$$\tag{2.2.4}$$

$$T(r,t) = \left(T^*(r^*,t^*) - T_0^*\right)/\left(T_a^* - T_0^*\right), \qquad \alpha = L/c\left(T_a^* - T_0^*\right),$$

where $k$ is the thermal conductivity, $\rho$ is the constant density, $L$ the latent heat of fusion and $c$ the constant heat capacity of the molten material. The positive constant $\alpha$ denotes the inverse Stefan number, while the constant $\lambda$ takes on values of 0, 1, and 2 specifying plane, cylinder and sphere respectively.

## 2.3 Known results

For the semi-infinite plane $(-\infty, 1)$ the standard Landau transformation takes the form $x = (1 - r)/(1 - R)$ and the classical Neumann solution (see Carslaw and Jaeger, 1959) is given by

$$T(r,t) = \alpha\gamma \int_x^1 e^{\frac{\gamma}{2}(1 - \xi^2)}d\xi, \qquad (2.3.1)$$

where $R(t) = 1 - (2\gamma t)^{\frac{1}{2}}$ while $\gamma$ denotes the positive root of the transcendental equation

$$\alpha\gamma \int_0^1 e^{\frac{\gamma}{2}(1 - \xi^2)}d\xi = 1, \qquad (2.3.2)$$

which are tabulated, for selected values of $\alpha$, in Carslaw and Jaeger (1959). Frequently equations (2.3.1) and (2.3.2) are written in terms of the error function. However, this change in convention should not cause any real confusion.

For the sphere Davis and Hill (1982) use essentially the transformation variables

$$x = \frac{1 - r}{1 - R}, \qquad y = 1 - R, \qquad \phi(x,y) = rT(r,t), \qquad (2.3.3)$$

together with an assumed series solution of the form

$$\phi(x,y) = \sum_{n=0}^{\infty} A_n(x)y^n, \qquad (2.3.4)$$

to obtain a semi-analytic series approximation. On substituting (2.3.3) with (2.3.4) into (2.2.1)-(2.2.3), they show that the $A_n(x)$ satisfy the equations

$$A''_0 + \gamma x A'_0 = 0,$$

$$A''_n + \gamma[xA'_n - nA_n] = f_n(x), \quad n = 1, 2, \ldots, \qquad (2.3.5)$$

with $\gamma$ again being the positive root of (2.3.2) and $f_n(x)$ given by

$$f_n(x) = -A''_{n-1} + \frac{1}{\alpha}\sum_{j=1}^{n} A'_j(1)\left[xA'_{n-j} - (n-j)A_{n-j}\right], \qquad n = 1, 2, \ldots \qquad (2.3.6)$$

The boundary conditions on the $A_n(x)$ are shown to be

$$A_0(0) = 1, \qquad A_0(1) = 0,$$

$$(2.3.7)$$

$$A_n(0) = 0, \qquad A_n(1) = 0, \qquad n = 1, 2, \ldots .$$

The first three terms of the series can be shown to be given by

$$A_0(x) = \alpha\gamma \int_x^1 e^{\frac{\gamma}{2}(1 - \xi^2)} d\xi,$$

$$A_1(x) = \frac{\alpha\gamma x}{(\gamma + 3)}\left\{1 - e^{\frac{\gamma}{2}(1 - x^2)}\right\},$$

$$(2.3.8)$$

$$A_2(x) = \frac{\alpha\gamma}{(\gamma + 3)^2}\left\{\alpha\gamma\mu(1 + \gamma x^2)\int_0^x e^{\frac{\gamma}{2}(1 - \xi^2)} d\xi \right.$$

$$\left. - \left[\mu(1 + \gamma) + \frac{\gamma}{2}(1 - x^2)\right]x e^{\frac{\gamma}{2}(1 - x^2)}\right\},$$

with

$$\mu = 6\left[\gamma^2 + 6\gamma + 3 + \alpha\gamma(\gamma + 5)\right]^{-1}. \qquad (2.3.9)$$

Here we note that $A_0(x)$ (the zero order approximation) is identical to the exact Neumann solution for the semi-infinite plane.

Following the method of Davis and Hill (1982), Hill and Dewynne (1986) use (for the cylindrical problem) the boundary fixing transformation

$$x = \frac{\log r}{\log R}, \qquad y = \log R, \qquad \phi(x, y) = T(r, t), \qquad (2.3.10)$$

together with (2.3.4) to find that $A_0(x)$ was identical to the $A_0(x)$ given by (2.3.8)$_1$ for the spherical case, while $A_1(x)$ was given by

$$A_1(x) = \frac{\alpha\gamma}{2}x\left\{(1 - x)e^{\frac{\gamma}{2}(1 - x^2)} - \int_x^1 e^{\frac{\gamma}{2}(1 - \xi^2)} d\xi + \frac{1}{(\gamma + 3)}\left[e^{\frac{\gamma}{2}(1 - x^2)} - 1\right]\right\}.$$

$$(2.3.11)$$

Unfortunately the algebraic complexities prevent them obtaining $A_2(x)$ explicitly. Nevertheless, using the formula derived by Davis and Hill (1982), namely

$$A'_n(1) = \int_0^1 f_n(\xi)\frac{W(1)}{W(\xi)}\frac{A_{n2}(\xi)}{A_{n2}(1)}d\xi, \qquad (2.3.12)$$

they are able to find $A'_2(1)$ which they use in determining an approximation for the boundary motion.

The boundary fixing series technique outlined above gives rise to particularly accurate numerical results and for large and small $\alpha$, admits the appropriate limiting solutions (see Davis and Hill, 1982 and Hill and Dewynne, 1986. In order to extend the technique to more complicated problems we first need to understand the nature of the series convergence, applicability to other types of boundary conditions, and the significance of the boundary fixing transformation. To this end, in the following three sections we outline the procedure for finding $A'_3(1)$ for the sphere, solve the spherical problem with Newton's boundary condition, and outline an alternate solution for the sphere respectively. The alternate solution allows the three problems (i.e. plane, cylinder and sphere) to be characterized by a single formula for the boundary fixing transformation.

## 2.4 Evaluating $A'_3(1)$

In order to determine $A'_3(1)$ we have from (2.3.2) and (2.3.5)

$$A''_3 + \gamma[xA'_3 - 3A_3] = f_3(x),\qquad (2.4.1)$$

where $f_3(x)$ is defined by

$$f_3(x) = -A''_2 + \frac{1}{\alpha}\sum_{j=1}^{3} A'_j(1)\left[xA'_{3-j} - (3-j)A_{3-j}\right].\qquad (2.4.2)$$

Now from the results given in Section 2.3 we can simplify (2.4.2) and deduce the following expression for $f_3(x)$, that is

$$f_3(x) = \left[B_1 - \gamma A'_3(1) + B_2x^2 + B_3x^4\right]xe^{\frac{\gamma}{2}(1-x^2)}$$
$$- \frac{3\alpha^2\gamma^3(6 + \gamma - K)}{2(3 + \gamma)^3(1 + \gamma + \alpha\gamma)} \int_0^x e^{\frac{\gamma}{2}(1-\xi^2)}d\xi,\qquad (2.4.3)$$

where the constants $B_1$, $B_2$ and $B_3$ are given by

$$B_1 = \frac{-\alpha\gamma^2}{4(3+\gamma)^3}\left[3(30+21\gamma+4\gamma^2)-(9+4\gamma)K\right],$$

$$B_2 = \frac{\alpha\gamma^3}{4(3+\gamma)^3}[3(20+7\gamma)-7K], \qquad (2.4.4)$$

$$B_3 = \frac{-3\alpha\gamma^4}{2(3+\gamma)^3},$$

and $K$ is defined by

$$K = \left\{\frac{(-6+15\gamma+12\gamma^2+\gamma^3)+\alpha\gamma(6+11\gamma+\gamma^2)}{(3+6\gamma+\gamma^2)+\alpha\gamma(5+\gamma)}\right\}. \qquad (2.4.5)$$

From equation (2.3.12) we have

$$A'_3(1) = \frac{1}{(3+\gamma)}\int_0^1 f_3(\xi)e^{-\frac{\gamma}{2}(1-\xi^2)}(3+\gamma\xi^2)\xi\,d\xi, \qquad (2.4.6)$$

which is the determining equation for $A'_3(1)$. On noting that $A'_3(1)$ occurs on both sides of this equation we finally obtain on simplification

$$A'_3(1) = \alpha\gamma K^*(3+\gamma)^{-3}, \qquad (2.4.7)$$

where the constant $K^*$ is defined by

$$K^* = \frac{1}{24R_4}[3R_1K - R_2 - \alpha\gamma R_3], \qquad (2.4.8)$$

with the constants $R_1$, $R_2$, $R_3$ and $R_4$ given in turn by

$$R_1 = (-135+170\gamma+121\gamma^2+14\gamma^3-2\gamma^4)+\alpha\gamma(135+105\gamma+16\gamma^2-2\gamma^3),$$

$$R_2 = (-2430+3915\gamma+4590\gamma^2+1575\gamma^3+182\gamma^4+2\gamma^5),$$

$$R_3 = (2430+3375\gamma+1395\gamma^2+180\gamma^3+2\gamma^4),$$

$$R_4 = (15+10\gamma+\gamma^2)(1+\gamma+\alpha\gamma).$$

$$(2.4.9)$$

Following the procedure described in Davis and Hill (1982), we obtain the following expression for the motion of the boundary

$$t = \frac{1}{\gamma} \left\{ \frac{(R-1)^2}{2} + \frac{(R-1)^3}{(3+\gamma)} + \frac{\rho_1(R-1)^4}{4(3+\gamma)^2} + \frac{\rho_2(R-1)^5}{5(3+\gamma)^3} + \cdots \right\}, \quad (2.4.10)$$

where the constants $\rho_1$ and $\rho_2$ are given by

$$\rho_1 = K - 3\gamma, \qquad \rho_2 = K^* + (3-\gamma)K + 3\gamma^2. \quad (2.4.11)$$

From (2.4.10) we observe that the time to complete melting is given by

$$t_c = \frac{1}{\gamma} \left\{ \frac{1}{2} - \frac{1}{(3+\gamma)} + \frac{\rho_1}{4(3+\gamma)^2} - \frac{\rho_2}{5(3+\gamma)^3} + \cdots \right\}. \quad (2.4.12)$$

Now for large $\alpha$ (small $\gamma$) we have from (2.3.2)

$$\frac{1}{\alpha} = \gamma \left\{ 1 + \frac{\gamma}{3} + O(\gamma^2) \right\}, \quad (2.4.13)$$

and from (2.4.5), (2.4.8) and (2.4.9) we find that

$$K = 3\gamma + O(\gamma^2), \qquad K^* = -9\gamma + O(\gamma^2), \quad (2.4.14)$$

so that $\rho_1$ and $\rho_2$ are both of order $\gamma^2$ and equation (2.4.12) yields

$$t_c = \frac{1}{\gamma} \left\{ \frac{1}{6} + \frac{\gamma}{9} + O(\gamma^2) \right\} = \frac{\alpha}{6} + \frac{1}{6} + O\left(\frac{1}{\alpha}\right). \quad (2.4.15)$$

Thus the pseudo steady state approximation as well as the order one correction emerge for large $\alpha$. Now for small $\alpha$ (large $\gamma$) we have from (2.3.2)

$$\alpha \left\{ \left(\frac{\pi\gamma}{2}\right)^{1/2} e^{\gamma/2} - \left[ 1 - \frac{1}{\gamma} + \frac{3}{\gamma^2} + O\left(\frac{1}{\gamma^3}\right) \right] \right\} = 1, \quad (2.4.16)$$

so that in this case

$$\gamma = 2\log(1/\alpha) + O[\log(\log(1/\alpha))]. \quad (2.4.17)$$

In addition for large $\gamma$ we have from (2.4.12)

$$t_c = \frac{1}{2\gamma} + O\left(\frac{1}{\gamma^2}\right), \quad (2.4.18)$$

and thus (2.4.16) and (2.4.17) yield the asymptotically correct small $\alpha$ estimate for the time to complete melting.

In order to indicate the convergence of (2.4.11) the successive approximations

$$t_{1c} = \frac{1}{\gamma}\left\{\frac{1}{2} - \frac{1}{(3+\gamma)}\right\},$$

$$t_{2c} = \frac{1}{\gamma}\left\{\frac{1}{2} - \frac{1}{(3+\gamma)} + \frac{\rho_1}{4(3+\gamma)^2}\right\}, \qquad (2.4.19)$$

$$t_{3c} = \frac{1}{\gamma}\left\{\frac{1}{2} - \frac{1}{(3+\gamma)} + \frac{\rho_1}{4(3+\gamma)^2} - \frac{\rho_2}{5(3+\gamma)^3}\right\},$$

are given in the final section for various values of $\alpha$.

## 2.5 Newton's cooling

Replacing the constant temperature condition $(2.2.2)_1$ with that of Newton's cooling condition, namely

$$T(1,t) + \beta\frac{\partial T}{\partial r}(1,t) = 1, \qquad (2.5.1)$$

while leaving equations (2.2.1), $(2.2.2)_2$, and (2.2.3) unaltered we describe briefly the solution procedure for the sphere ($\lambda = 2$).

Using the transformation variables given by (2.3.3) it is a simple matter to show that the system given by (2.2.1), $(2.2.2)_2$, (2.2.3) and (2.5.1) becomes

$$y\frac{\partial^2\phi}{\partial x^2} = \frac{1}{\alpha}\frac{\partial\phi}{\partial x}(1,y)\left\{x\frac{\partial\phi}{\partial x} - (y-1)\frac{\partial\phi}{\partial y}\right\}, \qquad (2.5.2)$$

subject to the boundary conditions

$$\beta\frac{\partial\phi}{\partial x}(0,y) + (1-\beta)(1-y)\phi(0,y) = (y-1), \qquad \phi(1,y) = 0, \qquad (2.5.3)$$

while the energy balance condition on the moving boundary becomes

$$\frac{\partial\phi}{\partial x}(1,y) = -\alpha y(y-1)\frac{dy}{dt}, \qquad y(0) = 1, \qquad (2.5.4)$$

noting that in deriving (2.5.2) we have utilized (2.5.4).

The above non-linear system (2.5.2)-(2.5.4) can be formally solved by assuming a series solution for $\phi(x,y)$ of the form

$$\phi(x,y) = \sum_{n=0}^{\infty} A_n(x)(y-1)^n, \qquad (2.5.5)$$

where $A_n(x)$ denote functions of $x$ only. From (2.5.2)-(2.5.4) and (2.5.5) we find that the functions $A_n(x)$ are determined by solving

$$A''_0 = \alpha^{-1} A'_0(1) x A'_0,$$

$$A''_n = -A''_{n-1} + \frac{1}{\alpha} \sum_{j=0}^{n} A'_j(1)\left[ xA'_{n-j} - (n-j)A_{n-j} \right], \qquad n = 1, 2, \ldots,$$

$$(2.5.6)$$

subject to the boundary conditions

$$A'_0(0) = 0, \qquad A_n(1) = 0, \quad n = 0, 1, \ldots,$$

$$\beta A'_1(0) + (1-\beta)A_0(0) = 1, \quad \beta A'_n(0) + (1-\beta)A_{n-1}(0) = 0, \quad n = 2, 3, \qquad (2.5.7)$$

where the primes denote differentiation with respect to $x$ and in (2.5.6) the argument of $A_n$ is understood to be $x$ unless otherwise indicated. From (2.5.4) and (2.5.5) we find that the motion of the moving boundary is obtained from

$$\sum_{n=0}^{\infty} A'_n(1)(y-1)^n = -\alpha y(y-1)\frac{dy}{dt}. \qquad (2.5.8)$$

From (2.5.6) and (2.5.7)$_1$ we find that $A_0(x)$ is identically zero while the remaining $A_n(x)$ are obtained simply by integrating equations of the form

$$A''_n(x) = P_n(x), \qquad (2.5.9)$$

where $P_n(x)$ denotes a polynomial expression in $x$ of degree $n-2$ ($n \geq 2$, $P_1(x) = 0$). This is in contrast to the problem with $\beta = 0$ which gives rise to the confluent hypergeometric equations (2.3.5).

Introducing new constants $\eta$ and $\delta$ defined by

$$\eta = \alpha(\beta-1), \qquad \delta = 2-\alpha, \qquad (2.5.10)$$

we find that the first five non zero $A_n(x)$ are as follows

$$A_1(x) = \frac{(x-1)}{\beta},$$

$$A_2(x) = \frac{(x-1)}{2\alpha\beta^2}(x + 1 - 2\eta),$$

$$A_3(x) = \frac{(x-1)}{6\alpha^2\beta^3}\left\{\eta x^2 + (3\delta - 11\eta)x + (3\delta - 14\eta + 6\eta^2)\right\},$$

$$A_4(x) = \frac{(x-1)}{24\alpha^3\beta^4}\left\{(4\eta - \delta)x^3 + (4\eta - \delta)(1 - 4\eta)x^2\right.$$

$$+ (104\eta^2 - 56\eta\delta - 68\eta + 5\delta + 12\delta^2 + 12)x$$

$$\left. - (24\eta^3 - 160\eta^2 + 68\eta\delta + 68\eta - 5\delta - 12\delta^2 - 12)\right\},$$

$$A_5(x) = \frac{(x-1)}{120\alpha^4\beta^5}\left\{\eta(4\eta - \delta)x^4 + (40\eta + 79\eta\delta - 136\eta^2 - 10 - 15\delta^2)x^3\right.$$

$$+ (60\eta + 200\eta^3 + 89\eta\delta - 256\eta^2 - 10 - 15\delta^2 + 20\eta\delta^2 - 100\eta^2\delta)x^2$$

$$+ (- 1000\eta^3 - 940\eta - 891\eta\delta + 2264\eta^2 + 800\eta^2\delta$$

$$- 340\eta\delta^2 + 60\delta^3 + 75\delta^2 + 220\delta + 50)x$$

$$+ (120\eta^4 - 1800\eta^3 + 1140\eta^2\delta - 1000\eta - 916\eta\delta - 400\eta\delta^2$$

$$\left. + 2604\eta^2 + 60\delta^3 + 75\delta^2 + 220\delta + 50)\right\}.$$

$$(2.5.11)$$

In particular the values of $A'_n(1)$ which are needed to determine the motion of the moving boundary are given by

$$A'_1(1) = \frac{1}{\beta},$$

$$A'_2(1) = \frac{1}{\alpha\beta^2}(1 - \eta),$$

$$A'_3(1) = \frac{1}{\alpha^2\beta^3}(\eta^2 - 4\eta + \delta),$$

$$(2.5.12)$$

$$A'_4(1) = \frac{1}{3\alpha^3\beta^4}(\delta + 3\delta^2 + 3 - 15\eta\delta - 3\eta^3 + 31\eta^2 - 16\eta),$$

$$A'_5(1) = \frac{1}{3\alpha^4\beta^5}(3\eta^4 - 65\eta^3 + 112\eta^2 - 46\eta + 3\delta^3 + 3\delta^2$$

$$+ 2 + 11\delta - 41\eta\delta + 46\eta^2\delta - 18\eta\delta^2),$$

From (2.5.8), (2.5.12) and the initial condition $y(0) = 1$ we can deduce the following asymptotic series solution for the motion of the moving boundary,

$$t = -\alpha\beta\left\{(y - 1) + (1 + 2\eta - \delta)\frac{(y - 1)^2}{2\alpha\beta}\right.$$

$$(\eta^2 + 3\eta - 1 - \eta\delta)\frac{(y - 1)^3}{3\alpha^2\beta^2} + (4\eta - \eta^2 - \delta)\frac{(y - 1)^4}{3\alpha^3\beta^3}$$

$$\left. +(5\eta^3 - 52\eta^2 + 28\eta - 5 - 5\delta^2 - 2\delta + 25\eta\delta)\frac{(y - 1)^5}{15\alpha^4\beta^4} + \cdots\right\}.$$

$$(2.5.13)$$

In particular an approximating expression for the time $t_c$ to complete melting can be obtained from (2.5.13) by setting $y$ to zero, thus

$$t_c = \alpha\gamma\left\{1 - \frac{(1 + 2\eta - \delta)}{2\alpha\beta} + \frac{(\eta^2 + 3\eta - 1 - \eta\delta)}{3\alpha^2\beta^2} - \frac{(4\eta - \eta^2 - \delta)}{3\alpha^3\beta^3} + \right.$$

$$\left. \frac{(5\eta^3 - 52\eta^2 + 28\eta - 5 - 5\delta^2 - 2\delta + 25\eta\delta)}{15\alpha^4\beta^4} + \cdots\right\}.$$

$$(2.5.14)$$

Numerical values of various estimates for $t_c$ obtained from (2.5.14) are given in the final section.

We observe from (2.5.13) on using (2.5.10) and neglecting terms of order $\alpha^{-1}$ and higher,

$$t = -\alpha\beta\left\{(y - 1) + \frac{(2\beta - 1)}{2\beta}(y - 1)^2 + \frac{(\beta - 1)}{3\beta}(y - 1)^3\right\}$$

$$+ \left\{\frac{(y - 1)^2}{2} - \frac{(\beta - 1)(y - 1)^3}{3\beta}\left[1 - \tau + \tau^2 - \cdots\right]\right\} + o(1),$$

$$(2.5.15)$$

where $\tau$ is defined by

$$\tau = \frac{(\beta - 1)(y - 1)}{\beta}. \qquad (2.5.16)$$

It is of interest to note that the exact motion correct up to order $\alpha^{-1}$ can be deduced from (2.5.15) by assuming that the series in the square brackets involving $\tau$ is the geometric series with sum $(1 + \tau)^{-1}$ (assuming $|\tau| < 1$). Simplifying the result we

obtain from (2.5.15)

$$t = -\frac{\alpha}{6}\left\{2(\beta - 1)y^3 + 3y^2 - (2\beta + 1)\right\} + \frac{(y - 1)^2}{6}\left\{\frac{(2\beta + 1) + (\beta - 1)y}{1 + (\beta - 1)y}\right\} + o(1),$$

$$(2.5.17)$$

which can of course be deduced more directly from an assumption of the form

$$T(r,t) = T_1(r,t) + T_2(r,t)/\alpha + T_3(r,t)/\alpha^2 + O(1/\alpha^3). \qquad (2.5.18)$$

Finally in this section we observe that the first term of (2.5.17) is precisely the pseudo steady state result and moreover that the pseudo steady state expression for $\phi(x,y)$ can be seen to arise from (2.5.5) and (2.5.11) by retaining only the terms of order one in the expression (2.5.11). We find that

$$\phi(x,y) = \frac{(x - 1)(y - 1)}{\beta}\left\{1 - \tau + \tau^2 - \tau^3 + \tau^4 - \cdots\right\} + o(1), \qquad (2.5.19)$$

where $\tau$ is given by (2.5.16). Again on assuming the series involving $\tau$ is the geometric series and that $|\tau| < 1$ we obtain in a straightforward manner

$$\phi(x,y) = \frac{(x - 1)(y - 1)}{[1 + (\beta - 1)y]} + o(1), \qquad (2.5.20)$$

which is precisely the pseudo steady state result.

## 2.6 Alternative solution for the sphere

Instead of (2.3.3) we make the following transformation of independent variables,

$$x = \frac{r^{-1} - 1}{R^{-1} - 1}, \quad y = R^{-1} - 1, \qquad (2.6.1)$$

and look for a solution of the form

$$T(r,t) = A_0(x) + A_1^*(x)y + A_2^*(x)y^2 + \cdots. \qquad (2.6.2)$$

In order to determine these functions we may either proceed directly as in Section 2.3 or we may simply reconcile the two expressions (2.3.4) and (2.6.2) by writing the

$(x, y)$ variables in (2.3.4) in terms of those defined by (2.6.1) and then expanding in powers of y and equating coefficients of $y^0$, $y^1$, and $y^2$. We find $A_0(x)$ is as usual given by (2.3.8)$_1$ while $A_1^*(x)$ and $A_2^*(x)$ are given by

$$A_1^*(x) = A_1(x) + x(1 - x)A_0'(x) + xA_0(x), \qquad (2.6.3)$$

$$A_2^*(x) = A_2(x) + (1 - x)[xA_1'(x) - A_1(x)] + x^2(1 - x)^2A_0''(x)/2, \qquad (2.6.4)$$

where $A_1(x)$ and $A_2(x)$ are defined by (2.3.8)$_2$ and (2.3.8)$_3$ respectively. These equations yield

$$A_1^*(x) = -\alpha\gamma x\left\{(1 - x)e^{\frac{\gamma}{2}(1 - x^2)} - \int_x^1 e^{\frac{\gamma}{2}(1 - \xi^2)} d\xi + \frac{1}{(\gamma + 3)}[e^{\frac{\gamma}{2}(1 - x^2)} - 1]\right\},$$
$$(2.6.5)$$

$$A_2^*(x) = A_2(x) + \alpha\gamma^2 x^3(1 - x)\left\{\frac{1}{(\gamma + 3)} + \frac{(1 - x)}{2}\right\}e^{\frac{\gamma}{2}(1 - x^2)}, \qquad (2.6.6)$$

where $A_2(x)$ is obtained from (2.3.8)$_3$ and (2.3.9). From (2.2.3) and (2.6.2) we may cast the motion of the boundary in the form

$$t = \gamma^{-1} \int_R^1 \frac{(1 - \xi)\xi^3 \, d\xi}{(\beta_1\xi^2 - \beta_2\xi + \beta_3)}, \qquad (2.6.7)$$

where $\beta_1$, $\beta_2$ and $\beta_3$ are defined by

$$\beta_1 = 1 + \delta_1 - \delta_2, \quad \beta_2 = \delta_1 - 2\delta_2, \quad \beta_3 = -\delta_2, \qquad (2.6.8)$$

where $\delta_1$ and $\delta_2$ are given by

$$\delta_1 = (\alpha\gamma)^{-1}\frac{dA_1^*(1)}{dx}, \quad \delta_2 = (\alpha\gamma)^{-1}\frac{dA_2^*(1)}{dx}. \qquad (2.6.9)$$

If we define $\psi(\xi)$ by

$$\psi(\xi) = \xi^3(\beta_1\xi^2 - \beta_2\xi + \beta_3)^{-1}, \qquad (2.6.10)$$

then from (2.6.6) and the Taylor series

$$\psi(\xi) = \psi(1) + (\xi - 1)\psi'(1) + (\xi - 1)^2\psi''(1)/2 + \cdots, \qquad (2.6.11)$$

we obtain for the motion of the boundary

$$t = \gamma^{-1}\left\{\frac{\psi(1)}{2}(R-1)^2 + \frac{\psi'(1)}{3}(R-1)^3 + \frac{\psi''(1)}{8}(R-1)^4 + \cdots\right\}. \quad (2.6.12)$$

Remarkably this equation can be shown to be identical to that obtained previously in Section 2.3 using variables essentially defined by (2.3.3).

## 2.7 Numerical results

In this section we compare our approximations with various perturbation, integral iteration and theoretical bounds against numerical solutions obtained by the enthalpy method of Voller and Cross (1981).

Figures 2.1 and 2.2 compare the approximations to the boundary motion given by (2.4.10) and the numerical solution obtained by the enthalpy method of Voller and Cross (1981), for $\alpha = 0.2$ and $\alpha = 2.0$ respectively. Clearly the procedure described in Sections 2.3 and 2.4 yields excellent approximations for even small values of $\alpha$. In order to indicate the convergence of (2.4.12) the successive approximations

$$t_{1c} = \frac{1}{\gamma}\left\{\frac{1}{2} - \frac{1}{(3+\gamma)}\right\},$$

$$t_{2c} = \frac{1}{\gamma}\left\{\frac{1}{2} - \frac{1}{(3+\gamma)} + \frac{\rho_1}{4(3+\gamma)^2}\right\}, \quad (2.7.1)$$

$$t_{3c} = \frac{1}{\gamma}\left\{\frac{1}{2} - \frac{1}{(3+\gamma)} + \frac{\rho_1}{4(3+\gamma)^2} - \frac{\rho_2}{5(3+\gamma)^3}\right\},$$

are given in Table 2.1 for various values of $\alpha$. In addition the pseudo steady state estimate and the order one corrected perturbation estimate are also included in the table. From these values the pseudo steady state estimate $\alpha/6$ and the order one corrected perturbation estimate $(\alpha + 1)/6$ provide lower and upper bounds respectively for the times to complete melting. These lower and upper bounds can

be verified rigorously by making use of the integral formulation of Theofanous and Lim (1971), and the physically obvious inequalities $0 \le T(r,t) \le 1$. The values given in Table 2.1 also reflect the excellent convergence of the series (2.4.12) even for very small values of $\alpha$. Furthermore $R = 0$ is the worst possible situation as far as the convergence of the series (2.4.10) is concerned. For example we would expect the estimate (2.4.10) for the times when $0 < R << 1$ to be more accurate. Table 2.2 compares estimate (2.4.10) with the pseudo steady state approximation, order one corrected perturbation estimate and the numerical solution of Voller and Cross (1981) for the motion of the boundary with $\alpha = 1.0$. Again the accuracy of estimate (2.4.10) is seen to be surprisingly good.

From (2.5.14) we obtain for the Newton's boundary condition case ($\beta \ne 0$) the following estimates for the times $t_c$ to complete melting

$$t_{1c}^* = \alpha\gamma \left\{ 1 - \frac{(1 + 2\eta - \delta)}{2\alpha\beta} + \frac{(\eta^2 + 3\eta - 1 - \eta\delta)}{3\alpha^2\beta^2} \right\},$$

$$t_{2c}^* = \alpha\gamma \left\{ 1 - \frac{(1 + 2\eta - \delta)}{2\alpha\beta} + \frac{(\eta^2 + 3\eta - 1 - \eta\delta)}{3\alpha^2\beta^2} - \frac{(4\eta - \eta^2 - \delta)}{3\alpha^3\beta^3} \right\},$$

$$t_{3c}^* = \alpha\gamma \left\{ 1 - \frac{(1 + 2\eta - \delta)}{2\alpha\beta} + \frac{(\eta^2 + 3\eta - 1 - \eta\delta)}{3\alpha^2\beta^2} - \frac{(4\eta - \eta^2 - \delta)}{3\alpha^3\beta^3} + \right.$$

$$\left. \frac{(5\eta^3 - 52\eta^2 + 28\eta - 5 - 5\delta^2 - 2\delta + 25\eta\delta)}{15\alpha^4\beta^4} \right\}.$$

$$(2.7.2)$$

From (2.5.17) with $y = 0$ we obtain the pseudo steady state and first order corrected perturbation estimates to $t_c$, namely

$$t_l = \alpha(2\beta + 1)/6, \qquad t_u = (\alpha + 1)(2\beta + 1)/6. \qquad (2.7.3)$$

Numerical values of the above estimates are given in Tables 2.3 and 2.4 for various values of $\alpha$ and $\beta = 5$, and various values of $\beta$ with $\alpha = 5$ respectively. Firstly these results indicate reasonable convergence of the series (2.5.14) and secondly they

are consistent with the theoretical bounds (2.7.3). Again, as in the $\beta = 0$ case, $R = 0$ is the worst possible situation as far as the convergence of the series (2.4.14) is concerned.

Figures 2.3 and 2.4 show the variation of position $R(t)$ with time for $\alpha = 2$ and $\alpha = 10$ respectively and three values of $\beta$. The numerical values based on (2.5.13) are clearly in general agreement with those of Shih and Chou (1971) and the numerical solution of Tao (1967). We note however the discrepancies for the time to complete melting with this work and Shih and Chou (1971) in the case where $\alpha = 2.0$ and $\beta = 4.0$. This observation is consistent with comments of Shih and Chou (1971) who indicate their semi-analytical procedure is more accurate for small $\beta$. In contrast the series (2.5.13) and (2.5.14) are seen to converge more rapidly for large values of $\beta$ and therefore in this sense the procedure described here is complementary to that of Shih and Chou (1971).

## 2.8 Discussion and conclusion

We may now rationalize Landau's transformation and the cylindrical and spherical boundary fixing transformations (2.3.10) and (2.6.1) respectively by

$$x = \frac{K_\lambda(1,r)}{K_\lambda(1,R)}, \qquad y = K_\lambda(1,R), \qquad (2.8.1)$$

where $K_\lambda(x,y)$ is introduced in Hill and Dewynne (1984) in the context of bounding the motion of the boundary and is defined by

$$K_\lambda(x,y) = \int_y^x \xi^{-\lambda} d\xi. \qquad (2.8.2)$$

We observe that $f(r) = K_\lambda(1,r)$ is simply the solution of

$$\frac{d^2 f}{dr^2} + \frac{\lambda}{r} \frac{df}{dr} = 0, \qquad (2.8.3)$$

such that

$$f(1) = 0, \qquad \frac{df}{dr}(1) = -1. \qquad (2.8.4)$$

This particular choice of $f(r)$ arises as follows. With

$$x = \frac{f(r)}{f(R)}, \qquad y = f(R), \qquad (2.8.5)$$

and $T(r,t) = \phi(x,y)$ we see that (2.2.1) becomes

$$\alpha\left\{\frac{\partial^2\phi}{\partial x^2}\left(\frac{df}{dr}\right)^2 + y\frac{\partial\phi}{\partial x}\left(\frac{d^2f}{dr^2} + \frac{\lambda}{r}\frac{df}{dr}\right)\right\} = \left(\frac{df}{dR}\right)^2\frac{\partial\phi}{\partial x}(1,y)\left(x\frac{\partial\phi}{\partial x} - y\frac{\partial\phi}{\partial y}\right), \quad (2.8.6)$$

and therefore the choice (2.8.3) provides the greatest simplification. We also observe for (2.6.1) that since $y \to \infty$ as $R \to 0$ it is natural to use an Euler transformation $y/(1 + y)$ which in this case is simply $1 - R$, namely that used in (2.3.3). This provides some justification for using Landau's transformation for the spherical problem. It will be seen that for more complicated moving boundary problems, these observations provide great insight into choosing the most appropriate new independent variables which not only fix the boundary but also lead to meaningful numerical results.

In conclusion, we note that the boundary fixing series method just described yields very simple yet highly accurate results which display all the subtle features of the numerical solutions. Furthermore, it lacks the usual problems associated with complicated singular perturbations (i.e singular behaviour for small $\alpha$ and boundary layer behaviour near $R = 0$), or messy integral iterations.
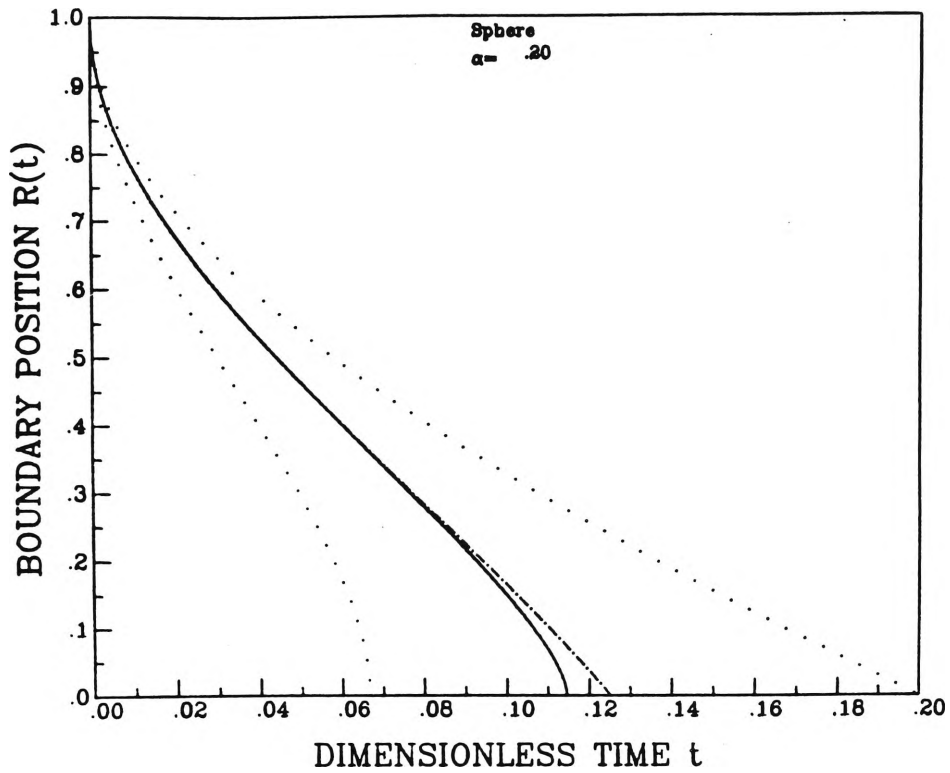
**Figure 2.1**    Comparison of the boundary fixing estimate $(-\cdot-\cdot-)$ and theoretical bounds $(\cdots)$ with numerical solution $(\rule{2cm}{0.4pt})$ for the boundary motion with $\alpha = 0.2$
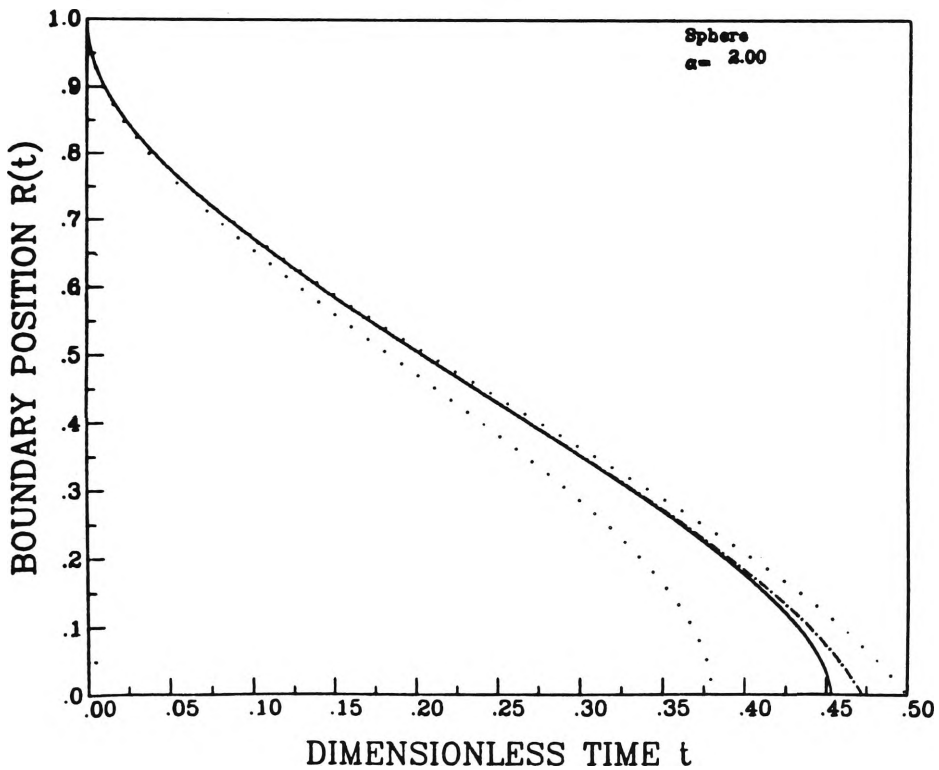


**Figure 2.2**    Comparison of the boundary fixing estimate $(-\cdot-\cdot-)$ and theoretical bounds $(\cdots)$ with numerical solution $(\rule{2cm}{0.4pt})$ for the boundary motion with $\alpha = 2.0$
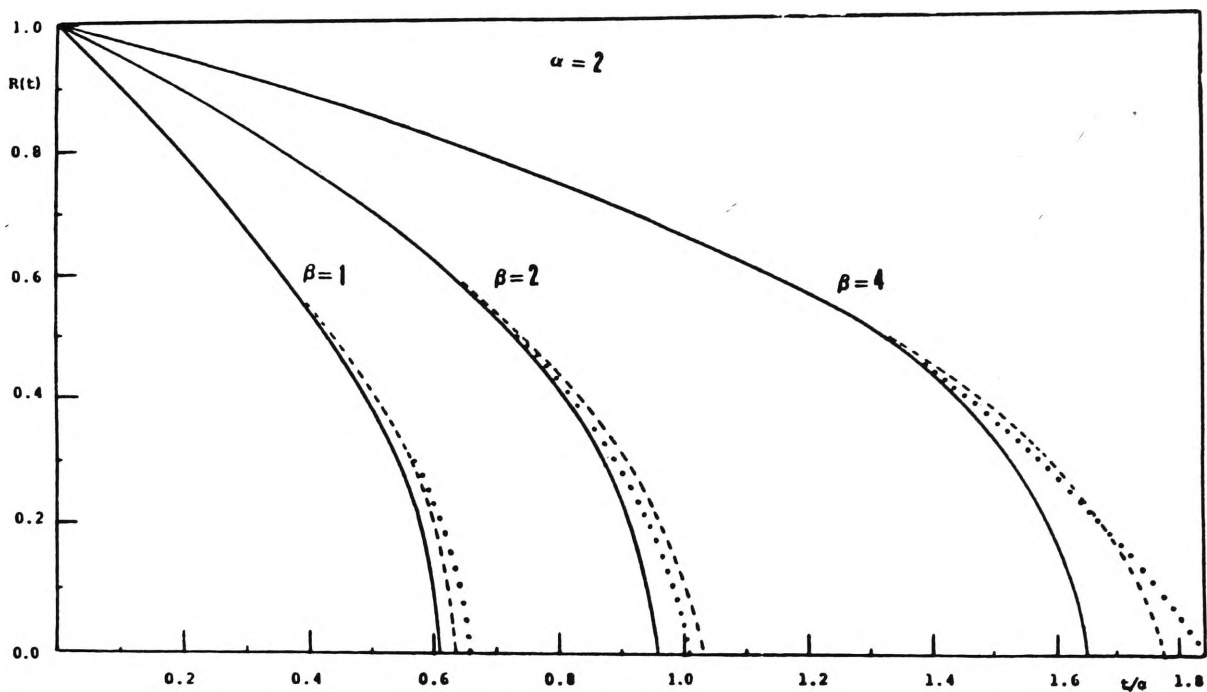
Figure 2.3     Comparison of the boundary fixing estimate $(\cdots)$,   with Shih and Chou (1971) (————),
and numerical solution of Tao (1967) $(-\ -\ -\ -)$ for $\alpha = 2$
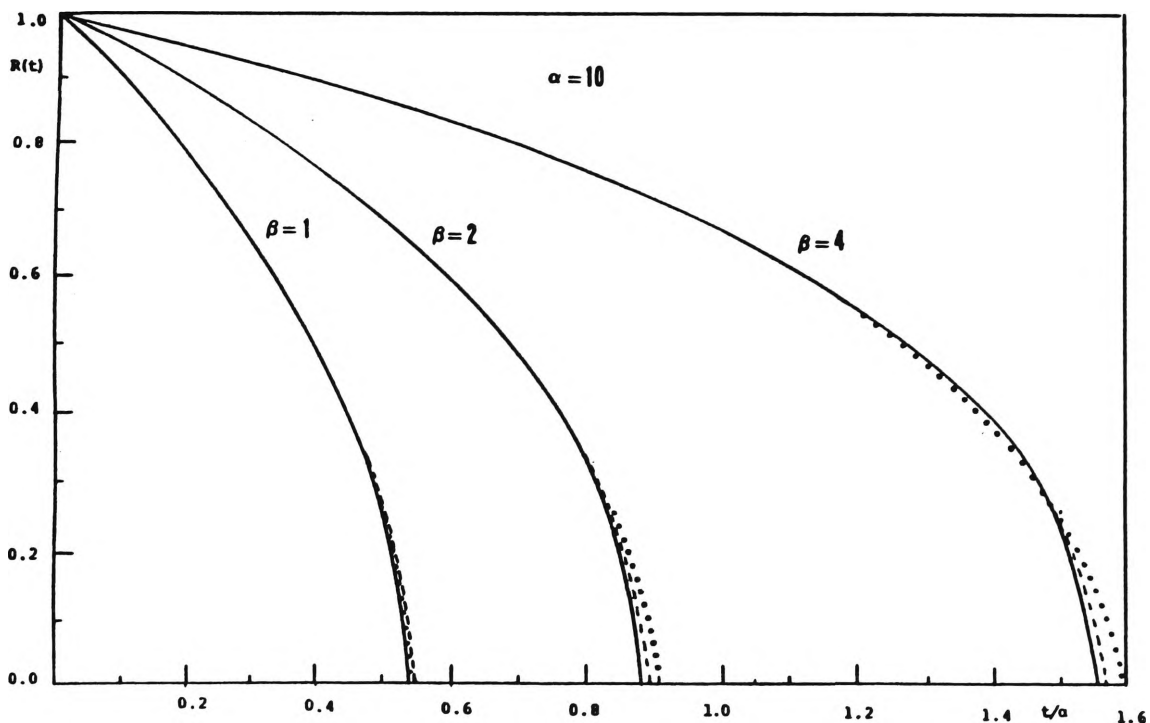


Figure 2.4     Comparison of the boundary fixing estimate $(\cdots)$,   with Shih and Chou (1971) (————),
and numerical solution of Tao (1967) $(-\ -\ -\ -)$ for $\alpha = 10$

| $R = 0$ $\alpha$ | $\alpha/6$ | $t_{c1}$ $(2.7.1)_1$ | $t_{c2}$ $(2.7.1)_2$ | $t_{c3}$ $(2.7.1)_3$ | Numer. Sol. | $(\alpha + 1)/6.$ |
|---|---|---|---|---|---|---|
| 0.01 | .0017 | .0582 | .0545 | .0526 | .0475 | .1683 |
| 0.02 | .0033 | .0678 | .0633 | .0611 | .0552 | .1700 |
| 0.05 | .0083 | .0861 | .0805 | .0774 | .0701 | .1750 |
| 0.10 | .0167 | .1069 | .0997 | .0962 | .0875 | .1833 |
| 0.20 | .0333 | .1378 | .1294 | .1252 | .1146 | .2000 |
| 0.50 | .0833 | .2079 | .1988 | .1938 | .1799 | .2500 |
| 1.00 | .1667 | .3052 | .2970 | .2919 | .2751 | .3333 |
| 2.00 | .3333 | .4829 | .4767 | .4724 | .4532 | .5000 |
| 5.00 | .8333 | .9921 | .9887 | .9860 | .9666 | 1.0000 |
| 10.00 | 1.6667 | 1.8291 | 1.8272 | 1.8256 | 1.8086 | 1.8333 |

Table 2.1    Numerical values of estimates defined by equations $(2.7.1)$, $\alpha/6$, $(\alpha + 1)/6$ and numerical solutions, for selected values of $\alpha$

| $\alpha = 1$ $R$ | Pseudo Steady State | Boundary Fix. Est. $(2.4.10)$ | Numerical Solution | Perturbation Estimate |
|---|---|---|---|---|
| 1.0 | .000000 | .000000 | .000000 | .000000 |
| 0.9 | .004667 | .006156 | .006162 | .006333 |
| 0.8 | .017333 | .023234 | .023243 | .024000 |
| 0.7 | .036000 | .049126 | .049134 | .051000 |
| 0.6 | .058667 | .081693 | .081683 | .085333 |
| 0.5 | .083333 | .118759 | .118665 | .125000 |
| 0.4 | .108000 | .158101 | .157765 | .168000 |
| 0.3 | .130667 | .197450 | .196462 | .212333 |
| 0.2 | .149333 | .234477 | .231906 | .256000 |
| 0.1 | .162000 | .266793 | .260403 | .297000 |
| 0.0 | .166667 | .291941 | .275163 | .333333 |

Table 2.2    Numerical values of estimates defined by equations $(2.4.10)$, the pseudo steady state estimate, order one corrected perturbation estimate and numerical solutions, for $\alpha = 1.0$

| $\beta = 5$ <br> $\alpha$ | Lower <br> Bound | $t^{*}_{c1}$ <br> $(2.7.3)_1$ | $t^{*}_{c2}$ <br> $(2.7.3)_2$ | $t^{*}_{c3}$ <br> $(2.7.3)_3$ | Upper <br> Bound |
|---|---|---|---|---|---|
| 5 | 9.17 | 9.92 | 10.09 | 10.17 | 11.00 |
| 10 | 18.33 | 19.09 | 19.28 | 19.41 | 20.12 |
| 15 | 27.50 | 28.26 | 28.46 | 28.60 | 29.33 |
| 20 | 36.67 | 37.43 | 37.63 | 37.78 | 38.50 |
| 25 | 45.83 | 46.60 | 46.80 | 46.95 | 47.67 |
| 30 | 55.00 | 55.76 | 55.97 | 56.12 | 56.83 |
| 35 | 64.17 | 64.93 | 65.14 | 65.29 | 66.00 |
| 40 | 73.33 | 74.10 | 74.31 | 74.46 | 75.17 |
| 45 | 82.50 | 83.27 | 83.47 | 83.63 | 84.33 |
| 50 | 91.67 | 92.43 | 92.64 | 92.80 | 93.50 |

Table 2.3     Numerical values of estimates defined by equations $(2.7.3)$ and bounds $(2.7.4)$ for various values of $\alpha$ and $\beta = 5.0$

| $\alpha = 5$ <br> $\beta$ | Lower <br> Bound | $t^{*}_{c1}$ <br> $(2.7.3)_1$ | $t^{*}_{c2}$ <br> $(2.7.3)_2$ | $t^{*}_{c3}$ <br> $(2.7.3)_3$ | Upper <br> Bound |
|---|---|---|---|---|---|
| 5 | 9.17 | 9.93 | 10.09 | 10.17 | 11.00 |
| 10 | 17.50 | 18.29 | 18.94 | 18.72 | 21.00 |
| 15 | 25.83 | 26.64 | 26.91 | 27.14 | 31.00 |
| 20 | 34.17 | 34.98 | 35.27 | 35.52 | 41.00 |
| 25 | 42.50 | 43.32 | 43.61 | 43.88 | 51.00 |
| 30 | 50.83 | 51.65 | 51.96 | 52.24 | 61.00 |
| 35 | 59.17 | 59.99 | 60.30 | 60.58 | 71.00 |
| 40 | 67.50 | 68.32 | 68.63 | 68.93 | 81.00 |
| 45 | 75.83 | 76.66 | 76.97 | 77.27 | 91.00 |
| 50 | 84.17 | 84.99 | 85.31 | 85.61 | 101.00 |

Table 2.4     Numerical values of estimates defined by equations $(2.7.3)$ and bounds $(2.7.4)$ for various values of $\beta$ and $\alpha = 5.0$

# CHAPTER THREE

# Planar Solidification with Newton Cooling

## 3.1 Introduction

In this chapter we consider the classical problem of the planar solidification of a liquid initialy uniformly at its freezing point, comprising the semi-infinite half-space with Newton cooling at the surface. By fixing the boundary we obtain two iterative analytic series solutions, the first valid for small times and the second valid for subsequent times. The technique employed is an extension of the method proposed in Chapter 2 for freezing a saturated liquid inside a spherical container. The major contribution of this chapter is the so-called large time solution which gives accurate results at all times apart from the small initial period at which the short time solution applies. In the limit of no Newton cooling at the surface the initial time interval, over which the short time solution is applicable, shrinks to zero, and the large time solution yields precisely the well known Neumann solution. In Section 3.2 we describe the physical problem in detail and formulate the equations in dimensionless form. In Section 3.3 we state known bounds and outline the method of solution. In Sections 3.4 and 3.5 we present main results for the short and large time cases respectively. A detailed numerical comparison and a discussion is presented in Section 3.6.

## 3.2 Governing equations

We suppose that the semi-infinite half-space $(0, \infty)$ consists of a molten material at its uniform fusion temperature $T_f$. At time zero we assume the plane $x^* = 0$ is surrounded by a coolant which is maintained at a constant temperature $T_0$. Under the usual assumptions the problem with Newton's cooling at the surface becomes in dimensionless variables

$$\frac{\partial \overline{T}}{\partial \overline{t}} = \frac{\partial^2 \overline{T}}{\partial \overline{x}^2}, \quad 0 < \overline{x} < \overline{X}(\overline{t}), \tag{3.2.1}$$

$$\overline{T}(0,\overline{t}) - \beta \frac{\partial \overline{T}}{\partial \overline{x}}(0,\overline{t}) = 1, \quad \overline{T}\big(\overline{X}(\overline{t}),\overline{t}\big) = 0, \tag{3.2.2}$$

$$\frac{\partial \overline{T}}{\partial \overline{x}}\big(\overline{X}(\overline{t}),\overline{t}\big) = -\alpha \frac{d\overline{X}}{d\overline{t}}, \quad \overline{X}(0) = 0, \tag{3.2.3}$$

where $\overline{T}(\overline{x}, \overline{t})$ and $\overline{X}(\overline{t})$ denote the non-dimensional temperature and the position of the moving boundary. The non-dimensional variables and constants $\alpha$ and $\beta$ are defined in terms of the "starred" physical parameters given by the equations

$$\overline{x} = \frac{x^*}{\ell}, \quad \overline{X} = \frac{X^*}{\ell}, \quad \overline{t} = \frac{kt^*}{\rho C \ell^2}, \quad \overline{T} = \frac{T_f - T^*}{T_f - T_0}, \tag{3.2.4}$$

$$\alpha = \frac{L}{C(T_f - T_0)}, \quad \beta = \frac{k}{h\ell}, \tag{3.2.5}$$

where $k$, $C$ and $\rho$ are respectively the thermal conductivity, heat capacity and density of the solid, $L$ is the latent heat of fusion, $h$ is the heat transfer coefficient and $\ell$ is any convenient length scale. In fact throughout we work with the following dimensionless variables

$$x = \frac{\overline{x}}{\beta}, \quad X = \frac{\overline{X}}{\beta}, \quad t = \frac{\overline{t}}{\beta^2}, \tag{3.2.6}$$

and $T(x, t) = \overline{T}(\overline{x}, \overline{t})$ so that problem (3.2.1) – (3.2.3) becomes

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < X(t), \tag{3.2.7}$$

$$T(0, t) - \frac{\partial T}{\partial x}(0, t) = 1, \quad T(X(t), t) = 0, \tag{3.2.8}$$

$$\frac{\partial T}{\partial x}(X(t),t) = -\alpha \frac{dX}{dt}(t), \quad X(0) = 0. \tag{3.2.9}$$

We have purposely noted the intermediate transformations (3.2.4), since it is important to identify the case of no Newton cooling at the surface, that is $\beta$ zero. This limiting case is somewhat obscured in the working variables (3.2.6). Perturbation solutions of (3.2.7) − (3.2.9) using $\alpha^{-1}$ as a small parameter are given in Pedroso and Domoto, (1973a), and Huang and Shih, (1975a,b) while standard integral iteration and heat balance methods are used in Siegel and Savino, (1966), Savino and Siegel, (1969), and Goodman, (1958) respectively. Other special methods and applications relating to the above problem can be found in Libby and Chen, (1965), Lock et al., (1969), Seeniraj, (1980), Cho and Sunderland, (1981) and Tao, (1981). Although a numerical solution of this problem can be effected by a finite difference enthalpy method (see, for example Voller and Cross, 1981) the implementation of the Newton cooling condition involves the step size and the required accuracy can only be achieved by taking extremely small step sizes. Thus computing time becomes expensive, especially for infinite domain problems.

In the following Section we briefly summarize simple known results and bounds for this problem and describe in general terms the method of solution adopted here. Since the details and calculations for the short and large time solutions are similar to those given in Chapter 2, only summaries of the main results are presented in Sections 3.3 and 3.4. Numerical results are given in the final section.

## 3.3 Known bounds and method of solution

The standard pseudo-steady state approximation to (3.2.7) − (3.2.9) is given by

$$T_{pss}(x,t) = \frac{X(t) - x}{1 + X(t)}, \quad t = \frac{\alpha}{2}X(t)[X(t) + 2], \tag{3.3.1}$$

where strictly speaking the motion of the boundary in this equation should be distinguished as the pseudo-steady state motion $X_{pss}(t)$. Dewynne and Hill (1984) show that $T(x,t)$ satisfies the integro-differential equation

$$T(x,t) = \frac{\partial}{\partial t} \int_x^{X(t)} (\xi - x)[\alpha + T(\xi,t)]\, d\xi,$$  (3.3.2)

while the exact motion of the moving boundary is formally determined from

$$t = \int_0^{X(t)} (1 + \xi)[\alpha + T(\xi,t)]\, d\xi.$$  (3.3.3)

From these equations and the first two inequalities of

$$0 \le T(x,t) \le T_{pss}(x,t) \le 1,$$  (3.3.4)

it follows that the motion satisfies the bounds

$$\frac{\alpha}{2} X(X + 2) \le t \le \frac{\alpha}{2} X(X + 2) + \frac{X^2(X + 3)}{6(X + 1)}.$$  (3.3.5)

We observe that the lower bound is simply the pseudo-steady state estimate while the upper bound can be shown to be the correct motion up to order $\alpha^{-1}$ (see Huang and Shih 1975a). By integrating (3.3.3) Hill and Dewynne (1984) show that an improved lower bound is

$$t^2 \ge \left[\frac{\alpha}{2} X(X + 2)\right]^2 + \frac{\alpha X^3}{12}(X + 4).$$  (3.3.6)

In terms of new variables defined by

$$y = \frac{x}{X(t)}, \quad z = X(t), \quad T(x,t) = \phi(y,z),$$  (3.3.7)

the problem (3.2.7) $-$ (3.2.9) becomes

$$\alpha \phi_{yy} = \phi_y(1,z)[y\phi_y - z\phi_z],$$  (3.3.8)

$$\phi_y(0,z) = z[\phi(0,z) - 1], \quad \phi(1,z) = 0,$$  (3.3.9)

$$\phi_y(1,z) = -\alpha z \frac{dz}{dt}, \quad z(0) = 0,$$  (3.3.10)

where subscripts denote partial derivatives and the arguments of $\phi$ and its derivatives are understood to be $(y,z)$ unless otherwise indicated. In the following Section we obtain a short time solution of the problem by assuming a series solution of the form

$$\phi(y,z) = \sum_{n=0}^{\infty} A_n(y)z^n. \tag{3.3.11}$$

For intermediate and large times we find that the convergence of this series is not improved by successive Euler transformations. However $(1 + z)^{-1}$ does provide an appropriate large time expansion variable. Accordingly we define further new variables by

$$y = \frac{x}{X(t)}, \quad Z = \frac{1}{1 + X(t)}, \quad T(x,t) = \psi(y,Z), \tag{3.3.12}$$

and the problem becomes

$$\alpha\psi_{yy} = \psi_y(1,Z)[y\psi_y + Z(1 - Z)\psi_Z], \tag{3.3.13}$$

$$Z\psi_y(0,Z) = (1 - Z)[\psi(0,Z) - 1], \quad \psi(1,Z) = 0, \tag{3.3.14}$$

$$\psi_y(1,Z) = \alpha(1 - Z)Z^{-3}\frac{dZ}{dt}, \quad Z(0) = 1. \tag{3.3.15}$$

In Section 3.5 we solve the problem by means of a series solution of the form

$$\psi(y,Z) = \sum_{n=0}^{\infty} B_n(y)Z^n. \tag{3.3.16}$$

Finally in this section we note that on equating expressions (3.3.11) and (3.3.16) and replacing $Z$ by $(1 + z)^{-1}$ it is a simple matter to deduce the following identity

$$A_n(y) = (-1)^n \sum_{j=0}^{\infty} \binom{n + j - 1}{j - 1} B_j(y), \tag{3.3.17}$$

and we observe that the inverse relations of (3.3.17) are not immediately apparent.

## 3.4 Short time solution

From (3.3.8), (3.3.9) and the assumed series solution (3.3.11) it is a straightforward matter to deduce a system of ordinary differential equations and boundary conditions for $A_n(y)$ which are solved recursively. The analysis involves simply integrating polynomials and is similar to that given in Chapter 2. The expressions obtained for the first six $A_n(y)$ are,

$$A_0(y) = 0,$$

$$A_1(y) = 1 - y,$$

$$A_2(y) = \frac{(y - 1)}{2\alpha}[(y - 1) + 2(\alpha + 1)],$$

$$A_3(y) = \frac{(y - 1)}{6\alpha^2}[\alpha(y - 1)^2 - 6(\alpha + 1)(y - 1) - 6(\alpha + 1)(\alpha + 2)],$$

$$A_4(y) = \frac{(y - 1)}{24\alpha^3}[-(3\alpha + 2)(y - 1)^3 - 4(\alpha + 1)(3\alpha + 2)(y - 1)^2$$
$$+ 12(\alpha + 1)(3\alpha + 5)(y - 1) + 8(\alpha + 1)(3\alpha^2 + 16\alpha + 17)],$$

$$A_5(y) = \frac{(y - 1)}{120\alpha^4}[-\alpha(3\alpha + 2)(y - 1)^4 + 10(\alpha + 1)(6\alpha + 7)(y - 1)^3$$
$$+ 20(\alpha + 1)(\alpha + 2)(6\alpha + 7)(y - 1)^2 - 40(\alpha + 1)(6\alpha^2 + 25\alpha + 23)(y - 1)$$
$$- 40(\alpha + 1)(3\alpha^3 + 31\alpha^2 + 81\alpha + 60)].$$

$$(3.4.1)$$

From these expressions and (3.3.10) we find on integration that the motion of the boundary is given by

$$t = \alpha X + (\alpha + 1)X^2\left\{\frac{1}{2} - \frac{X}{3\alpha} + \frac{(\alpha + 2)}{3\alpha^2}X^2 - \frac{(5\alpha^2 + 27\alpha + 29)}{15\alpha^3}X^3 + \cdots\right\}.$$

$$(3.4.2)$$

We observe that the pseudo-steady state emerges from (3.3.11) and (3.4.1) by retaining only the order one contribution and neglecting terms of order $\alpha^{-1}$ and higher powers, namely

$$\phi(y, z) = -(y - 1)z[1 - z + z^2 - z^3 + z^4 + \cdots] + O(\alpha^{-1}),  \quad (3.4.3)$$

which, on assuming the series in (3.4.3) is geometric gives precisely (3.3.1)$_1$. For the motion (3.4.2), if we retain terms of order $\alpha$ and order one, that is

$$t = \frac{\alpha}{2}X(X + 2) + \frac{X^2}{2} - \frac{X^3}{3}[1 - X + X^2 + \cdots] + O(\alpha^{-1}), \qquad (3.4.4)$$

then the order one corrected motion given in (3.3.5) emerges assuming the series in (3.4.4) is geometric with sum $(1 + X)^{-1}$.

From numerical values of the following estimates of the motion obtained from (3.4.2),

$$t_1(X) = \alpha X + (\alpha + 1)X^2\left\{\frac{1}{2} - \frac{X}{3\alpha} + \frac{(\alpha + 2)}{3\alpha^2}X^2\right\},$$

$$t_2(X) = \alpha X + (\alpha + 1)X^2\left\{\frac{1}{2} - \frac{X}{3\alpha} + \frac{(\alpha + 2)}{3\alpha^2}X^2 - \frac{(5\alpha^2 + 27\alpha + 29)}{15\alpha^3}X^3\right\},$$

$$\qquad (3.4.5)$$

it is apparent from these results that these estimates apply only for sufficiently small values of $X$. For example the condition $X \leq \frac{\alpha}{(\alpha + 1)(\alpha + 2)}$ is sufficient to ensure that both $t_1(X)$ and $t_2(X)$ satisfy the inequalities (3.3.5) for all values of $\alpha$. However for large $\alpha$ these estimates are applicable beyond this value. We note that in the 'barred' variables this condition becomes $\overline{X} \leq \frac{\alpha\beta}{(\alpha + 1)(\alpha + 2)}$ and therefore the range of validity of the short time solution in the limit of no Newton cooling on the surface ($\beta$ zero) shrinks to zero. From the following Section it is apparent that the large time solution yields the exact Neumann solution in this limit.

## 3.5 Large time solution

From (3.3.13), (3.3.14) and the assumed series solution (3.3.16) we may show that $B_n(y)$ satisfy an ordinary differential equation of the form

$$B_n'' + \gamma(yB_n' + nB_n) = f_n(y), \quad (n \geq 0), \qquad (3.5.1)$$

where primes denote differentiation with respect to y, $\gamma = -B'_0(1)/\alpha$, $f_0(y)$ is zero and for $n \geq 1$,

$$f_n(y) = (n-1)\gamma B_{n-1} + \frac{1}{\alpha} \sum_{j=1}^{n} B'_j(1)[y B'_{n-j} + (n-j)B_{n-j} - (n-j-1)B_{n-j-1}],$$

(3.5.2)

with the convention $B_{-1}$ is taken to be zero. Further, the boundary conditions are

$$B_0(0) = 1, \quad B_1(0) = B'_0(0), \quad B_n(0) = B'_{n-1}(0) + B_{n-1}(0) \quad (n \geq 2),$$

$$B_n(1) = 0 \quad (n \geq 0).$$

(3.5.3)

The analysis of the above is similar to that given in Chapter 2.

For $B_0(y)$ we obtain

$$B_0(y) = \alpha\gamma \int_y^1 e^{\frac{\gamma}{2}(1-\xi^2)} d\xi,$$

(3.5.4)

where $\gamma$ is determined as a positive root of the transcendental equation

$$\alpha\gamma \int_0^1 e^{\frac{\gamma}{2}(1-\xi^2)} d\xi = 1.$$

(3.5.5)

For $n \geq 1$ we may deduce the following expression for $B_n(y)$,

$$B_n(y) = \int_y^1 f_n(\xi)[B_{n1}(y)B_{n2}(\xi) - B_{n1}(\xi)B_{n2}(y)]e^{\frac{\gamma}{2}\xi^2} d\xi + B'_n(1)B_{n1}(1)e^{\frac{\gamma}{2}} B_{n2}(y),$$

(3.5.6)

where $B_{n1}(y)$ and $B_{n2}(y)$ are linearly independent solutions of the homogeneous equation (3.5.1) such that

$$B_{n1}(y) = \frac{d^n}{dy^n}\left[\int_y^1 e^{-\frac{\gamma}{2}\xi^2} d\xi\right], \quad B_{n2}(y) = -B_{n1}(y) \int_y^1 \frac{e^{-\frac{\gamma}{2}\xi^2}}{B_{n1}(\xi)^2} d\xi. \quad (3.5.7)$$

For example the first three functions $B_{n1}(y)$ are given by

$$B_{11}(y) = -e^{-\frac{\gamma}{2}y^2}, \quad B_{21}(y) = \gamma y e^{-\frac{\gamma}{2}y^2}, \quad B_{31}(y) = \gamma(1 - \gamma y^2)e^{-\frac{\gamma}{2}y^2}. \quad (3.5.8)$$

With $B_n(y)$ given by (3.5.6) the determining equation for the unknown $B_n'(1)$ results from (3.5.6) and the boundary conditions (3.5.3)$_1$.

After long but straightforward calculations the final expressions for $n = 1, 2$ and 3 are

$$B_1(y) = -\alpha\gamma(1 - y)e^{\frac{\gamma}{2}(1 - y^2)},$$

$$B_2(y) = \frac{\alpha\gamma^2}{2}y(1 - y)^2 e^{\frac{\gamma}{2}(1 - y^2)},$$

$$B_3(y) = \frac{\alpha\gamma^2}{6}e^{\frac{\gamma}{2}(1 - y^2)}\left\{(1 - \gamma y^2)(1 - y)^3 \right.$$

$$\left. + 2\left[y(e^{\frac{\gamma}{2}} - e^{\frac{\gamma}{2}y^2}) + (1 - \gamma y^2)\int_y^1 e^{\frac{\gamma}{2}\xi^2}d\xi\right]\left(\int_0^1 e^{\frac{\gamma}{2}\xi^2}d\xi\right)^{-1}\right\}. \tag{3.5.9}$$

We make the following two observations concerning the above derivations. Firstly for $B_2(y)$ we see from (3.5.2), (3.5.7)$_2$ and (3.5.8)$_2$ that the term involving $B_2'(1)$ in $B_2(y)$ has a logarithmic singularity unless $B_2'(1)$ is zero. Remarkably the remaining terms in $B_2(y)$ accommodates this requirement. Secondly, the identity

$$f_3(y) = -\frac{\alpha\gamma^2}{2(1 - \gamma y^2)}\frac{d}{dy}\left\{(1 - y)^2(1 - \gamma y^2)^2 e^{\frac{\gamma}{2}(1 - y^2)}\right\} - \gamma B_3'(1)y e^{\frac{\gamma}{2}(1 - y^2)}, \tag{3.5.10}$$

is an important equation for simplifying (3.5.6) for $n = 3$.

From (3.5.4) and (3.5.9) we obtain the following expression for $B_n'(1)$,

$$B_0'(1) = -\alpha\gamma, \quad B_1'(1) = \alpha\gamma, \quad B_2'(1) = 0, \quad B_3'(1) = -\alpha\gamma^2 e^{\frac{\gamma}{2}}\left(3\int_0^1 e^{\frac{\gamma}{2}\xi^2}d\xi\right)^{-1}, \tag{3.5.11}$$

and on integrating (3.3.15) we find that the motion of the boundary becomes

$$\gamma t = \frac{X}{2}(X + 2) - \frac{\gamma e^{\frac{\gamma}{2}X}}{3(1 + X)}\left(\int_0^1 e^{\frac{\gamma}{2}\xi^2}d\xi\right)^{-1} + \cdots. \tag{3.5.12}$$

We note that the significance of $B_2'(1)$ zero is that there results in no *log Z* contribution on integrating (3.3.15). We also note that for large $\alpha$ (small $\gamma$) we obtain from (3.5.12) exactly the order one corrected motion given in (3.3.5) on using the approximation $\alpha^{-1} \approx \gamma(1 + \frac{\gamma}{3})$ which follows from (3.5.5).

# 3.6 Numerical results

Numerical values of the short time motion obtained from (3.4.5) can be shown, for small enough X, to lie between the improved lower bound given by (3.3.6) and the upper bound given by (3.3.5). Figures 3.1 and 3.2 demonstrate the validity of $(3.4.5)_2$ for $\alpha = 5.0$ and $\alpha = 10.0$. For small X it lies between the upper and lower bounds and agrees with the perturbation solution of Huang and Shih (1975a). It is clearly inapplicable for large X. Numerical values for the large time motion (3.5.12) also lie between the improved lower bound (3.3.6) and the upper bound (3.3.5) for all the times except for a very small initial period. Figure 3.3 illustrates the large time solution for $\alpha = 0.3$ for which the perturbation solution is grossly inadequate. Clearly the large time motion is contained by the upper and lower bounds. The relation of the large time motion to the perturbation solution of Huang and Shih (1975a) is shown in Figure 3.4 for $\alpha = 1.0$. For increasing $\alpha$, Huang and Shih (1975a) and the large time motion are in complete agreement. In both Figures 3.3 and 3.4 the small initial period for which the large time motion does not apply is not discernible on the particular scales chosen. Figures 3.5 and 3.6 illustrate the convergent nature of the large time temperature series (3.3.16) for $\alpha = 0.1$, $X(t) = 5.0$, and $\alpha = 1.0$, $X(t) = 2.0$ respectively.

In Table 3.1 are tabulated various short time estimates for t for $X(t) = 0.006$, for a range of values of $\alpha$. With the exception of $\alpha = 0.01$, the short time solution (3.4.2) is seen to lie between the upper bound (3.3.5) and the improved lower bound (3.3.6). It is also seen that the short time solution is in excellent agreement with the tabulated numerical results, and superior to the perturbation estimate of Huang and Shih (1975a). In Table 3.2 are tabulated various large time estimates for $t$ for $X(t) = 20.0$, again for the same range of values of $\alpha$ as in Table 3.1. The large time solution (3.5.12) is seen always to lie between the upper bound (3.3.5)

and the improved lower bound (3.5.12), and to be in very close agreement with the numerical results. As expected, the perturbation estimate of Huang and Shih (1975a) diverges sharply for small $\alpha$. Tables 3.3 and 3.5 illustrate the ranges of validity of the short and large time solutions for $\alpha = 0.1$ and $\alpha = 1.0$ respectively. Unfortunately, for small $\alpha$ (i.e $\alpha \leq 1.0$) and intermediate values of $X(t)$, (i.e. $0.1 < X(t) < 1.0$), the validity of the two series do not overlap. Tables 3.5 and 3.6 show the excellent convergence of the large time temperature estimate (3.3.16) compared to the numerical solution.
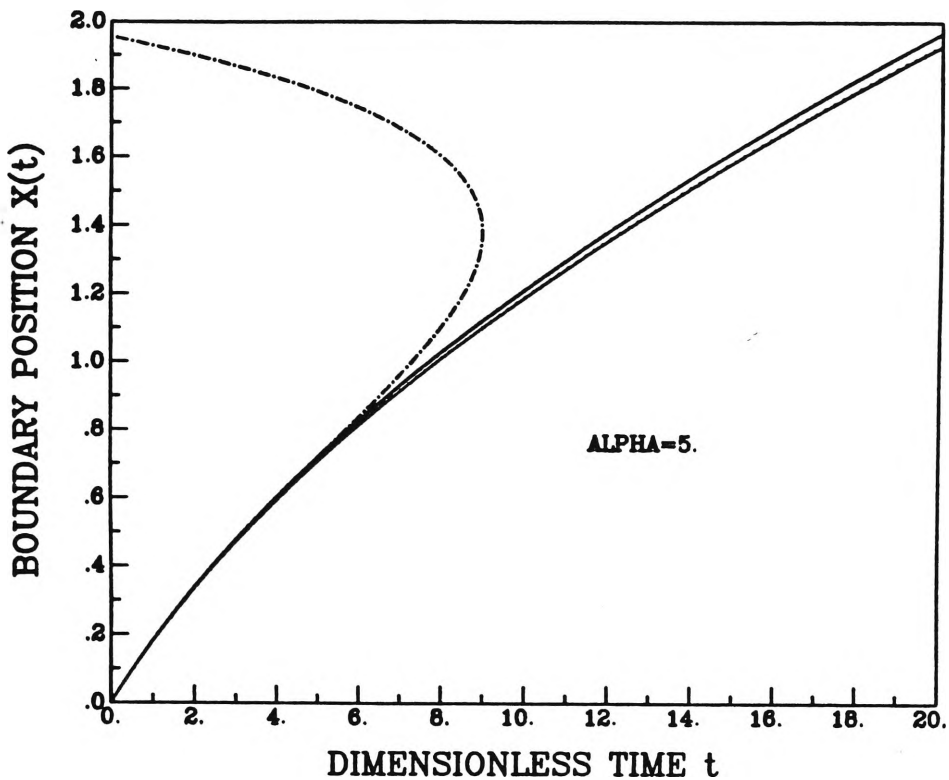
Figure 3.1  Short time boundary motion ($-\cdot-\cdot-\cdot$) compared with bounds ($\underline{\qquad}$) and perturbation estimate of Huang and Shih ($\cdots$)   for $\alpha\ =\ 5.0$
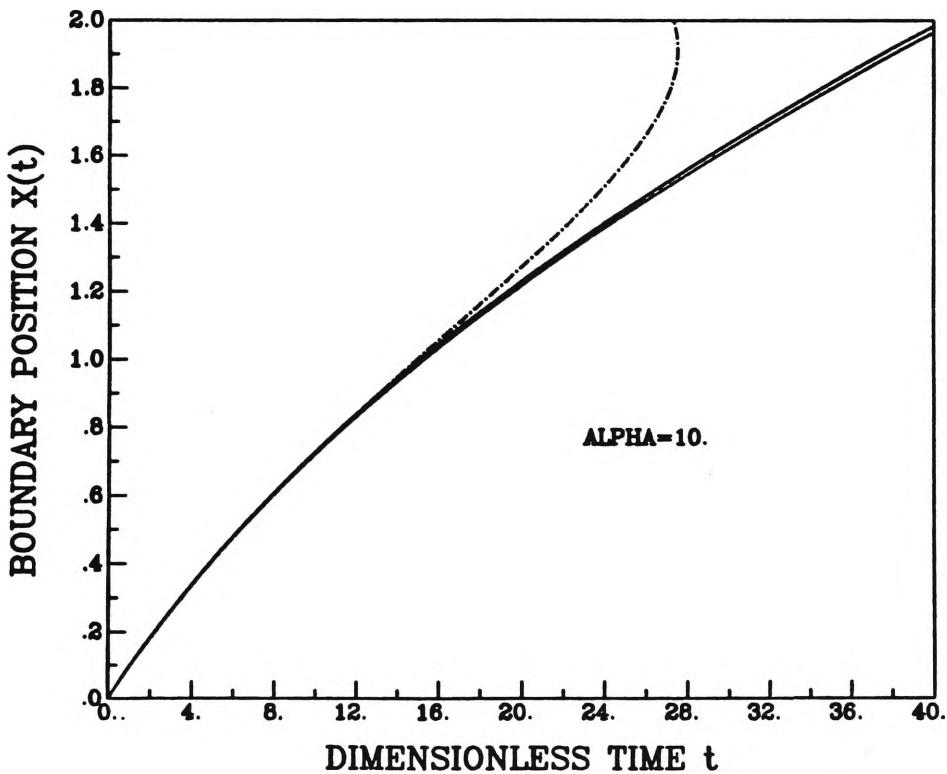


Figure 3.2  Short time boundary motion ($-\cdot-\cdot-\cdot$) compared with bounds ($\underline{\qquad}$) and perturbation estimate of Huang and Shih ($\cdots$)   for $\alpha\ =\ 10.0$
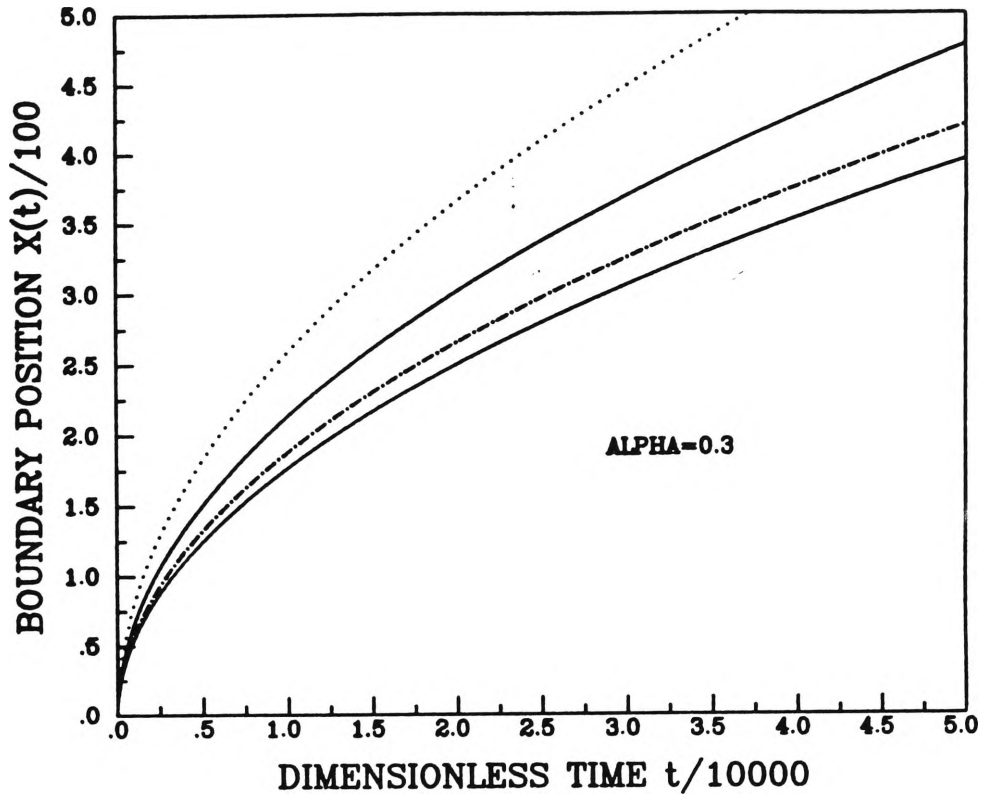
Figure 3.3    Large time boundary motion ( — · — · — · ) compared with bounds ( ———— ) and perturbation estimate of Huang and Shih ( · · · · ) for $\alpha = 0.3$
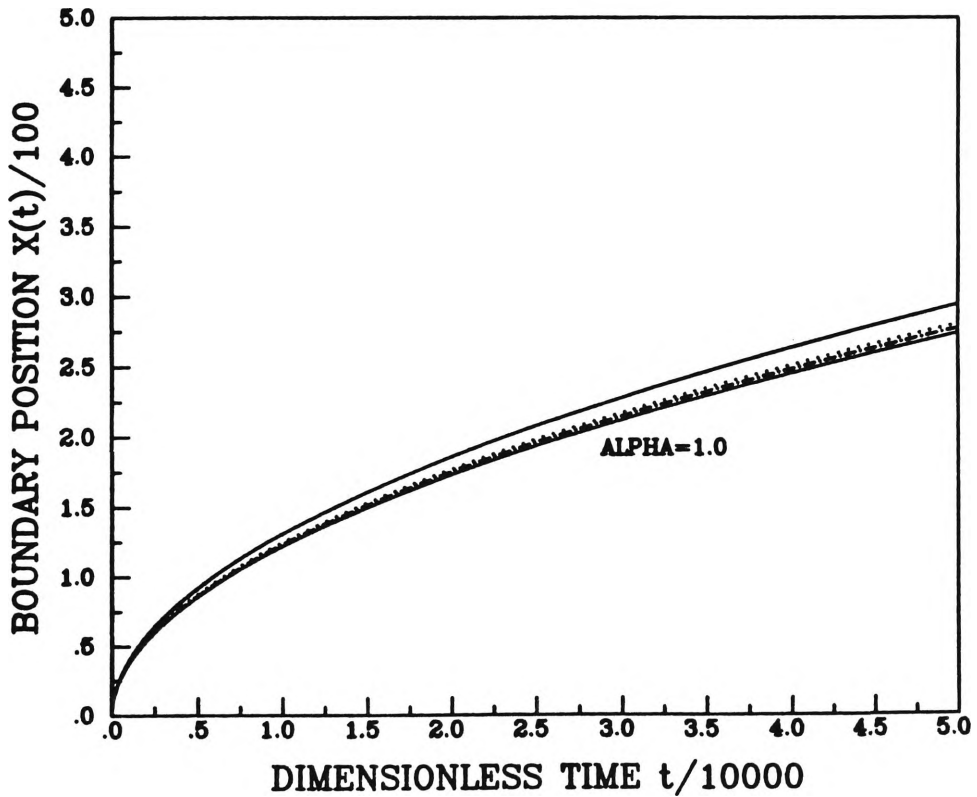


Figure 3.4    Large time boundary motion ( — · — · — · ) compared with bounds ( ———— ) and perturbation estimate of Huang and Shih ( · · · · ) for $\alpha = 1.0$
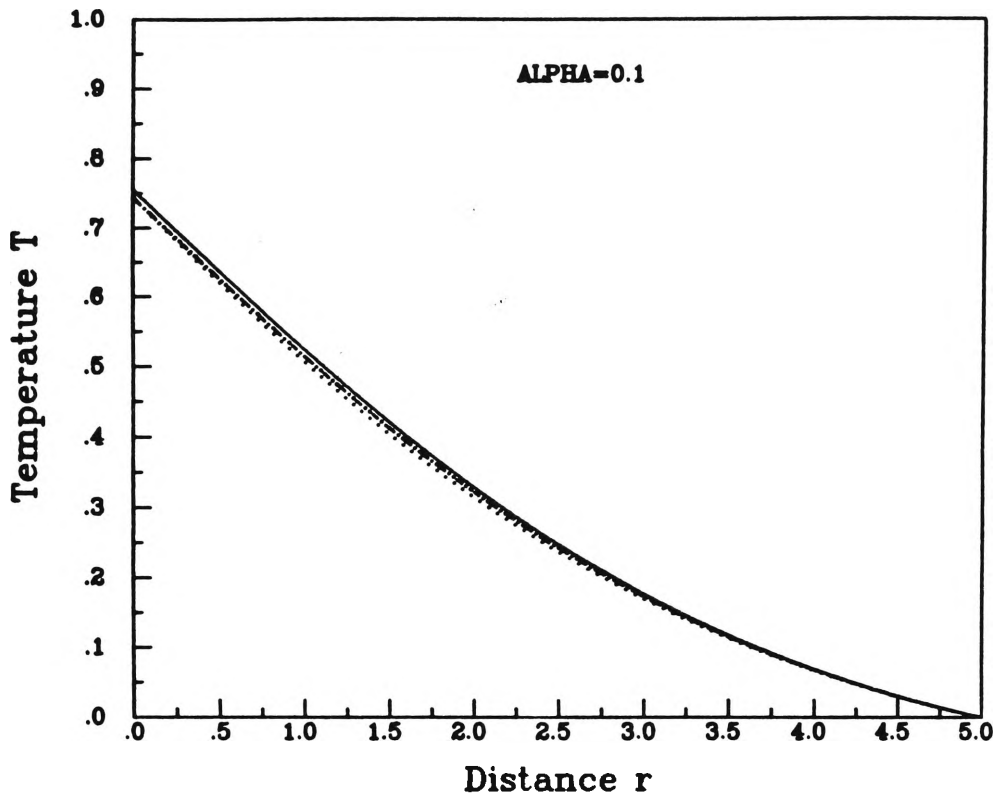
Figure 3.5    Convergence of large time temperature estimate for $\alpha = 0.1$ and $X(t) = 5.0$: Two terms ($\cdots$), Three terms ($-\cdot-\cdot-$), Four terms (———)
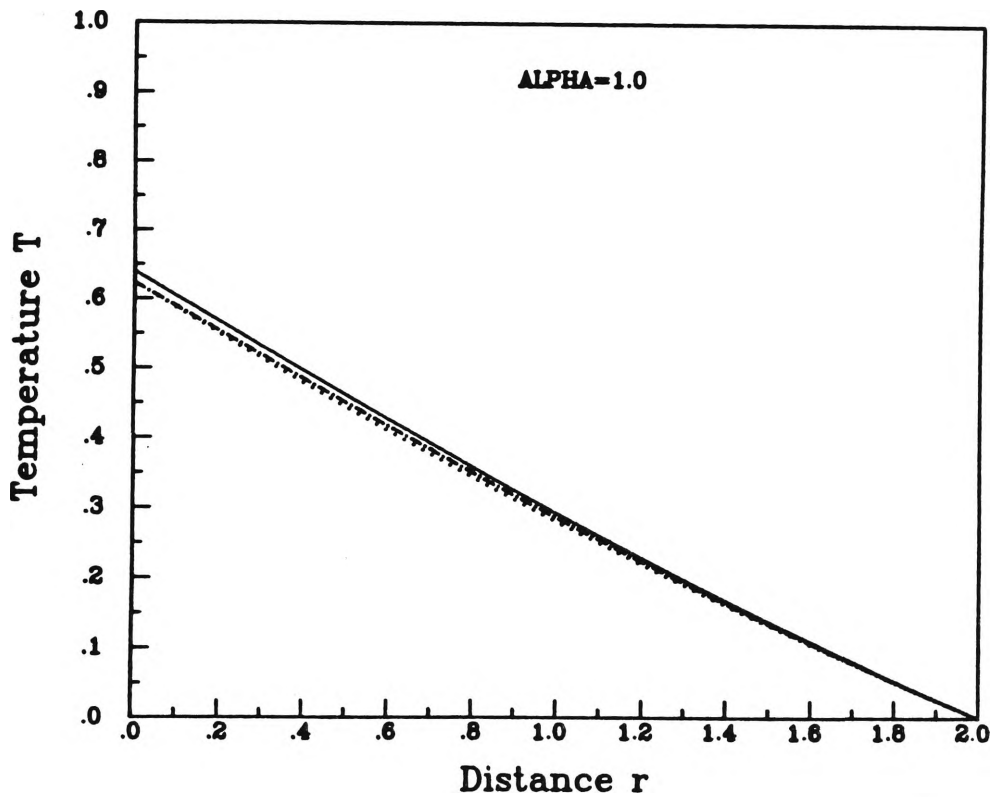


Figure 3.6    Convergence of large time temperature estimate for $\alpha = 1.0$ and $X(t) = 2.0$: Two terms ($\cdots$), Three terms ($-\cdot-\cdot-$), Four terms (———)

| $X(t) = 0.006$ α | Lower Bound (3.3.6) | Huang and Shih | Short Time (3.4.2) | Numer. Sol. | Upper Bound (3.3.5) |
|---|---|---|---|---|---|
| 0.01 | .000066 | .000032 | .000064 | .000074 | .000078 |
| 0.02 | .000126 | .000125 | .000135 | .000135 | .000138 |
| 0.05 | .000307 | .000316 | .000318 | .000318 | .000319 |
| 0.10 | .000603 | .000619 | .000619 | .000619 | .000620 |
| 0.20 | .001210 | .001221 | .001221 | .001221 | .001222 |
| 0.50 | .003024 | .003027 | .003027 | .003027 | .003027 |
| 1.00 | .006024 | .006036 | .006036 | .006036 | .006036 |
| 2.00 | .012042 | .012054 | .012054 | .012054 | .012054 |
| 5.00 | .030096 | .030108 | .030108 | .030108 | .030108 |
| 10.00 | .060186 | .060198 | .060198 | .060198 | .060198 |
| 20.00 | .120366 | .120378 | .120378 | .120378 | .120378 |

Table 3.1    Various short time estimates of time $t$ for $X(t) = 0.006$, for a range of α values

| $X(t) = 20.00$ α | Lower Bound (3.3.6) | Huang and Shih | Large Time (3.5.12) | Numer. Sol. | Upper Bound (3.3.5) |
|---|---|---|---|---|---|
| 0.01 | 12.83 | ...... | 30.35 | 31.78 | 75.21 |
| 0.02 | 18.42 | ...... | 37.37 | 38.45 | 77.42 |
| 0.05 | 30.34 | ...... | 51.47 | 52.18 | 84.02 |
| 0.10 | 45.65 | ...... | 68.81 | 69.29 | 95.02 |
| 0.20 | 71.67 | ...... | 97.33 | 97.61 | 117.02 |
| 0.50 | 141.77 | 148.37 | 171.14 | 171.28 | 183.02 |
| 1.00 | 253.77 | 279.46 | 285.70 | 285.76 | 293.02 |
| 2.00 | 474.97 | 507.18 | 508.83 | 508.84 | 513.02 |
| 5.00 | 1136.78 | 1170.91 | 1171.18 | 1171.18 | 1173.02 |
| 10.00 | 2236.09 | 2272.00 | 2272.06 | 2272.06 | 2273.02 |
| 20.00 | 4436.21 | 4472.51 | 4472.53 | 4472.53 | 4473.02 |

Table 3.2    Various large time estimates of time $t$ for $X(t) = 20.00$, for a range of α values

| $\alpha = 0.1$ <br> $X(t)$ | Lower <br> Bound <br> (3.3.6) | Huang <br> and <br> Shih | Short <br> Time <br> (3.4.2) | Large <br> Time <br> (3.5.12) | Numer. <br> Sol. | Upper <br> Bound <br> (3.3.5) |
|---|---|---|---|---|---|---|
| 0.01 | .001021 | .001051 | .001052 | -.005215 | .001052 | .001055 |
| 0.02 | .002085 | .002183 | .002196 | -.010233 | .002199 | .002217 |
| 0.05 | .005521 | .005657 | .005670 | -.024158 | .006128 | .006335 |
| 0.10 | .012017 | .008744 | -.003750 | -.043854 | .014059 | .015199 |
| 0.20 | .027641 | -.015405 | -.609200 | -.071697 | .034257 | .039778 |
| 0.50 | .092702 | -.471710 | -68.218751 | -.084848 | .123771 | .159722 |
| 1.00 | .253311 | -2.188087 | ....... | .050737 | .353671 | .483333 |
| 2.00 | .748331 | -7.287741 | ....... | .700569 | 1.084149 | 1.511111 |
| 5.00 | 3.526684 | -31.992459 | ....... | 4.831460 | 5.283219 | 7.305555 |
| 10.00 | 12.355835 | ....... | ....... | 18.26771 | 18.683154 | 25.696969 |
| 20.00 | 45.650848 | ....... | ....... | 68.813652 | 69.300589 | 95.015872 |

Table 3.3      Various short and large time estimates of time $t$ for increasing values of $X(t)$ with $\alpha = 0.1$

| $\alpha = 1.0$ <br> $X(t)$ | Lower <br> Bound <br> (3.3.6) | Huang <br> and <br> Shih | Short <br> Time <br> (3.4.3) | Large <br> Time <br> (3.5.12) | Numer. <br> Sol. | Upper <br> Bound <br> (3.3.5) |
|---|---|---|---|---|---|---|
| 0.01 | .01066 | .01009 | .01009 | .00883 | .01009 | .01010 |
| 0.02 | .02026 | .02039 | .02039 | .01788 | .02039 | .02039 |
| 0.05 | .05166 | .05242 | .05243 | .04628 | .05243 | .05246 |
| 0.10 | .10662 | .10941 | .10945 | .09766 | .10947 | .10970 |
| 0.20 | .22627 | .23582 | .23526 | .21480 | .23658 | .23778 |
| 0.50 | .66144 | .70399 | .53750 | .67018 | .71247 | .72222 |
| 1.00 | 1.63299 | 1.76037 | -4.80000 | 1.73678 | 1.78603 | 1.83333 |
| 2.00 | 4.47214 | 4.87102 | ......... | 4.91664 | 4.99554 | 5.11111 |
| 5.00 | 20.00000 | 21.95849 | ......... | 22.40162 | 22.48571 | 23.05555 |
| 10.00 | 69.04105 | 75.97225 | ......... | 77.63900 | 77.72583 | 79.69697 |
| 20.00 | 253.77155 | 279.45779 | ......... | 285.69498 | 286.27549 | 293.01587 |

Table 3.4      Various short and large time estimates of time $t$ for increasing values of $X(t)$ with $\alpha = 1.0$

| $R(t) = 5.0$ $\alpha = 1.0$ $r$ | Two-Terms | Three-Terms | Four-Terms | Numerical Solution |
|---|---|---|---|---|
| 0.0 | .81175 | .81175 | .81376 | .81351 |
| 0.5 | .71842 | .71939 | .72114 | .72084 |
| 1.0 | .62695 | .62847 | .62996 | .62964 |
| 1.5 | .53773 | .53944 | .54068 | .54036 |
| 2.0 | .45109 | .45272 | .45373 | .45344 |
| 2.5 | .36734 | .36871 | .36951 | .36925 |
| 3.0 | .28675 | .28776 | .28837 | .28815 |
| 3.5 | .20955 | .21018 | .21061 | .21045 |
| 4.0 | .13592 | .13623 | .13650 | .13640 |
| 4.5 | .06603 | .06615 | .06624 | .06619 |
| 5.0 | .00000 | .00000 | .00000 | .00000 |

Table 3.5     Convergence of large time temperature estimate for $\alpha = 1.0$ and $R(t) = 5.0$

| $R(t) = 5.0$ $\alpha = 5.0$ $r$ | Two-Terms | Three-Terms | Four-Terms | Numerical Solution |
|---|---|---|---|---|
| 0.0 | .82810 | .82810 | .82855 | .82845 |
| 0.5 | .74233 | .74255 | .74293 | .74276 |
| 1.0 | .65698 | .65732 | .65764 | .65748 |
| 1.5 | .57214 | .57253 | .57279 | .57263 |
| 2.0 | .48789 | .48828 | .48849 | .48834 |
| 2.5 | .40435 | .40468 | .40485 | .40471 |
| 3.0 | .32159 | .32184 | .32197 | .32185 |
| 3.5 | .23969 | .23985 | .23995 | .23979 |
| 4.0 | .15975 | .15883 | .15888 | .15883 |
| 4.5 | .07882 | .07884 | .07887 | .07893 |
| 5.0 | .00000 | .00000 | .00000 | .00000 |

Table 3.6     Convergence of large time temperature estimate for $\alpha = 5.0$ and $R(t) = 5.0$

# CHAPTER FOUR

# Two Phase Melting of Cylinders and Spheres

## 4.1 Introduction

This chapter is concerned with the extension of the boundary fixing series technique to full two phase cylindrical and spherical problems. The analysis is presented in terms of melting, but with minor changes the same results apply to freezing. For such problems the technique involves introducing a transformation which fixes three points: the origin, the moving boundary, and the outer surface of the cylinder or sphere, thus the original moving boundary problem is transformed into a fixed boundary problem. Furthermore, for the case of the two phase semi-infinite plane the method is shown to yield the exact similarity solution. In Section 4.2, we describe the physical problem in detail and formulate equations in dimensionless form. In Section 4.3 we discuss the procedure for choosing the optimal boundary fixing transformations and method of solution. In Sections 4.4 and 4.5, we present the analysis and results for the cylinder and the sphere respectively. Numerical results and discussion are given in Section 4.6.

## 4.2 Governing equations

The problem considered here is that of a subcooled two phase circular cylinder or sphere, of radius $a^*$, initially at temperature $T_i$. At time zero, the temperature of the outer boundary, $r^* = a^*$, is raised to, $T_{a^*}$, a value above the freezing temperature, $T_f$, and maintained constant thereafter. To simplify the problem, the thermal properties in each phase are assumed constant and the volumetric expansion

or contraction due to phase transformation is neglected. Further free convection currents in the liquid phase are ignored. Based on these assumptions the governing equations and boundary conditions can be written in dimensionless form as

$$\frac{\partial T_\ell}{\partial t} = \left[\frac{\partial^2 T_\ell}{\partial r^2} + \frac{\lambda}{r}\frac{\partial T_\ell}{\partial r}\right], \quad R(t) < r < 1, \qquad (\textit{liquid region}) \quad (4.2.1)$$

$$\frac{\partial T_s}{\partial t} = \kappa\left[\frac{\partial^2 T_s}{\partial r^2} + \frac{\lambda}{r}\frac{\partial T_s}{\partial r}\right], \quad 0 < r < R(t), \qquad (\textit{solid region}) \quad (4.2.2)$$

$$T_\ell(1,t) = 1, \quad T_\ell(R(t),t) = T_s(R(t),t) = \frac{\partial T_s}{\partial r}(0,t) = 0, \quad T_s(r,0) = -V,$$
$$(4.2.3)$$

$$\frac{\partial T_\ell}{\partial r}(R(t),t) - \frac{\partial T_s}{\partial r}(R(t),t) = -\alpha\frac{dR}{dt}, \quad R(0) = 1, \qquad (4.2.4)$$

where $T_\ell(r,t)$, $T_s(r,t)$ are the dimensionless temperatures in the liquid and solid respectively, $r$ and $t$ are the position and time variables, $\alpha$ and $\kappa$ are positive constants and all of these quantities are given in terms of the starred physical quantities by

$$T_\ell = \frac{T_\ell^* - T_f}{T_a^* - T_f}, \quad T_s = \frac{k_s}{k_\ell}\frac{T_s^* - T_f}{T_a^* - T_f}, \quad r = \frac{r^*}{a^*}, \quad t = \frac{k_\ell t^*}{\rho c_\ell a^{*2}},$$

$$R(t) = \frac{R^*(t^*)}{a^*}, \quad \alpha = \frac{L}{c_\ell(T_a^* - T_f)}, \quad \kappa = \frac{k_s c_\ell}{k_\ell c_s}, \quad -V = \frac{T_i - T_f}{T_a^* - T_f}.$$
$$(4.2.5)$$

The constant $\lambda$ takes on values 1 and 2 specifying cylinder or sphere respectively, while $\alpha$ and $V$ are positive constants. We note that the system is non-dimensionalized such that the temperatures in the solid and the liquid are bounded by $-V \leq T_s \leq 0 \leq T_\ell \leq 1$.

Here we remark that on replacing the zero flux condition at the origin with a constant temperature condition at $r = -\infty$, then for $\lambda = 0$ the corresponding planar problem has the exact solution

$$T_\ell(r,t) = \frac{1}{\mathrm{erf}\left(\sqrt{\gamma/2}\right)}\left[\mathrm{erf}\left(\sqrt{\gamma/2}\right) - \mathrm{erf}\left(\sqrt{\gamma/2}\,x\right)\right], \qquad R(t) < r < 1 \,,$$

$$T_S(r,t) = \frac{-V}{\mathrm{erfc}\left(\sqrt{\gamma/2\kappa}\right)}\left[\mathrm{erfc}\left(\sqrt{\gamma/2\kappa}\right) - \mathrm{erfc}\left(\sqrt{\gamma/2\kappa}\,x\right)\right], \quad -\infty < r < R(t) \,,$$

$$(4.2.6)$$

where $x$ is given by

$$x = \frac{1-r}{1-R(t)}, \qquad \text{with} \quad R(t) = 1 - \sqrt{2\gamma t}\,, \qquad (4.2.7)$$

while $\gamma$ satisfies the transcendental equation

$$\alpha\gamma = \sqrt{\frac{2\gamma}{\pi}}\left\{\frac{e^{-\gamma/2}}{\mathrm{erf}\left(\sqrt{\gamma/2}\right)} - \frac{Ve^{-\gamma/2\kappa}}{\sqrt{\kappa}\,\mathrm{erfc}\left(\sqrt{\gamma/2\kappa}\right)}\right\}. \qquad (4.2.8)$$

However, no such exact solutions are available for the cylinder or the sphere, which lead us to the development of the following solution technique.

## 4.3 Method of solution

The method of solution consists of introducing a transformation which simultaneously fixes the three points 0, $R(t)$ and 1. We assume a boundary fixing transformation of the form,

$$x = \frac{f(r)}{f(R)}, \qquad y = f(R), \qquad (4.3.1)$$

and

$$T_\ell(r,t) = \phi_\ell(x,y), \qquad T_S(r,t) = V[-1 + \phi_s(x,y)], \qquad (4.3.2)$$

where $f(r)$ is determined subsequently such that

$$f(1) = 0, \qquad |f(0)| = \infty. \qquad (4.3.3)$$

Thus the liquid region $[R(t), 1]$ is transformed to $[0, 1]$, the solid region $[0, R(t)]$ to $[1, \infty]$ and the original moving boundary problem is transformed into a fixed

boundary problem. From (4.3.1) and (4.3.2) equations (4.2.1) and (4.2.2) become on using (4.2.4),

$$\left\{ \frac{\partial^2 \phi_\ell}{\partial x^2} + y \left( \frac{df}{dr} \right)^{-2} \left[ \frac{d^2 f}{dr^2} + \frac{\lambda}{r} \frac{df}{dr} \right] \frac{\partial \phi_\ell}{\partial x} \right\}$$

$$= \frac{1}{\alpha} \left( \frac{df}{dR} / \frac{df}{dr} \right)^2 \left[ \frac{\partial \phi_\ell}{\partial x}(1,y) - V \frac{\partial \phi_s}{\partial x}(1,y) \right] \left[ x \frac{\partial \phi_\ell}{\partial x} - y \frac{\partial \phi_\ell}{\partial y} \right], \ 0 \le x \le 1, \tag{4.3.4}$$

$$\kappa \left\{ \frac{\partial^2 \phi_s}{\partial x^2} + y \left( \frac{df}{dr} \right)^{-2} \left[ \frac{d^2 f}{dr^2} + \frac{\lambda}{r} \frac{df}{dr} \right] \frac{\partial \phi_s}{\partial x} \right\}$$

$$= \frac{1}{\alpha} \left( \frac{df}{dR} / \frac{df}{dr} \right)^2 \left[ \frac{\partial \phi_\ell}{\partial x}(1,y) - V \frac{\partial \phi_s}{\partial x}(1,y) \right] \left[ x \frac{\partial \phi_s}{\partial x} - y \frac{\partial \phi_s}{\partial y} \right], \ 1 \le x \le \infty. \tag{4.3.5}$$

Clearly these equations are simplified if $f(r)$ is chosen so that it satisfies the homogeneous equation

$$\frac{d^2 f}{dr^2} + \frac{\lambda}{r} \frac{df}{dr} = 0. \tag{4.3.6}$$

In this case (4.3.4) and (4.3.5) become

$$\frac{\partial^2 \phi_\ell}{\partial x^2} = \frac{1}{\alpha} \left( \frac{df}{dR} / \frac{df}{dr} \right)^2 \left[ \frac{\partial \phi_\ell}{\partial x}(1,y) - V \frac{\partial \phi_s}{\partial x}(1,y) \right] \left[ x \frac{\partial \phi_\ell}{\partial x} - y \frac{\partial \phi_\ell}{\partial y} \right], 0 \le x \le 1,$$

$$\tag{4.3.7}$$

$$\kappa \frac{\partial^2 \phi_s}{\partial x^2} = \frac{1}{\alpha} \left( \frac{df}{dR} / \frac{df}{dr} \right)^2 \left[ \frac{\partial \phi_\ell}{\partial x}(1,y) - V \frac{\partial \phi_s}{\partial x}(1,y) \right] \left[ x \frac{\partial \phi_s}{\partial x} - y \frac{\partial \phi_s}{\partial y} \right], 1 \le x \le \infty.$$

$$\tag{4.3.8}$$

These equations are solved assuming formal series solutions of the form

$$\phi_\ell(x,y) = \sum_{n=0}^{\infty} A_n(x) y^n, \quad \phi_s(x,y) = \sum_{n=0}^{\infty} B_n(x) y^n, \tag{4.3.9}$$

where $A_n(x)$ and $B_n(x)$ denote functions of x only, the first two of which are derived in the following two sections for cylinders and spheres respectively.

## 4.4 Cylindrical melting

From (4.3.1),(4.3.3) and (4.3.6) with $\lambda = 1$, we have new independent variables

$$x = \frac{\ln r}{\ln R}, \quad y = \ln R, \tag{4.4.1}$$

so that in terms of (4.3.2) and (4.3.9), the system given by (4.2.1)-(4.2.4), with $\lambda = 1$ becomes

$$\frac{\partial^2 \phi_\ell}{\partial x^2} = \frac{1}{\alpha} e^{2(x-1)y} \left[\frac{\partial \phi_\ell}{\partial x}(1,y) - V\frac{\partial \phi_s}{\partial x}(1,y)\right]\left[x\frac{\partial \phi_\ell}{\partial x} - y\frac{\partial \phi_\ell}{\partial y}\right], 0 \le x \le 1, \quad (4.4.2)$$

$$\kappa\frac{\partial^2 \phi_s}{\partial x^2} = \frac{1}{\alpha} e^{2(x-1)y} \left[\frac{\partial \phi_\ell}{\partial x}(1,y) - V\frac{\partial \phi_s}{\partial x}(1,y)\right]\left[x\frac{\partial \phi_s}{\partial x} - y\frac{\partial \phi_s}{\partial y}\right], 1 \le x \le \infty,$$

$$(4.4.3)$$

subject to boundary and initial conditions

$$\phi_\ell(0,y) = 1, \quad \phi_\ell(1,y) = 0, \quad \phi_s(1,y) = 1, \quad \frac{\partial \phi_s}{\partial x}(\infty,y) = 0, \quad (4.4.4)$$

$$\phi_s(\infty,0) = 0, \quad (4.4.5)$$

while the energy balance condition on the moving boundary interface becomes

$$\frac{\partial \phi_\ell}{\partial x}(1,y) - V\frac{\partial \phi_s}{\partial x}(1,y) = -\alpha y e^{2y}\frac{dy}{dt}, \quad y(0) = 0. \quad (4.4.6)$$

Substituting (4.3.9) into (4.4.2)-(4.4.6) and equating like powers of $y$ yields two systems of ordinary linear differential equations for the $A_n(x)$'s and $B_n(x)$'s, namely

$$A''_0 + \gamma x A'_0 = 0, \qquad \kappa B''_0 + \gamma x B'_0 = 0, \qquad (4.4.7)$$

$$A''_n + \gamma(xA'_n - nA_n) = R_n(x), \kappa B''_n + \gamma(xB'_n - nB_n) = S_n(x), \quad (4.4.8)$$

where the $R_n(x)$'s and $S_n(x)$'s are given by

$$R_n(x) = \frac{1}{\alpha}\sum_{j=1}^{n}\Gamma_j(x)\left[xA'_{n-j} - (n-j)A_{n-j}\right],$$

$$(4.4.9)$$

$$S_n(x) = \frac{1}{\alpha}\sum_{j=1}^{n}\Gamma_j(x)\left[xB'_{n-j} - (n-j)B_{n-j}\right],$$

with $\gamma$ and $\Gamma_n(x)$ given by

$$\gamma = \frac{-1}{\alpha}[A'_0(1) - VB'_0(1)], \quad \Gamma_n(x) = \sum_{j=0}^{n} a_j\frac{[2(x-1)]^{n-j}}{(n-j)!}, \quad n = 1, 2, \ldots$$

$$(4.4.10)$$

and the $a_n$'s are

$$a_n = A'_n(1) - VB'_n(1), \quad n = 0, 1, \ldots . \tag{4.4.11}$$

Primes denote differentiation with respect to x and the arguments of $A_n$'s and $B_n$'s are understood to be x unless otherwise indicated. From (4.3.9) we see that the boundary conditions (4.4.4) are satisfied provided

$$A_0(0) = 1, A_0(1) = 0, \quad B_0(1) = 1, B'_0(\infty) = 0,$$
$$A_n(0) = 0, A_n(1) = 0, \quad B_n(1) = 0, B'_n(\infty) = 0, \tag{4.4.12}$$

and the energy balance condition yields

$$\sum_{n=0}^{\infty} a_n y^n = -\alpha y e^{2y} \frac{dy}{dt}, \quad y(0) = 0. \tag{4.4.13}$$

Solving (4.4.7) subject to (4.4.12)$_1$ yields

$$A_0(x) = \frac{1}{L_\ell} \int_x^1 e^{\frac{\gamma}{2}(1-\xi^2)} d\xi, \quad B_0(x) = \frac{1}{L_s} \int_x^\infty e^{\frac{\gamma}{2\kappa}(1-\xi^2)} d\xi, \tag{4.4.14}$$

where the $L_\ell$ and $L_s$ are given by

$$L_\ell = \int_0^1 e^{\frac{\gamma}{2}(1-\xi^2)} d\xi, \quad L_s = \int_1^\infty e^{\frac{\gamma}{2\kappa}(1-\xi^2)} d\xi, \tag{4.4.15}$$

and $\gamma$ satisfies the transcendental equation

$$\alpha\gamma = \frac{1}{L_\ell} - V\frac{1}{L_s}. \tag{4.4.16}$$

With x given by (4.2.7)$_1$ it is seen that (4.4.14)-(4.4.16) yields the exact solution for the plane.

Solving (4.4.8) subject to (4.4.12)$_2$, with $n = 1$ yields

$$A_1(x) = \frac{x}{6L_\ell} \left\{ [a + 3(1 - x)]e^{\frac{\gamma}{2}(1-x^2)} - 3\int_x^1 e^{\frac{\gamma}{2}(1-\xi^2)} d\xi - a \right\},$$

$$B_1(x) = \frac{1}{6L_s} \left\{ \left[ \frac{\kappa}{\gamma}(b - 3) + x[a + 3(1 - x)] \right] e^{\frac{\gamma}{2\kappa}(1-x^2)} - bx \int_x^\infty e^{\frac{\gamma}{2\kappa}(1-\xi^2)} d\xi \right\}, \tag{4.4.17}$$

where the constants $a$ and $b$ are given by

$$a = \frac{3\left[\alpha + \frac{\kappa V}{\gamma(\kappa - \gamma L_s)}\right]}{\left[3\alpha + \frac{1}{L_\ell} + \frac{V}{L_s}\left(\frac{1}{\gamma} - \frac{1}{\kappa}\right) + \frac{V}{(\kappa - \gamma L_s)}\right]}, b = \frac{\frac{3\kappa}{(\kappa - \gamma L_s)}\left[2\alpha + \frac{1}{L_\ell} + \frac{1}{L_\ell}\left(\frac{1}{\gamma} - \frac{1}{\kappa}\right)\right]}{\left[3\alpha + \frac{1}{L_\ell} + \frac{V}{L_s}\left(\frac{1}{\gamma} - \frac{1}{\kappa}\right) + \frac{V}{(\kappa - \gamma L_s)}\right]}.$$
(4.4.18)

From (4.4.13) and (4.4.16) the motion of the boundary is given approximately by

$$t \approx \frac{1}{\gamma} \int_0^y \frac{\xi e^{2\xi} d\xi}{[1 + \xi(1 - a)/2]} .$$
(4.4.19)

Numerical results indicate that this is adequately approximated by expanding the denominator binomialy, and integrating to obtain

$$t \approx \frac{1}{8\gamma}\left\{2\left[(1 - R^2) + 2R^2 \ln R\right] + (1 - a)\left[(1 - R^2) + 2R^2 \ln R - 2R^2(\ln R)^2\right]\right\},$$
(4.4.20)

from which it is apparent that an estimate for the time to complete melting $t_c$ is

$$t_c \approx (3 - a)/8\gamma .$$
(4.4.21)

## 4.5 Spherical melting

From (4.3.1), (4.3.3) and (4.3.6) with $\lambda = 2$, the new independent variables for the sphere are

$$x = \frac{r^{-1} - 1}{R^{-1} - 1} , \quad y = R^{-1} - 1 ,$$
(4.5.1)

so that from (4.3.2) the system given by (4.2.1)-(4.2.4) becomes

$$\frac{\partial^2 \phi_\ell}{\partial x^2} = \frac{1}{\alpha}\left(\frac{1 + y}{1 + xy}\right)^4\left[\frac{\partial \phi_\ell}{\partial x}(1, y) - V\frac{\partial \phi_s}{\partial x}(1, y)\right]\left[x\frac{\partial \phi_\ell}{\partial x} - y\frac{\partial \phi_\ell}{\partial y}\right], 0 \leq x \leq 1, (4.5.2)$$

$$\kappa\frac{\partial^2 \phi_s}{\partial x^2} = \frac{1}{\alpha}\left(\frac{1 + y}{1 + xy}\right)^4\left[\frac{\partial \phi_\ell}{\partial x}(1, y) - V\frac{\partial \phi_s}{\partial x}(1, y)\right]\left[x\frac{\partial \phi_s}{\partial x} - y\frac{\partial \phi_s}{\partial y}\right], 1 \leq x \leq \infty,$$
(4.5.3)

subject to the same boundary and initial conditions (4.4.4) and (4.4.5), while the energy balance condition on the moving boundary becomes

$$\frac{\partial \phi_\ell}{\partial x}(1,y) - V\frac{\partial \phi_s}{\partial x}(1,y) = -\alpha y(1 + y)^{-4}\frac{dy}{dt}, \quad y(0) = 0. \tag{4.5.4}$$

Again if we assume a formal series solution as given by (4.3.9), we obtain the differential equations as given by (4.4.7)-(4.4.11) but with different polynomials $\Gamma_n(x)$. The energy balance condition (4.5.4) becomes

$$\sum_{n=0}^{\infty} a_n y^n = -\alpha y(1 + y)^{-4}\frac{dy}{dt}, \quad y(0) = 0, \tag{4.5.5}$$

where again the $a_n$'s are defined by (4.4.11).

Solving for $A_0(x)$ and $B_0(x)$ yields the same solutions as given for the cylinder by (4.4.14), (4.4.15) and (4.4.16). Further $A_1(x)$ and $B_1(x)$ coincide with (4.4.17) apart from a multiplicative factor, thus

$$A_1(x) = \frac{-x}{3L_\ell}\left\{[a + 3(1 - x)]e^{\frac{\gamma}{2}(1-x^2)} - 3\int_x^1 e^{\frac{\gamma}{2}(1-\xi^2)}\,d\xi - a\right\},$$

$$B_1(x) = \frac{-1}{3L_s}\left\{\left[\frac{\kappa}{\gamma}(b - 3) + x[a + 3(1 - x)]\right]e^{\frac{\gamma}{2\kappa}(1-x^2)} - bx\int_x^\infty e^{\frac{\gamma}{2\kappa}(1-\xi^2)}\,d\xi\right\}, \tag{4.5.6}$$

where again the constants $a$ and $b$ are given by $(4.4.18)_1$ and $(4.4.18)_2$ respectively. From (4.5.5) and (4.5.6) we obtain the following estimate for the motion of the boundary

$$t \approx \frac{1}{\gamma}\int_0^y \frac{(1 + \xi)^{-4}\xi\,d\xi}{[1 + (a - 1)\xi]}, \tag{4.5.7}$$

which can be integrated exactly to obtain

$$t \approx \frac{(1 - R)}{6\gamma(a - 2)^3}\left[2(a - 2)^2R^2 + (a - 2)(2a - 1)R + (2a^2 + a - 4)\right]$$

$$- \frac{(a - 1)^2}{\gamma(a - 2)^4}\log|(a - 1) + (2 - a)R|, \tag{4.5.8}$$

from which we may readily deduce that an estimate for the time to complete melting is given by

$$t_c \approx \frac{(2a^2 + a - 4)}{6\gamma(a - 2)^3} - \frac{(a - 1)^2}{\gamma(a - 2)^4}\log|a - 1|. \tag{4.5.9}$$

## 4.6 Numerical results and discussion

In this section we compare our approximations with the exact numerical solution obtained by the enthalpy method of Voller and Cross (1981) and the perturbation solution of Jiji and Weinbaum (1978). Figure 4.1 compares the approximation to the boundary motion for the cylinder given by (4.4.19) with that of Jiji and Weinbaum (1978), given by their equation (89) and the numerical solution obtained by the enthalpy method. Figure 4.2 compares the approximation to the boundary motion for the sphere given by (4.5.7) or (4.5.8) with the numerical solution. Clearly the procedure described here yields compatible numerical results and (4.4.21) and (4.5.9) are useful simple approximations for times to complete melting. For the temperature profiles for both the cylinder and sphere, two terms of the series yield outer phase temperature approximations which are well behaved, while the inner phase approximation is singular for large times.

To a certain extent we may eliminate this large time singularity (i.e. $y = \ln R$ and $y = R^{-1} - 1$), if for both the cylinder and sphere we make transformations of the form

$$X = \frac{1 - r}{1 - R}, \quad Y = 1 - R, \quad \Phi_\ell(X, Y) = \phi_\ell(x, y), \quad \Phi_s(X, Y) = \phi_s(x, y),$$

$$(4.6.1)$$

where now $\Phi_\ell$ and $\Phi_s$ are assumed to have formal series solutions in the nonsingular $Y$, with coefficients $\overline{A}_n(X)$ and $\overline{B}_n(X)$. We note that these variables cannot be used directly to solve the problem since $r = 0$ is not fixed. For the sphere, we remark that the variable Y given by $(4.6.1)_2$ results from applying an Euler transformation $y/(1 + y)$ to the singular variable $(4.5.1)_2$. However, no such simple interpretation exists for the cylindrical case. The functions $\overline{A}_n$ and $\overline{B}_n$ can be found simply by rewriting $\phi_\ell$ and $\phi_s$ in terms of the new independent variables $X$ and $Y$ and equating coefficients of like powers of $Y$. $\overline{A}_0$ and $\overline{B}_0$ turn out to have exactly the

same functional form as $A_0$ and $B_0$, while $\overline{A}_1$ and $\overline{B}_1$ for the cylinder and sphere are given respectively by

$$\overline{A}_1(X) = \frac{-X}{6L_\ell}\left\{a\left[e^{\frac{\gamma}{2}(1-X^2)} - 1\right] - 3\int_X^1 e^{\frac{\gamma}{2}(1-\xi^2)}\,d\xi\right\},$$

$$\overline{B}_1(X) = \frac{1}{6L_s}\left\{\left[\left[\frac{\kappa}{\gamma}(b-3) + X[a \qquad\qquad ]\right]e^{\frac{\gamma}{2\kappa}(1-X^2)} - bX\int_X^\infty e^{\frac{\gamma}{2\kappa}(1-\xi^2)}\,d\xi\right\},$$

$$(4.6.2)$$

and

$$\overline{A}_1(X) = \frac{-X}{3L_\ell}\left\{a\left[e^{\frac{\gamma}{2}(1-X^2)} - 1\right] - 3\int_X^1 e^{\frac{\gamma}{2}(1-\xi^2)}\,d\xi\right\},$$

$$\overline{B}_1(X) = \frac{1}{3L_s}\left\{\left[\left[\frac{\kappa}{\gamma}(b-3) + X[a \qquad\qquad )\right]\right]e^{\frac{\gamma}{2\kappa}(1-X^2)} - bX\int_X^\infty e^{\frac{\gamma}{2\kappa}(1-\xi^2)}\,d\xi\right\}.$$

$$(4.6.3)$$

Figures 4.3 and 4.4 show the temperature profiles corresponding to only one term of the series and these are seen to be in reasonable agreement with the enthalpy profiles. Numerical results based on the first two terms of each series indicate well behaved temperature approximations to both the outer and inner phases. However the additional terms do not increase the accuracy of the one term profiles shown in Figure 4.3 and 4.4 and therefore these graphs are not included. These results indicate that a genuine improvement on the one term profiles may only be achieved by including the first three terms in the series approximations. However the analysis involved is considerably more complicated than that presented here and this extension has not been attempted.

In Table 4.1 estimates obtained from numerically evaluating equations, (4.4.21) and Jiji and Weinbaum's (89), for times to complete melting, $t_c$, are compared with the numerical solutions. For the comparison both $\kappa$ and $V$ were chosen to be 1.0, while $\alpha$ was varied from 1.0 to 100.0. As seen from the table, for $\alpha$ close to unity, (i.e. $\alpha \approx 1.0$), both the series and perturbation estimates are out by about 50%. However, as would be expected, for increasing $\alpha$ the accuracy of the estimates from

both the methods is seen to improve. For $\alpha$ = 100.0 both the methods yield estimates with less than 10% error. In Table 4.2 estimates for the boundary motion with $\kappa$ = 1.0, $V$ = 1.0, and $\alpha$ = 1.0 are tabulated and compared with numerical solutions. We note that for small times, ($R(t) > 0.8$), the boundary fixing method yields a very accurate estimate. Unfortunately, Jiji and Weinbaum restricted their analysis to the very special case where the thermal diffusivities in both the phases are identical (i.e. $\kappa$ = 1.0), restricting possible comparisons. Furthermore, no such perturbation estimates have as yet been worked out for two phase spheres.
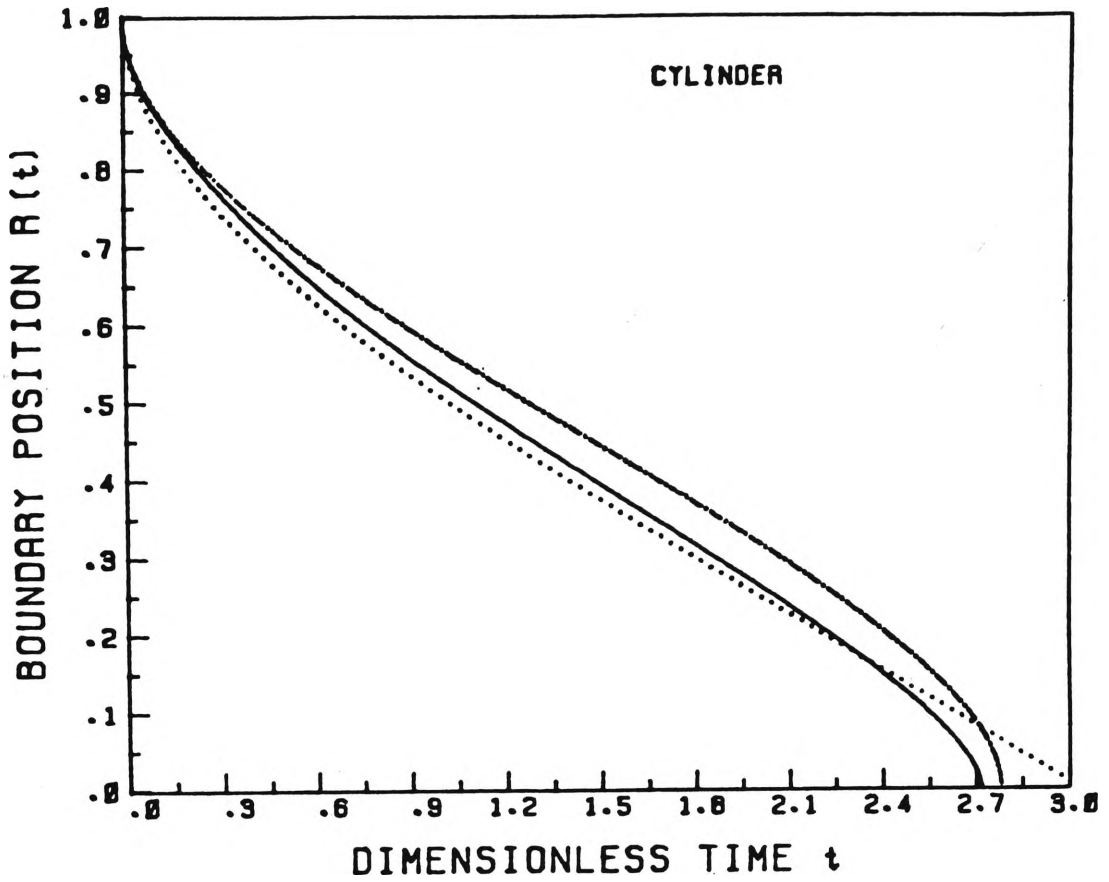
**Figure 4.1**    Comparison of the boundary fixing estimate ($-\cdot-\cdot-$) and perturbation estimate ($\cdots$), with numerical estimate ($\text{————}$) for the boundary motion for the cylinder with $\alpha = 10, \kappa = 1,$ and $V = 1$
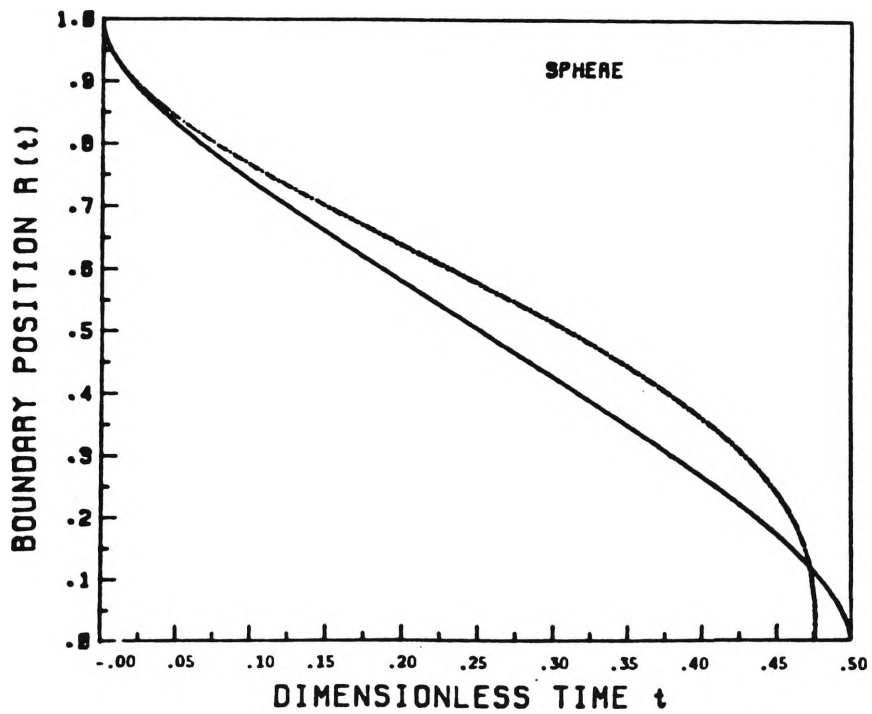


**Figure 4.2**    Comparison of the boundary fixing estimate ($-\cdot-\cdot-$) with numerical estimate ($\text{————}$) for the boundary motion for the sphere with $\alpha = 2, \kappa = 1,$ and $V = 1$
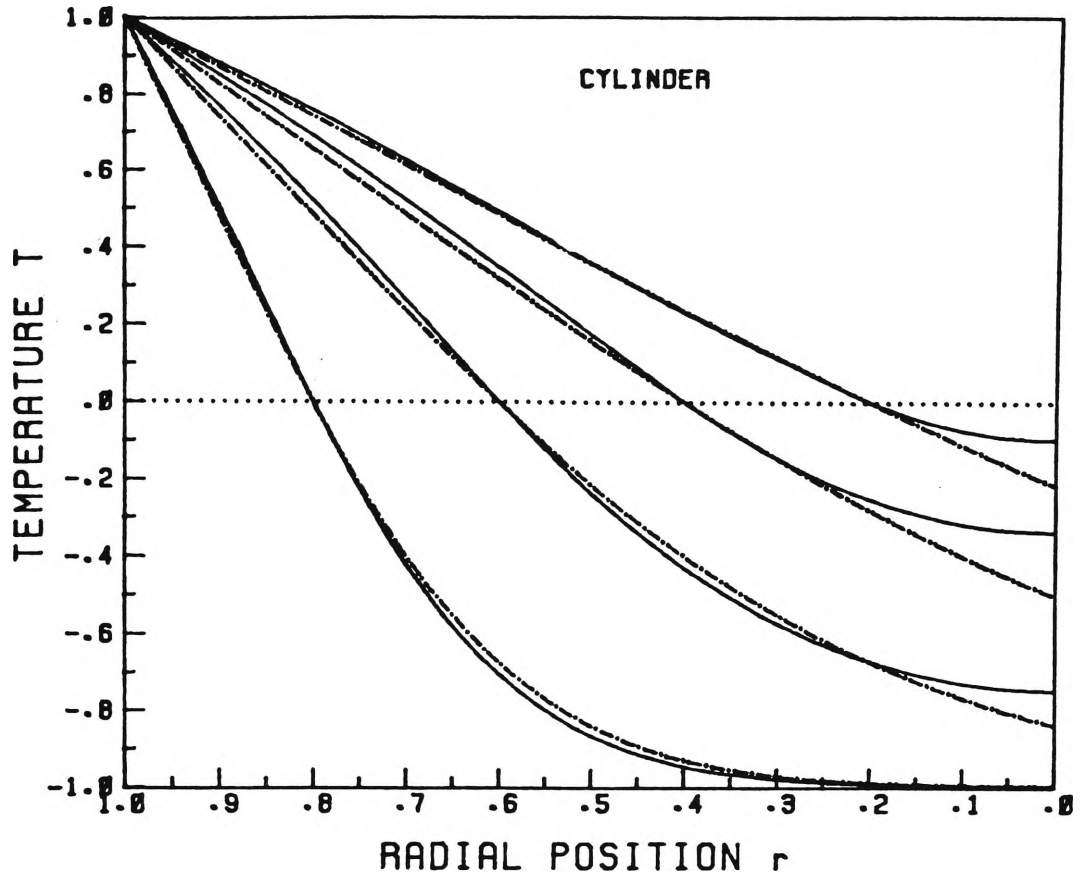
**Figure 4.3**     One term temperature profile for the cylinder with $\alpha = 0.01$, $\kappa = 0.5$, and $V = 1$
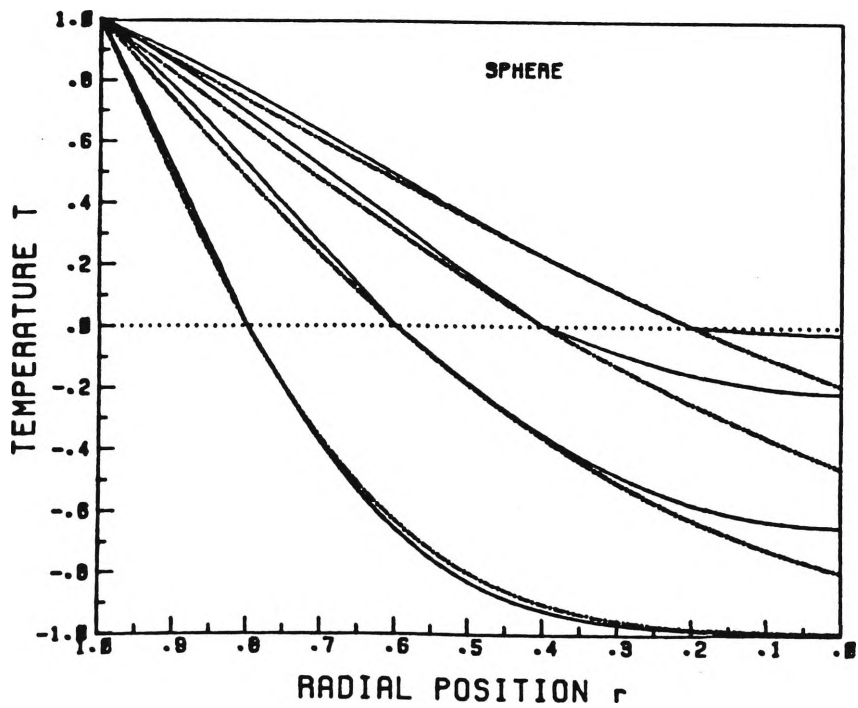


**Figure 4.4**     One term temperature profile for the sphere with $\alpha = 0.1$, $\kappa = 1$, and $V = 1$

| $\kappa = 1.0$<br>$V = 1.0$<br>$\alpha$ | Jiji & Weinbaum's<br>Perturbation<br>Solution | Boundary<br>Fixing series<br>(4.4.21) | Numerical<br>Solution |
|---|---|---|---|
| 1.0 | 0.29 | 0.68 | 0.48 |
| 3.0 | 0.87 | 1.17 | 0.98 |
| 5.0 | 1.46 | 1.65 | 1.47 |
| 10.0 | 2.91 | 2.78 | 2.72 |
| 20.0 | 5.83 | 4.99 | 5.21 |
| 30.0 | 8.74 | 7.17 | 7.71 |
| 40.0 | 11.66 | 9.32 | 10.21 |
| 50.0 | 14.57 | 11.46 | 12.71 |
| 100.0 | 29.15 | 22.04 | 25.23 |

Table 4.1    Various estimates for times, $t_c$, to complete melting, $R(t_c) = 0.0$, for a two phase cylinder with $\kappa = 1.0$, $V = 1.0$, and selected values of $\alpha$

| $\kappa = 1.0$<br>$V = 1.0$<br>$\alpha = 1.0$ | Jiji & Weinbaum's<br>Perturbation<br>Solution | Boundary<br>Fixing series<br>(4.4.20) | Numerical<br>Solution |
|---|---|---|---|
| 0.9 | 0.034 | 0.016 | 0.016 |
| 0.8 | 0.068 | 0.062 | 0.057 |
| 0.7 | 0.100 | 0.131 | 0.112 |
| 0.6 | 0.131 | 0.218 | 0.172 |
| 0.5 | 0.161 | 0.315 | 0.230 |
| 0.4 | 0.189 | 0.416 | 0.287 |
| 0.3 | 0.216 | 0.513 | 0.342 |
| 0.2 | 0.242 | 0.598 | 0.397 |
| 0.1 | 0.267 | 0.661 | 0.447 |
| 0.0 | 0.291 | 0.684 | 0.476 |

Table 4.2    Comparison of various estimates for the boundary motion for a two phase cylinder with $\alpha = 1.0$, $\kappa = 1.0$, and $V = 1.0$

# CHAPTER FIVE

# Heterogeneous Moving Boundary Problems

## 5.1 Introduction

The present chapter is concerned with the application, evaluation, and comparisons between two analytic methods for moving boundary problems. The analysis is presented in terms of melting heterogeneous single-phase planes, cylinders and spheres. By heterogeneous we mean that at least one of the thermal properties is a function of position. In Section 5.2, we describe the physical problems in detail and formulate equations in dimensionless form. In Section 5.3, we apply the formal boundary fixing series technique and derive the first two terms which are subsequently used to generate accurate temperature and boundary motion estimates shown to be valid for both small and large values of $\alpha$. In Section 5.4, we introduce a new and simple polynomial approximation technique for moving boundary problems. The first four terms of the approximation are found and used to generate approximations for both temperature profiles and boundary motions which are accurate for a large range of $\alpha$. For completeness, asymptotic properties and extensions to higher order approximations are presented at the end of the section. A detailed numerical comparison between the estimates, theoretical upper and lower bounds, and numerical solutions is presented in Section 5.5. In closing, recommendations for using particular methods for various ranges of $\alpha$ are made.

## 5.2 Governing equations

The problems considered here will be the melting of an idealized plane of width $a^*$, a cylinder and sphere of radius $a^*$, containing a solid initially at its fusion temperature $T_0^*$. At time zero, $t^* = 0$, the temperature, $T^*$, at the outer boundary, $r^* = a^*$, is raised to the value, $T_a^*$, above the melting point, $T_0^*$, and maintained at this constant thereafter. To simplify the problem the volumetric expansion or contraction due to the phase change is neglected and the thermal properties of the system are assumed to be independent of temperature. Based on these simplifications the governing equation and boundary conditions can be written in dimensionless form as

$$r^\lambda \frac{\partial T}{\partial t} = \frac{\partial}{\partial r}\left(r^\lambda D(r)\frac{\partial T}{\partial r}\right), \quad R(t) < r < 1, \tag{5.2.1}$$

subject to the boundary and initial conditions

$$T(1,t) = 1, \quad T(R,t) = 0, \quad T(r,0) = 0, \tag{5.2.2}$$

and the heat balance (Stefan) condition on the moving boundary

$$D(R)\frac{\partial T}{\partial r}(R,t) = -\alpha \frac{dR}{dt}, \quad R(0) = 1. \tag{5.2.3}$$

Here, $T(r,t)$ denotes the non-dimensional temperature, and the non-dimensional variables $r$, $t$, $R(t)$ and $D(r)$ and constant $\alpha$ are given in terms of the starred physical quantities

$$r = \frac{r^*}{a^*}, \qquad t = \frac{k(0)}{\rho c a^{*2}}t^*, \qquad R(t) = \frac{1}{a^*}R^*(t^*), \qquad D(r) = \frac{k(r^*)}{k(0)},$$

$$T(r,t) = \left(T^*(r^*,t^*) - T_0^*\right)/\left(T_a^* - T_0^*\right), \qquad \alpha = L/c\left(T_a^* - T_0^*\right), \tag{5.2.4}$$

where $k(r^*)$ is the inhomogeneous thermal conductivity with $k(0)$ being non-zero, $\rho$ is the constant density, $L$ the latent heat of fusion, and $c$ the constant heat capacity of the molten material. The positive constant $\alpha$ denotes the inverse Stefan number,

while the constant $\lambda$ takes on values of 0, 1, and 2 specifying planar, cylindrical and spherical geometries respectively.

## 5.3 Boundary fixing series technique

In this section we derive the first two terms of a formal series solution. The two terms will then be used to obtain estimates for both the temperature profiles and boundary motions valid for large and small values of $\alpha$ . Following the procedure of previous chapters, we introduce a boundary fixing transformation of the form

$$x = \frac{f(r)}{f(R)}, \quad y = f(R), \quad \phi(x,y) = T(r,t), \tag{5.3.1}$$

where $f(r)$ is determined such that $f(1) = 0$. Thus the region $[R(t), 1]$ is transformed to $[0, 1]$, and the original moving boundary problem is transformed into a fixed boundary problem. Substituting (5.3.1) into (5.2.1) yields

$$\frac{D(r)}{D(R)}\left(\frac{df}{dr}\Big/\frac{df}{dR}\right)^2\frac{\partial^2\phi}{\partial x^2} + \frac{f(R)}{D(R)}\left(\frac{df}{dR}\right)^{-2}\left[\frac{d^2f}{dr^2} + \left(\frac{D'(r)}{D(r)} + \frac{\lambda}{r}\right)\frac{df}{dr}\right]\frac{\partial\phi}{\partial x}$$
$$= \frac{1}{\alpha}\frac{\partial\phi}{\partial x}(1,y)\left[x\frac{\partial\phi}{\partial x} - y\frac{\partial\phi}{\partial y}\right]. \tag{5.3.2}$$

Clearly equation (5.3.2) is simplified greatly provided $f(r)$ is chosen so that it satisfies the homogeneous equation

$$\frac{d^2f}{dr^2} + \left(\frac{D'(r)}{D(r)} + \frac{\lambda}{r}\right)\frac{df}{dr} = 0. \tag{5.3.3}$$

With the boundary fixing transformation defined by (5.3.1), (5.3.3) and $f(1) = 0$,the system (5.2.1)-(5.2.3) becomes

$$\frac{D(r)}{D(R)}\left(\frac{df}{dr}\Big/\frac{df}{dR}\right)^2\frac{\partial^2\phi}{\partial x^2} = \frac{1}{\alpha}\frac{\partial\phi}{\partial x}(1,y)\left[x\frac{\partial\phi}{\partial x} - y\frac{\partial\phi}{\partial y}\right], \quad 0 < x < 1, \tag{5.3.4}$$

subject to the fixed boundary and initial conditions

$$\phi(0,y) = 1, \quad \phi(1,y) = 0, \quad \phi(x,0) = 0, \tag{5.3.5}$$

and the energy balance condition on the moving boundary becomes

$$\frac{\partial \phi}{\partial x}(1,y) = -\alpha \left[\frac{y}{D(R)f'(R)^2}\right] \frac{dy}{dt}, \quad y(0) = 0. \tag{5.3.6}$$

From (5.3.3) and the required boundary fixing condition $f(1) = 0$, we have the transformation function $f(r)$ is given by

$$f(r) = \int_r^1 \frac{d\xi}{D(\xi)\xi^\lambda} = K_\lambda(1,r), \quad \text{with} \quad K_\lambda(x,y) = \int_x^y \frac{d\xi}{\xi^\lambda D(\xi)}. \tag{5.3.7}$$

Assuming a formal series solution of the form

$$\phi(x,y) = \sum_{n=0}^{\infty} A_n(x)y^n, \tag{5.3.8}$$

substituting (5.3.8) into (5.3.4)-(5.3.6), expanding and equating coefficients of like powers of $y$, the following system of ordinary linear differential equations is obtained

$$A''_0 + \gamma[xA'_0] = 0,$$
$$A''_n + \gamma[xA'_n - nA_n] = F_n(x), \quad n = 1,2,\ldots, \tag{5.3.9}$$

where the functions $F_n(x)$'s are given by

$$F_n(x) = -\sum_{j=0}^{n-1} A''_j Q_{n-j}(x) + \frac{1}{\alpha}\sum_{j=1}^{n} A'_j(1)[xA'_{n-j} - (n-j)A_{n-j}], \tag{5.3.10}$$

and the argument of the $A_n$'s are understood to be $x$, unless otherwise indicated. The boundary conditions (5.3.5) become

$$A_0(0) = 1, \quad A_0(1) = 0,$$
$$A_n(0) = 0, \quad A_n(1) = 0, \quad n = 1,2,\ldots, \tag{5.3.11}$$

while (5.3.6) becomes

$$\sum_{n=0}^{\infty} A'_n(1)y^n = -\alpha \left[\frac{y}{D(R)f'(R)^2}\right] \frac{dy}{dt}, \quad y(0) = 0. \tag{5.3.12}$$

We have also used in equation (5.3.9) the notation

$$A'_0(1) = -\alpha\gamma. \tag{5.3.13}$$

From equation (5.3.12) we note that only the constants $A'_n(1)$ are required to fully determine the motion of the boundary. The functions $Q_n(x)$ in equation (5.3.10) are easily found by assuming the existence of the series expansion

$$\frac{D(r)}{D(R)}\left(\frac{df}{dr}\Big/\frac{df}{dR}\right)^2 = 1 + \sum_{n=1}^{\infty} Q_n(x)y^n. \tag{5.3.14}$$

where, for example, $Q_1(x)$, (which will be required presently) is given by

$$Q_1(x) = \mu(x - 1), \qquad \text{with} \quad \mu = D'(1) + 2\lambda D(1). \tag{5.3.15}$$

Solving equation (5.3.9) subject to (5.3.11)$_1$ gives the solution for $A_0(x)$, namely

$$A_0(x) = \alpha\gamma \int_x^1 e^{\frac{\gamma}{2}(1-\xi^2)} d\xi, \tag{5.3.16}$$

where $\gamma$ is the positive root of the transcendental equation

$$\alpha\gamma \int_0^1 e^{\frac{\gamma}{2}(1-\xi^2)} d\xi = 1. \tag{5.3.17}$$

Substituting results (5.3.16) and (5.3.17) into (5.3.10) and using (5.3.15) yields

$$F_1(x) = -\gamma[\alpha\gamma\mu(x - 1) + A'_1(1)]e^{\frac{\gamma}{2}(1-x^2)}. \tag{5.3.18}$$

Solving (5.3.9)$_2$ subject to boundary conditions (5.3.11)$_2$ while using result (5.3.18) gives the solution for $A_1(x)$

$$A_1(x) = \frac{\alpha\gamma\mu x}{4(3+\gamma)}\left\{[(3+\gamma)x - (4+\gamma)]e^{\frac{\gamma}{2}(1-x^2)} + (3+\gamma)\int_x^1 e^{\frac{\gamma}{2}(1-\xi^2)} d\xi + 1\right\}, \tag{5.3.19}$$

from which, on differentiating and setting $x = 1$, we find that $A'_1(1)$ is given by

$$A'_1(1) = \alpha\gamma\delta, \qquad \text{with} \quad \delta = \frac{\gamma\mu}{4(3+\gamma)}. \tag{5.3.20}$$

Substituting results (5.3.13) and (5.3.20) into (5.3.12), integrating and returning to original variables $r$, $t$ yields the following boundary motion estimate

$$t \approx \frac{1}{\gamma} \int_{R(t)}^1 \xi^\lambda K_\lambda(1, \xi)[1 + \delta K_\lambda(1, \xi)] d\xi, \tag{5.3.21}$$

provided that the diffusivity $D(r)$ is non-zero throughout the range of integration.

For the case $D(r) = 1 + (\epsilon r)^2$, the constant $\delta$ is given by

$$\delta = \frac{\gamma}{2(3 + \gamma)}\left[\lambda + \epsilon^2(\lambda + 1)\right]. \qquad (5.3.22)$$

while the function $K_\lambda$ is given by $(5.3.7)_2$.

We note that the expanding variable, $y$, can become very large and even singular for certain values of $R(t)$ causing (5.3.21) to yield bad estimates. To eliminate this singularity we introduce a new transformation given by

$$\Phi(x,z) = \phi(x,y), \quad \text{with} \quad z = (1 - R(t)), \qquad (5.3.23)$$

expanding $y$ in terms of $z$ and equating coefficients of like powers of $z$ yields

$$t \approx \frac{1}{\gamma}\int_R^1 \xi^\lambda K_\lambda(1,\xi)[1 + \delta(\xi - 1)/D(1)]d\xi, \qquad (5.3.24)$$

a non singular expression for the motion of the boundary.

From equations (5.3.20) and (5.3.22) with $\epsilon = 0$ and $\lambda = 0$, that is for the homogeneous plane, it is easy to see that $A'_1(1)$ is zero, from which it quickly follows that $A_1(x)$ must be identically zero. Substituting $A_1(x) \equiv 0$ into $(5.3.9)_2$ and using result (5.3.16) yields

$$A''_2 + \gamma[xA'_2 - 2A_2] = -\gamma x A'_2(1)e^{\frac{\gamma}{2}(1-x^2)}, \qquad (5.3.25)$$

and solving (5.3.25) subject to homogeneous boundary conditions $(5.3.11)_2$ gives $A_2(x) \equiv 0$. Repeating the process eliminates all the remaining $A_n(x)$'s leaving the exact solution $A_0(x)$ as given by (5.3.16).

## 5.4 Polynomial approximations

In this section we introduce a new polynomial technique for moving boundary problems. The technique yields simple and quick approximations for both temperature profiles and boundary motions. The method of solution consists of representing

$T(r,t)$ by a series of the form

$$T(r,t) = \sum_{n=0}^{\infty} a_n(R) U_\lambda^n(r,R), \tag{5.4.1}$$

where the coefficients $a_n$ are independent of 'r'. while the function $U_\lambda(r,R)$ is left to be determined later based on some simplification criteria. Since the number of boundary conditions is limited, it is necessary to assume that the temperature $T$ can be approximated accurately by terminating the series at a cubic in $U_\lambda$, namely

$$u(r,t) \approx a_0(R) + a_1(R) U_\lambda(r,R) + a_2(R) U_\lambda^2(r,R) + a_3(R) U_\lambda^3(r,R). \tag{5.4.2}$$

Four boundary conditions are required to determine the coefficients $a_0(R)$, $a_1(R)$, $a_2(R)$ and $a_3(R)$ uniquely. Boundary conditions $(5.2.2)_1$ and $(5.2.2)_2$ are the obvious first two. Boundary condition $(5.2.3)$ can not be used directly since it would introduce unknown $dR/dt$ terms into the coefficients, therefore two other boundary conditions must somehow be generated. Differentiating both boundary conditions $(5.2.2)_1$ and $(5.2.2)_2$ with respect to time $t$ yields

$$\frac{\partial T}{\partial t}(1,t) = 0, \qquad \frac{\partial T}{\partial t}(R,t) = -\frac{\partial T}{\partial r}(R,t)\frac{dR}{dt}. \tag{5.4.3}$$

Substituting $(5.4.3)_1$ and $(5.4.3)_2$ into the governing equation $(5.2.1)$ and using condition $(5.2.3)$ for $dR/dt$ yields

$$\frac{\partial}{\partial r}\left(r^\lambda D(r)\frac{\partial T}{\partial r}\right) = 0, \quad r = 1, \qquad r^\lambda D(r)\left(\frac{\partial T}{\partial r}\right)^2 = \alpha \frac{\partial}{\partial r}\left(r^\lambda D(r)\frac{\partial T}{\partial r}\right), \quad r = R. \tag{5.4.4}$$

Condition $(5.4.4)_1$ is a simple statement that at the fixed boundary, with constant temperature condition, the pseudo-steady state holds exactly. Condition $(5.4.4)_2$ is considerably harder to interpret physically. Substituting approximation $(5.4.2)$ into $(5.4.4)_1$ and $(5.4.4)_2$ generates

$$\frac{\partial}{\partial r}\left(r^\lambda D(r)\frac{\partial U_\lambda}{\partial r}\right)\left(a_1 + 2a_2 U_\lambda + 3a_3 U_\lambda^2\right) + r^\lambda D(r)\left(\frac{\partial U_\lambda}{\partial r}\right)^2 (2a_2 + 6a_3 U_\lambda) = 0, \tag{5.4.5}$$

and

$$r^\lambda D(r) \left[ \frac{\partial U_\lambda}{\partial r} (a_1 + 2a_2 U_\lambda + 3a_3 U_\lambda^2) \right]^2 = \alpha \left\{ \left[ \frac{\partial}{\partial r} \left( r^\lambda D(r) \frac{\partial U_\lambda}{\partial r} \right) (a_1 + 2a_2 U_\lambda + 3a_3 U_\lambda^2) \right] \right.$$

$$\left. + \left[ r^\lambda D(r) \left( \frac{\partial U_\lambda}{\partial r} \right)^2 (2a_2 + 6a_3 U_\lambda) \right] \right\},$$

$$(5.4.6)$$

the last two required boundary conditions. From (5.4.5) and (5.4.6) it is clear that a great simplification will result if $U_\lambda(r, R)$ satisfies the homogeneous system

$$\frac{\partial}{\partial r} \left( r^\lambda D(r) \frac{\partial U_\lambda}{\partial r} \right) = 0, \quad R \leq r \leq 1, \qquad (5.4.7)$$

subject to the boundary conditions

$$U_\lambda(1, R) = 1, \qquad U_\lambda(R, R) = 0. \qquad (5.4.8)$$

On solving (5.4.7) and (5.4.8) we find

$$U_\lambda(r, R) = \frac{K_\lambda(r, R)}{K_\lambda(1, R)}, \qquad (5.4.9)$$

where the function $K_\lambda$ is given by equation $(5.3.7)_2$, identifying $U_\lambda(r, R)$ as the pseudo-steady state solution of (5.2.1)-(5.2.3). From $(5.2.2)_1$, $(5.2.2)_2$, (5.4.5) and (5.4.6) with (5.4.7)-(5.4.9), the coefficients $a_0$, $a_1$, $a_2$ and $a_3$ are found by solving the algebraic system

$$0 = a_0, \qquad 1 = a_1 + a_2 + a_3, \qquad 0 = a_1^2 - 2\alpha a_2, \qquad 0 = a_2 + 3a_3. \quad (5.4.10)$$

With (5.4.9) and (5.4.10) the temperature approximation (5.4.2) is now fully defined.

Multiplying equation $(5.2.3)_1$ by $dt(D(r)\partial T/\partial r)^{-1}$, integrating from $R(t)$ to 1 and using (5.4.2) with (5.4.9) and (5.4.10), the motion of the boundary can be approximated by

$$t \approx \frac{1}{\zeta} \Sigma_\lambda(R), \qquad (5.4.11)$$

with $\Sigma_\lambda(R)$ and $1/\zeta$ given by

$$\Sigma_\lambda(R) = \int_R^1 \xi^\lambda K_\lambda(1, \xi) d\xi, \qquad \frac{1}{\zeta} = \frac{\alpha}{2} \left( 1 + \sqrt{1 + \frac{4}{3\alpha}} \right). \qquad (5.4.12)$$

Alternatively, dropping boundary condition (5.4.4)$_1$, and instead, multiplying equation (5.2.1) by $dr$, integrating from $R(t)$ to 1 and using boundary condition (5.2.3) yields

$$D(1)\frac{\partial T}{\partial r}(1,t) = -\left[\alpha R^\lambda + \frac{d\theta}{dR}\right]\frac{dR}{dt}, \quad R(0) = 1, \qquad (5.4.13)$$

which is usually refered to as Goodman's heat-balance integral equation. Here $\theta$ is essentially a measure of the total thermal energy of the molten region and is given by

$$\theta = \int_{R(t)}^{1} r^\lambda T(r,t)dr. \qquad (5.4.14)$$

However, the nonlinear nature of the heat-balance condition makes it very difficult to solve analytically, even the simplest cases. For example, Goodman (1958), after much effort, was able to solve for the homogeneous plane and obtain the following boundary motion estimate

$$t \approx \frac{1}{2q}(1 - R)^2, \quad \text{with} \quad \frac{2}{\alpha} = \left[\frac{q^3 + 18q^2 + 72q}{3(12 - q)}\right], \qquad (5.4.15)$$

which has the following asymptotic estimates for large and small $\alpha$

$$t \sim \frac{\alpha}{2}\left(1 + \frac{1}{3\alpha} - \frac{5}{72\alpha^2}\right)(1 - R)^2 \quad \text{(large } \alpha\text{)}, \quad t \sim \frac{1}{24}(1 - R)^2 \quad \text{(small } \alpha\text{)}.$$
$$(5.4.16)$$

Expanding (5.4.11) and (5.4.12) for large and small $\alpha$ yields the following asymptotic estimates for the plane

$$t \sim \frac{\alpha}{2}\left(1 + \frac{1}{3\alpha} - \frac{1}{9\alpha^2}\right)(1 - R)^2 \quad \text{(large } \alpha\text{)}, \quad t \sim \sqrt{\frac{\alpha}{3}}(1 - R)^2 \quad \text{(small } \alpha\text{)}.$$
$$(5.4.17)$$

For large $\alpha$ estimates (5.4.16)$_1$ and (5.4.17)$_1$ are seen to be in very close agreement. However, for small $\alpha$ (5.4.16)$_2$ degenerates leaving (5.4.17)$_2$ as the more accurate estimate. For more complicated diffusivities and other geometries Goodman's heat-balance equation (5.4.13) must be solved numerically, while equation (5.4.11) is a useful estimate for all geometries and any radially dependent diffusivity $D(r)$.

Better polynomial estimates can be obtained by assuming that $T(r, t)$ can be approximated by a higher order polynomial, namely

$$T(r,t) \approx \sum_{n=0}^{2N+1} a_n(R) U_\lambda^n(r,R),$$ (5.4.18)

subject to the "natural" boundary conditions $(5.2.2)_1$ and $(5.2.2)_2$, and the generated conditions

$$\frac{d^n T}{d t^n}(1,t) = 0, \qquad \frac{d^n T}{d t^n}(R,t) = 0, \qquad \text{for} \quad n = 1, \dots N.$$ (5.4.19)

With the condition (5.2.3) used to eliminate $dR/dt$ and the governing equation used to replace the time derivatives with space derivatives we find again that $U_\lambda(r,R)$ is as given by (5.4.9) while the new estimate for the boundary motion is given by

$$t \approx \alpha \int_R^1 \frac{\xi^\lambda K_\lambda(1,\xi) d\xi}{a_1(\xi)},$$ (5.4.20)

where $a_1$ is no longer a constant but a function of $R$ which must be found numerically by solving a set of algebraic equations similar to that of (5.4.10).

## 5.5 Numerical results and discussion

In this final section we present a detailed numerical comparison between the analytical estimates and an adaption of the explicit finite-difference enthalpy method of Voller and Cross (1981), which will serve as the principle basis for assessing the applicability and accuracy of the various analytic approximations. In all our comparisons we have set the diffusivity $D(r)$ to be $D(r) = 1 + (\epsilon r)^2$.

Figures 5.1, 5.2, 5.3, and 5.4 compare the upper and lower bounds for the boundary motion of Dewynne (see Dewynne, 1985) with the polynomial approximation (5.4.11), the boundary fixing series approximation (5.3.21), and the numerical solution. Figure 5.1 shows the various approximations for the cylinder with $\alpha = 0.1$ and $\epsilon = 0.0$, Figure 5.2, the various approximations for the sphere with $\alpha = 0.1$

and $\epsilon$ = 0.0, and Figures 5.3 and 5.4 the various approximations for the cylinder and plane with $\alpha$ = 1.0 and $\epsilon$ = 0.5. In all the four cases the boundary fixing series technique provides the best estimate for both the motion of the boundary and the times to complete melting. The polynomial approximation technique provides estimates which are close to, but not always within, the lower bound, as shown in Figure 5.2. The upper bound (also being the two term perturbation estimate) diverges sharply as the moving boundary, $R(t)$, approaches the center. Figures 5.5 and 5.6 compare the boundary fixing series approximation for the temperature profiles with that of the polynomial approximation and the numerical solution for the cylinder and sphere respectively, with $\alpha$ = 10.0, $\epsilon$ = 0.5 and equally spaced values of $R(t)$. In both cases the polynomial approximation technique is seen to yield the superior temperature estimate.

In Tables 5.1 and 5.2 various estimates for the times to complete melting for a large range of $\alpha$ and selected values of $\epsilon$ are tabulated and compared with the numerical solution for the cylinder and sphere. For small $\alpha$, the upper bound estimate is highly inaccurate with errors over 100 %. The lower bound and the polynomial approximation technique are seen to yield better estimates with errors of about 70 %, while the boundary fixing series technique is shown to yield the best estimate with errors of the order of 25 %. For large $\alpha$ all the methods yield good estimates, with the two term perturbation estimate the best. In Table 5.3 various estimates for the times to complete melting for $\alpha$ = 1.0 and a range of $\epsilon$ are tabulated and compared with the numerical solution. For all the $\epsilon$ values tested it is seen that the boundary fixing series technique yields the better estimate. In Table 5.4 the various estimates for the boundary motion for the cylinder with $\alpha$ = 2.0 and $\epsilon$ = 0.3 are tabulated and compared with the numerical solution. It is surprising to note that for small times, $(R(t) \geq 0.8)$, the polynomial estimate yields the best

agreement with the numerical solution. We also note here that the performance of all the methods appear to be independent of the particular choice of $\epsilon$.

In conclusion, the following recommendations for using particular methods for various ranges of $\alpha$ are made:

1. For large values of $\alpha$, ($\alpha > 10.0$), one can use the bounding technique of Dewynne to produce tight theoretical upper and lower bounds for both the boundary motion and times to complete melting. We also note here that for this range of $\alpha$ the numerical enthalpy method requires a large number of iterations making it computationally expensive.

2. For intermediate values of $\alpha$, ($0.1 < \alpha < 10.0$), the boundary fixing series technique of section 5.3 can be used to produce reliable estimates for the boundary motion, while the polynomial approximation technique of Section 5.4 for temperature profile estimates.

3. For small values of $\alpha$, ($\alpha < 0.1$), the only analytic expression presently available is the exact similarity solution, discussed in Section 5.3, for the homogeneous plane. It would appear that further effort to derive analytic expressions is required in this range of $\alpha$, where only numerical solutions exist.
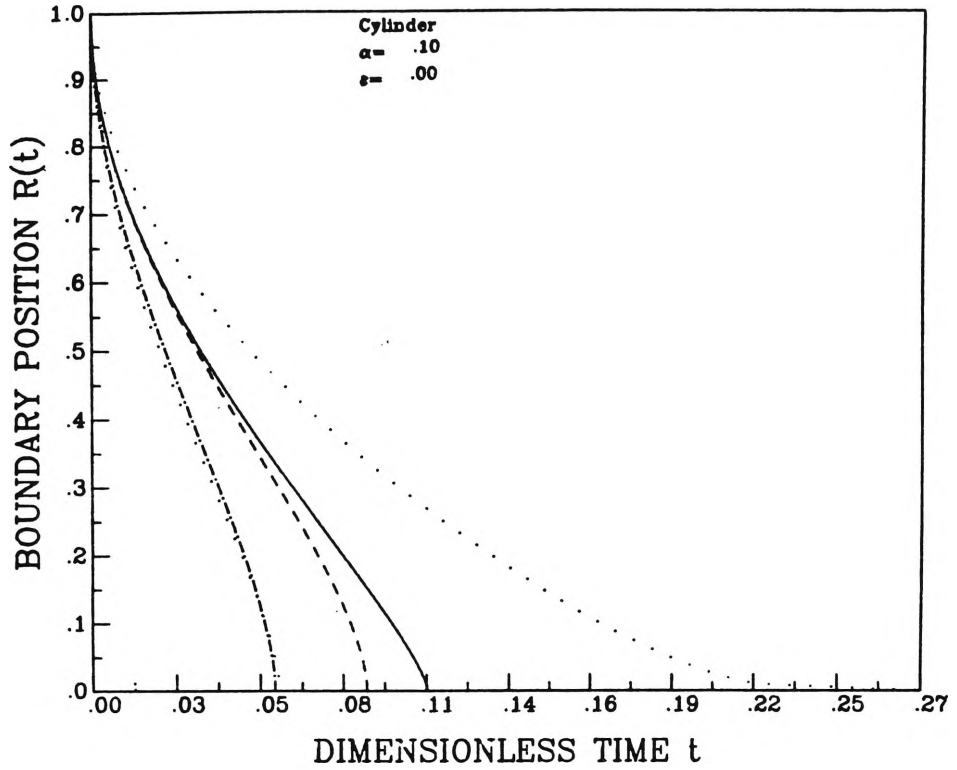
Figure 5.1  Comparison of boundary fixing estimate ($-\cdot-\cdot-$), polynomial estimate ($\cdots$), and bounds ($---$), with numerical boundary motion ($\longrightarrow$) for the cylinder with $\alpha = 0.1$, and $\epsilon = 0.0$
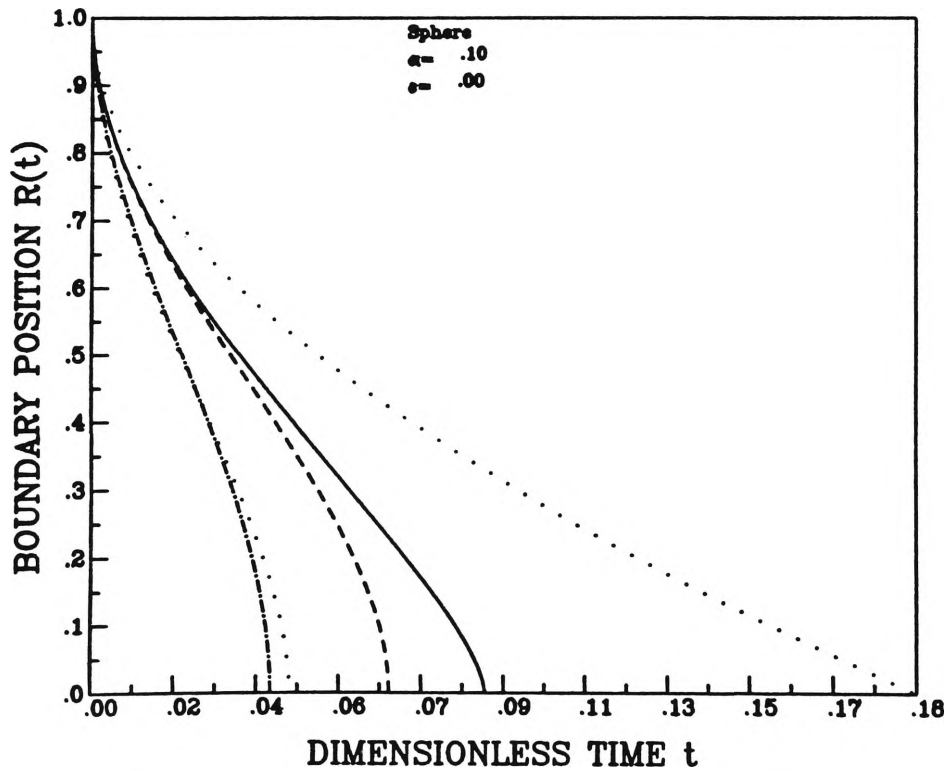


Figure 5.2  Comparison of boundary fixing estimate ($-\cdot-\cdot-$), polynomial estimate ($\cdots$), and bounds ($---$), with numerical boundary motion ($\longrightarrow$) for the sphere with $\alpha = 0.1$, and $\epsilon = 0.0$
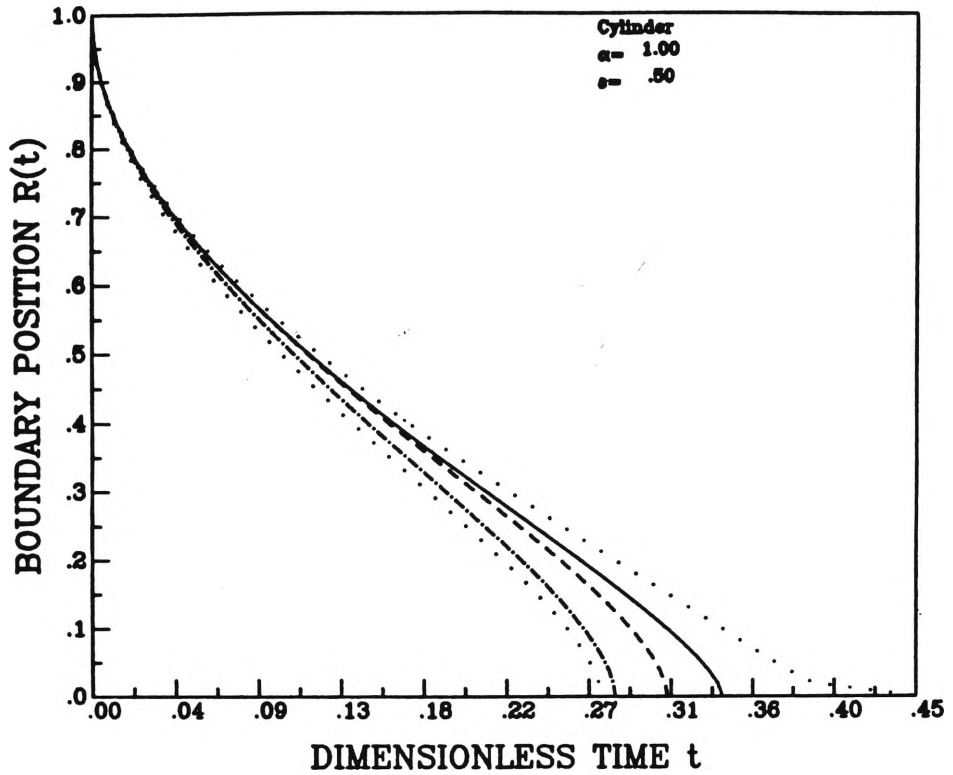
**Figure 5.3**   Comparison of boundary fixing estimate ($-\cdot-\cdot-$), polynomial estimate ($\cdot\cdot\cdot$), and bounds ($-\ -\ -$), with numerical boundary motion (━━━━) for the cylinder with $\alpha =$ **10** and $\epsilon = 0.5$
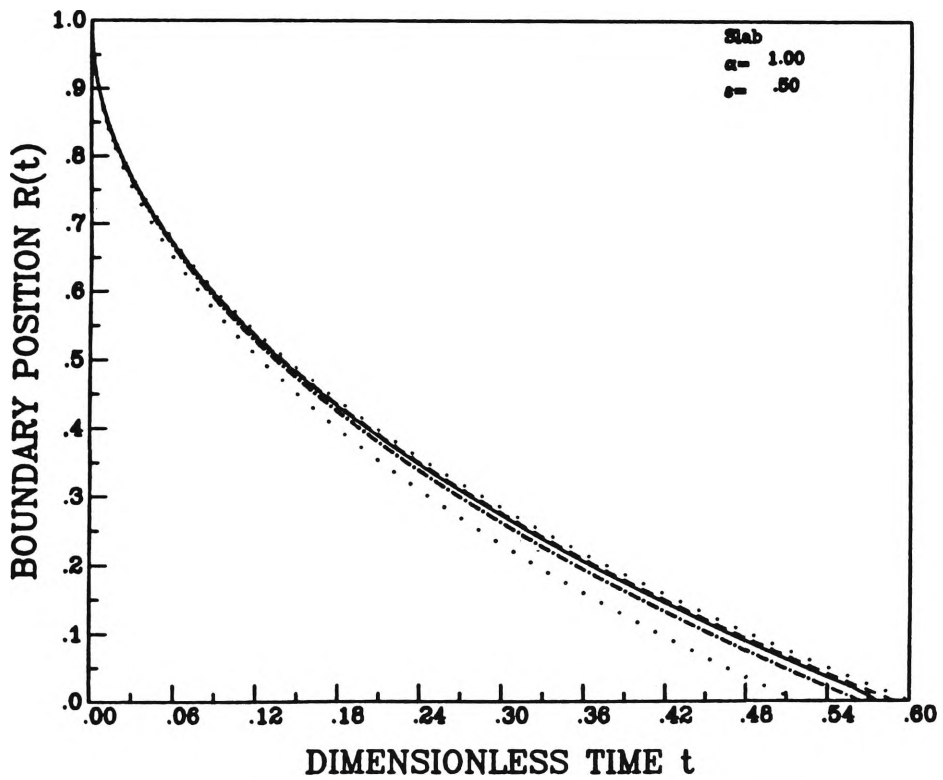


**Figure 5.4**   Comparison of boundary fixing estimate ($-\cdot-\cdot-$), polynomial estimate ($\cdot\cdot\cdot$), and bounds ($-\ -\ -$), with numerical boundary motion (━━━━) for the plane with $\alpha = $ **1.0**, and $\epsilon = 0.5$
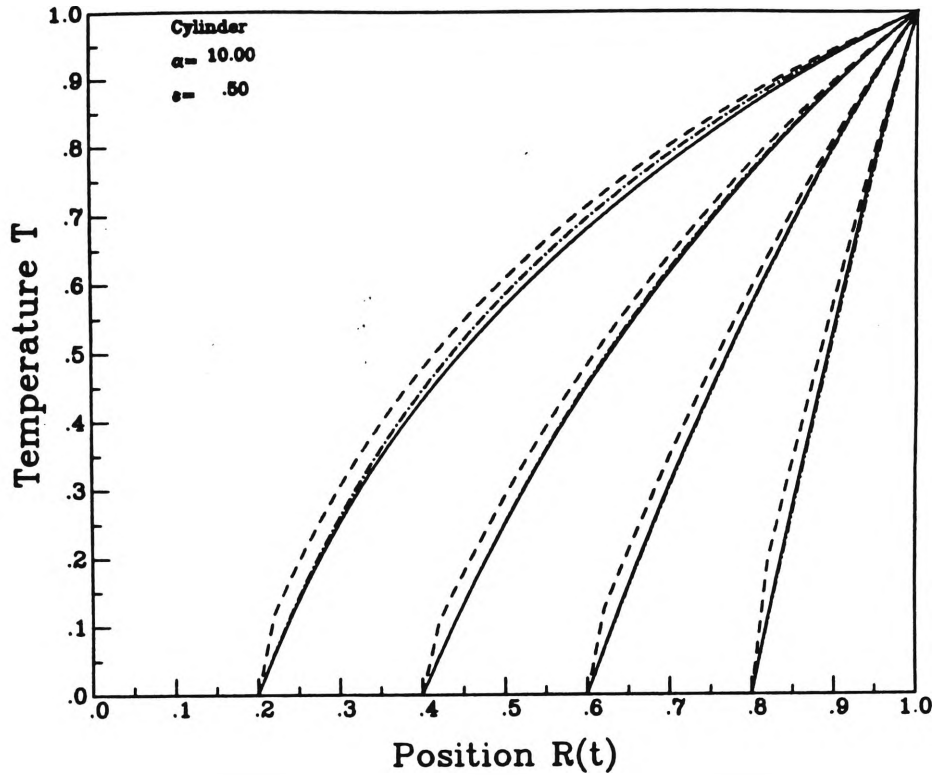
**Figure 5.5** Comparison of boundary fixing series approximation ($- \cdot - \cdot -$), polynomial approximation

($\cdot \cdot \cdot \cdot$), with numerical estimate (——————) for the temperature profiles of the cylinder with

$\alpha = 10.0, \epsilon = 0.5$, and equally spaced values of $R(t)$
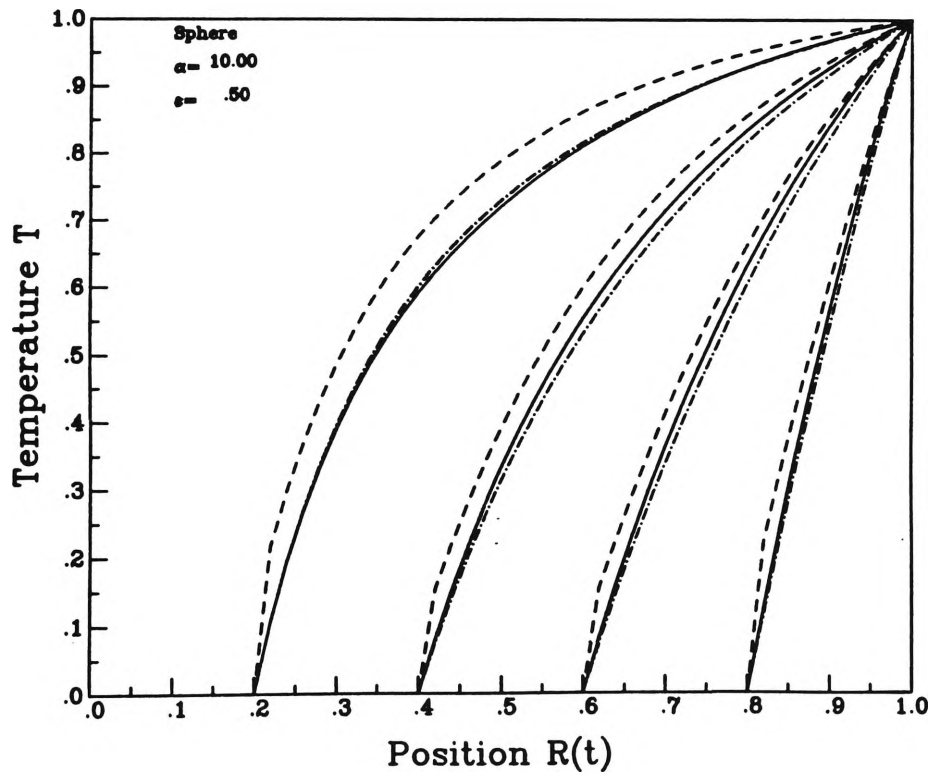


**Figure 5.6** Comparison of boundary fixing series approximation ($- \cdot - \cdot -$), polynomial approximation

($\cdot \cdot \cdot \cdot$), with numerical estimate (——————) for the temperature profiles of the sphere with

$\alpha = 10.0, \epsilon = 0.5$, and equally spaced values of $R(t)$

| $\epsilon = 0.0$ $\alpha$ | Lower Bound | Polynomial Approx. (5.4.11) | Boundary Fix. Series (5.3.24) | Numerical Solution | Upper Bound |
|---|---|---|---|---|---|
| 0.10 | 0.0612 | 0.0598 | 0.9038 | 0.1103 | 0.2750 |
| 0.25 | 0.1082 | 0.1098 | 0.1400 | 0.1649 | 0.3125 |
| 0.50 | 0.1767 | 0.1821 | 0.2112 | 0.2412 | 0.3750 |
| 0.75 | 0.2420 | 0.2500 | 0.2782 | 0.3118 | 0.4375 |
| 1.00 | 0.3061 | 0.3159 | 0.3435 | 0.3800 | 0.5000 |
| 2.50 | 0.6846 | 0.6994 | 0.7251 | 0.7715 | 0.8750 |
| 5.00 | 1.3110 | 1.3284 | 1.3530 | 1.4072 | 1.5000 |
| 7.50 | 1.9364 | 1.9549 | 1.9791 | 2.0375 | 2.1250 |
| 10.00 | 2.5617 | 2.5807 | 2.6046 | 2.6659 | 2.7500 |
| 25.00 | 6.3121 | 6.3322 | 6.3557 | 6.4241 | 6.5000 |

Table 5.1      Various estimates for times, $t_c$, to complete reaction, $(R(t_c) = 0)$, for a cylinder with selected values of $\alpha$, and $\epsilon$ zero

| $\epsilon = 0.0$ $\alpha$ | Lower Bound | Polynomial Approx. (5.4.11) | Boundary Fix. Series (5.3.24) | Numerical Solution | Upper Bound |
|---|---|---|---|---|---|
| 0.10 | 0.0440 | 0.0398 | 0.0662 | 0.0876 | 0.1833 |
| 0.25 | 0.0768 | 0.0732 | 0.1007 | 0.1265 | 0.2083 |
| 0.50 | 0.1236 | 0.1214 | 0.1494 | 0.1798 | 0.2500 |
| 0.75 | 0.1677 | 0.1666 | 0.1948 | 0.2284 | 0.2916 |
| 1.00 | 0.2108 | 0.2106 | 0.2388 | 0.2750 | 0.3333 |
| 2.50 | 0.4639 | 0.4662 | 0.4944 | 0.5397 | 0.5833 |
| 5.00 | 0.8819 | 0.8855 | 0.9136 | 0.9660 | 1.0000 |
| 7.50 | 1.2990 | 1.3032 | 1.3311 | 1.3875 | 1.4166 |
| 10.10 | 1.7159 | 1.7204 | 1.7483 | 1.8073 | 1.8333 |
| 25.00 | 4.2163 | 4.2212 | 4.2494 | 4.3152 | 4.3333 |

Table 5.2      Various estimates for times, $t_c$, to complete reaction, $(R(t_c) = 0)$, for a sphere with selected values of $\alpha$, and $\epsilon$ zero

| $\alpha = 1.0$ $\epsilon$ | Lower Bound | Polynomial Approx. (5.4.11) | Boundary Fix. Series (5.3.24) | Numerical Solution | Upper Bound |
|---|---|---|---|---|---|
| 0.1 | 0.3047 | 0.3143 | 0.3420 | 0.3776 | 0.4975 |
| 0.2 | 0.3004 | 0.3097 | 0.3376 | 0.3720 | 0.4902 |
| 0.3 | 0.2936 | 0.3025 | 0.3305 | 0.3636 | 0.4787 |
| 0.4 | 0.2848 | 0.2930 | 0.3212 | 0.3539 | 0.4638 |
| 0.5 | 0.2744 | 0.2820 | 0.3102 | 0.3404 | 0.4462 |
| 0.6 | 0.2630 | 0.2698 | 0.2980 | 0.3267 | 0.4270 |
| 0.7 | 0.2510 | 0.2571 | 0.2851 | 0.3124 | 0.4069 |
| 0.8 | 0.2388 | 0.2442 | 0.2719 | 0.2978 | 0.3864 |
| 0.9 | 0.2267 | 0.2314 | 0.2586 | 0.2833 | 0.3662 |
| 1.0 | 0.2149 | 0.2189 | 0.2456 | 0.2691 | 0.3465 |

Table 5.3     Various estimates for times, $t_C$, to complete reaction, $(R(t_C) = 0)$, for a cylinder with selected values of $\epsilon$, and $\alpha = 1.0$

| $\alpha = 2.0$ $\epsilon = 0.3$ $R(t)$ | Lower Bound | Polynomial Approx. (5.4.11) | Boundary Fix. Series (5.3.24) | Numerical Solution | Upper Bound |
|---|---|---|---|---|---|
| 0.9 | 0.0096 | 0.0102 | 0.0104 | 0.0101 | 0.0105 |
| 0.8 | 0.0374 | 0.0395 | 0.0403 | 0.0397 | 0.0407 |
| 0.7 | 0.0814 | 0.0857 | 0.0877 | 0.0871 | 0.0889 |
| 0.6 | 0.1391 | 0.1460 | 0.1502 | 0.1498 | 0.1528 |
| 0.5 | 0.2078 | 0.2175 | 0.2246 | 0.2252 | 0.2297 |
| 0.4 | 0.2895 | 0.2961 | 0.3070 | 0.3099 | 0.3164 |
| 0.3 | 0.3631 | 0.3769 | 0.3923 | 0.3994 | 0.4090 |
| 0.2 | 0.4390 | 0.4537 | 0.4738 | 0.4880 | 0.5024 |
| 0.1 | 0.5028 | 0.5168 | 0.5412 | 0.5667 | 0.5905 |
| 0.0 | 0.5358 | 0.5484 | 0.5752 | 0.6144 | 0.7182 |

Table 5.4     Comparison of various estimates for the boundary motion for a cylinder with $\alpha = 2.0$ and $\epsilon = 0.3$

# CHAPTER SIX

# Moving Boundary Problems with Internal Heat Loss

## 6.1 Introduction

In this chapter we look at melting of planes, cylinders and spheres which are accompanied by internal heat loss. Specifically we consider problems where throughout the newly formed molten region heat is being lost at a rate proportional to its temperature. In Section 6.2, we describe the physical problem in detail and formulate equations in dimensionless form. A short discussion is also given pertaining to the analogous shrinking core problem frequently used in chemical reaction models. In such problems it is usually hypothesised that a second reaction, behind the moving front, is taking place assumed to be pseudo first order. For both the melting and shrinking core models appropriate non-dimensionalizations are given. In Section 6.3 we give some known results and bounds. In Section 6.4 we discuss the strategy for choosing the boundary fixing transformation and method of solution. The new transformation will be shown to be a generalization on the previously used transformations. It will also be shown later that no other boundary fixing transformation can suffice. In Sections 6.5, 6.6 and 6.7 we present the analysis and results for the plane, cylinder and sphere respectively. In each case, the first two nontrivial terms are used to obtain accurate boundary motion estimates. Numerical results and a brief discussion are given in the final section.

## 6.2 Governing equations

The problems considered here will be the melting of an idealized plane of width $a^*$, a cylinder and sphere of radius $a^*$, containing a solid initially at its fusion temperature $T_0^*$. At time zero, $t^* = 0$, the temperature, $T^*$, at the outer boundary, $r^* = a^*$, is raised to the value, $T_a^*$, above the melting point, $T_0^*$, and maintained at this constant thereafter. Furthermore, it is assumed that there is a heat loss throughout the molten region which is proportional to the temperature. As in the previous chapters, to simplify the problem, the volumetric expansion or contraction due to the phase change is neglected and the thermal properties of the system are assumed to be independent of temperature. Based on these simplifications the governing equation and boundary conditions can be written in dimensionless form as

$$r^\lambda \frac{\partial T}{\partial t} = \frac{\partial}{\partial r}\left(r^\lambda \frac{\partial T}{\partial r}\right) - \nu^2 r^\lambda T, \quad R(t) < r < 1, \tag{6.2.1}$$

subject to the boundary and initial conditions

$$T(1,t) = 1, \quad T(R,t) = 0, \quad T(r,0) = 0, \tag{6.2.2}$$

and the heat balance (Stefan) condition on the moving boundary

$$\frac{\partial T}{\partial r}(R,t) = -\alpha \frac{dR}{dt}, \quad R(0) = 1. \tag{6.2.3}$$

Here, $T(r,t)$ denotes the non-dimensional temperature, and the non-dimensional variables $r$, $t$, $R(t)$ and constants $\alpha$ and $\nu^2$ are given in terms of the starred physical quantities

$$r = \frac{r^*}{a^*}, \quad t = \frac{k}{\rho c a^{*2}} t^*, \quad R(t) = \frac{1}{a^*} R^*(t^*), \quad \nu^2 = \frac{\nu_1 a^{*2}}{k},$$
$$\tag{6.2.4}$$
$$T(r,t) = \left(T^*(r^*,t^*) - T_0^*\right)\big/\left(T_a^* - T_0^*\right), \quad \alpha = L\big/c\left(T_a^* - T_0^*\right),$$

where $k$ is the thermal conductivity, $\rho$ is the constant density, $L$ the latent heat of fusion, $c$ the constant heat capacity of the molten material, and $\nu_1$ is the non-negative rate constant for the heat loss. As always, the positive constant $\alpha$ denotes

the inverse Stefan number, while the constant $\lambda$ takes on values of 0, 1, and 2 specifying plane, cylinder and sphere respectively.

Alternatively, replacing $T(r,t)$ with $c(r,t)$ (the concentration of a diffusing reactant), the system (6.2.1)-(6.2.3) is frequently used to describe a liquid-solid (or gas-solid) chemical reaction. The incoming reactant, $c(r,t)$, is assumed to react instantaneously with at least one of the solid reactants, giving rise to a moving "shrinking core" reaction front. Under such conditions, the constants $\alpha$ and $\nu^2$ have to be defined by new physical quantities, namely

$$\alpha = \frac{\rho\omega}{c_0}, \quad \text{and} \quad \nu^2 = \frac{a^{*2}\nu_2}{D}, \tag{6.2.5}$$

where, $\rho$, $\omega$, and $c_0$ denote the density, diffusivity, and constant boundary concentration of the liquid reactant respectively, $\omega$ the stoichiometric coefficient for the reaction on the moving front, and $\nu_2$ the pseudo-first order rate constant for the reaction behind the moving boundary.

## 6.3 Known results and bounds

The standard pseud-steady state approximation to (6.2.1)-(6.2.3) can be shown to be given by

$$T_{pss}(r,R) = \frac{K_\lambda(r,R)}{K_\lambda(1,R)}, \quad t_{pss} = \alpha\Sigma_\lambda(R), \tag{6.3.1}$$

with

$$K_0(r,R) = \frac{1}{\nu}\sinh[\nu(r-R)],$$

$$K_1(r,R) = I_0(\nu r)K_0(\nu R) - I_0(\nu R)K_0(\nu r), \tag{6.3.2}$$

$$K_2(r,R) = \frac{1}{\nu r R}\sinh[\nu(r-R)],$$

and

$$\Sigma_0(R) = \frac{1}{\nu^2}[\cosh[\nu(1 - R)] - 1],$$

$$\Sigma_1(R) = \frac{1}{\nu^2}[\nu R[I_0(\nu)K_1(\nu R) - I_1(\nu R)K_0(\nu)] - 1], \qquad (6.3.3)$$

$$\Sigma_2(R) = \frac{1}{\nu^3}[\nu R \cosh[\nu(1 - R)] - \nu + \sinh[\nu(1 - R)]],$$

where the functions $I_0(x)$, $K_0(x)$ and $I_1(x)$, $K_1(x)$ denote the two linearly independent modified Bessel functions of orders 0 and 1 respectively.

Dewynne and Hill, (1985) showed that the temperature $T(r, t)$ satisfies the integro-differential equation

$$T(r, t) = \frac{\partial}{\partial t} \int_{R(t)}^{r} \xi^\lambda K_\lambda(r, \xi)[\alpha + T(\xi, t)]d\xi, \qquad (6.3.4)$$

while the time $t$, as a function of the boundary position $R$, satisfies the integral equation

$$t = \int_{R}^{1} K_\lambda(1, \xi)[\alpha + T(\xi, t)]d\xi, \qquad (6.3.5)$$

where the functions $K_\lambda$ are as given by equation (6.3.2) for $\lambda$ taking on values 0, 1, and 2. From these equations, and the physically obvious inequality

$$0 \le T(r, t) \le 1, \qquad (6.3.6)$$

it follows instantly that the motion of the boundary satisfies the bounds

$$\alpha \Sigma_\lambda(R) \le t \le (\alpha + 1)\Sigma_\lambda(R). \qquad (6.3.7)$$

Here we observe that the lower bound is simply the pseudo-steady state approximation. Furthermore, substituting the pseudo-steady state approximation (6.3.1)$_1$ into (6.3.5) Krishnamurthy and Shah (1979), obtained, at least for the spherical case, an iterated first correction to the pseudo-steady state approximation. However, such iterations become extremely complicated with very little or no improvements.

Introducing the notation $t_{cpss} = t_{pss}(0)$, i.e. the pseudo-steady state estimate for the time to complete melting, we have from $(6.3.1)_2$ and $(6.3.3)$ that

$$t_{cpss} = \frac{\alpha}{\nu^2}[\cosh \nu - 1] \qquad \text{(plane)},$$

$$t_{cpss} = \frac{\alpha}{\nu^2}[I_0(\nu) - 1] \qquad \text{(cylinder)}, \qquad (6.3.8)$$

$$t_{cpss} = \frac{\alpha}{\nu^3}[\sinh \nu - \nu] \qquad \text{(sphere)}.$$

As for all pseudo-steady state approximations, the estimates (6.3.8), as indicated by bounds (6.3.7), can be expected to yield reasonable results for large $\alpha$. Improvements on bounds (6.3.7) can be found in Dewynne and Hill (1985), however, for brevity, we only reference them here.

## 6.4 Method of solution

Generalizing the procedure of previous chapters, the method of solution involves the introduction of a boundary fixing transformation of a new form, namely

$$x = \frac{f(r,R)}{f(1,R)}, \qquad y = g(R), \qquad \phi(x,y) = T(r,t), \qquad (6.4.1)$$

where the function $f(r,R)$ is such that $f(R,R) = 0$. Thus the region $[R(t), 1]$ is transformed to $[0,1]$, and the original moving boundary problem is transformed into a fixed boundary problem. Using a slightly different approach from Chapters 4 and 5 to choose the transformation function $f$, we define $f$ to be

$$f(r,R) = K_\lambda(r,R), \qquad (6.4.2)$$

where the function $K_\lambda$ is as given by (6.3.2). The transformed equations are then solved by assuming a formal series solution of the form

$$\phi(x,y) = \sum_{n=0}^{\infty} A_n(x)y^n, \qquad (6.4.3)$$

where the $A_n(x)$ are functions of $x$ only. Unlike in the previous chapters where the variable $y$ was chosen to be given by $y = f(R)$, here we choose $g(R)$ such that $y$ is given by

$$y = \nu(1 - R), \tag{6.4.4}$$

the reason for which will become apparent later.

In the following three sections we will derive explicit expressions for $A_0(x)$ and $A_1(x)$ for the plane, cylinder, and sphere case respectively.

## 6.5 Planar melting

From (6.4.1), (6.4.2) and (6.4.4) with $\lambda = 0$, we have that the new independent variables $x$ and $y$ are given by

$$x = \frac{\sinh[\nu(r - R)]}{\sinh[\nu(1 - R)]}, \qquad y = \nu(1 - R), \tag{6.5.1}$$

so that in terms of $(6.4.1)_3$ and (6.5.1) the system given by (6.2.1)-(6.2.3) with $\lambda = 0$ becomes

$$[1 + b^2 x^2]\frac{\partial^2 \phi}{\partial x^2} + b^2 x \frac{\partial \phi}{\partial x} - b^2 \phi = \frac{-1}{\alpha}\frac{\partial \phi}{\partial x}(0, y)\left\{\left[ax - (1 + b^2 x^2)^{\frac{1}{2}}\right]\frac{\partial \phi}{\partial x} - b\frac{\partial \phi}{\partial y}\right\}, \tag{6.5.2}$$

subject to the boundary conditions

$$\phi(1, y) = 1, \qquad \phi(0, y) = 0, \tag{6.5.3}$$

and the energy balance condition on the moving boundary becomes

$$\frac{\partial \phi}{\partial x}(0, y) = \frac{\alpha b}{\nu^2}\frac{dy}{dt}, \qquad y(0) = 0. \tag{6.5.4}$$

For convenience, in equations (6.5.2) and (6.5.4), we have introduced new variables $a$ and $b$ which are given by

$$a = \cosh(y), \qquad b = \sinh(y). \tag{6.5.5}$$

Substituting (6.4.3) into (6.5.2)-(6.5.4), equating coefficients of like powers of $y$, yields the following system of ordinary linear differential equations

$$A''_0 + \gamma(x - 1)A'_0 = 0,$$

$$A''_n + \gamma[(x - 1)A'_n - nA_n] = F_n(x),$$

(6.5.6)

where the functions $F_n(x)$ can easily be calculated. For example, $F_1(x)$ and $F_2(x)$ are given by

$$F_1(x) = \frac{-1}{\alpha}[A'_1(0)(x - 1)A'_0],$$

$$F_2(x) = \frac{-1}{\alpha}[A'_1(0)[(x - 1)A'_1 - A_1] + A'_2(0)[(x - 1)A'_0]]$$

$$- \left[x^2 A''_0 + xA'_0 - A_0\right].$$

(6.5.7)

The boundary conditions (6.5.3) become

$$A_0(1) = 1, \qquad A_0(0) = 0,$$

$$A_n(1) = 0, \qquad A_n(0) = 0, \qquad n = 1, 2, \ldots,$$

(6.5.8)

while the energy balance condition (6.5.4) becomes

$$\sum_{n=0}^{\infty} A'_n(0)y^n = \frac{\alpha}{v^2}\sinh(y)\frac{dy}{dt}, \qquad y(0) = 0.$$

(6.5.9)

In equation (6.5.6) we have used the notation

$$\gamma = \frac{1}{\alpha}A'_0(0).$$

(6.5.10)

From equations (6.5.9) we note that only the constants $A'_n(0)$ are required to fully determine the motion of the boundary.

Solving (6.5.6)$_1$ subject to (6.5.8)$_1$ yields

$$A_0(x) = \alpha\gamma \int_0^x e^{-\frac{\gamma}{2}[(1-\xi)^2 - 1]}d\xi,$$

(6.5.11)

where $\gamma$ is the positive root of the transcendental equation

$$\alpha\gamma \int_0^1 e^{-\frac{\gamma}{2}[(1-\xi)^2 - 1]}d\xi = 1.$$

(6.5.12)

Taking the limit as $\nu$ tends to zero in equation $(6.5.1)_1$, equations $(6.5.11)$ and $(6.5.12)$ can easily be shown to reduce to the classical Neumann solution.

Solving $(6.5.6)_2$ with $n = 1$ and $F_1(x)$ as given by $(6.5.7)_1$ and subject to boundary conditions $(6.5.8)_2$ yields

$$A_1(x) = 0, \tag{6.5.13}$$

from which it follows that

$$A'_1(0) = 0. \tag{6.5.14}$$

Results $(6.5.13)$ and $(6.5.14)$ are easily verified by back substitution.

Solving $(6.5.6)_2$ with $n = 2$ and $F_2(x)$ as given by $(6.5.7)_2$ and subject to boundary conditions $(6.5.8)_2$ yields, after some effort (see Appendix)

$$A'_2(0) = \frac{\alpha}{6} \left[ \frac{12(1 - \alpha\gamma) - 4\gamma + \gamma^2(7 + \gamma)}{4(1 + \alpha\gamma) + \gamma(7 + \gamma)} \right]. \tag{6.5.15}$$

By inspection of equation $(6.5.6)_2$, it is a simple matter to see that $A_3(x)$, like $A_1(x)$, must be identically zero. Moreover, all the odd terms, that is $A_{2n+1}(x)$, are identically zero.

Substituting results $(6.5.10)$, $(6.5.14)$ and $(6.5.15)$ into equation $(6.5.9)$ and integrating yields the following boundary motion estimate

$$t \approx \frac{1}{\gamma\nu^2} \int_0^y \frac{\sinh(\xi)}{1 + \epsilon\xi^2} d\xi, \tag{6.5.16}$$

where $\epsilon$ is given by

$$\epsilon = \frac{A'_2(0)}{A_0(0)}. \tag{6.5.17}$$

Using the asymptotic expansion for $\alpha$, namely

$$\alpha\gamma \sim 1 - \frac{\gamma}{3} + \frac{2}{45}\gamma^2, \tag{6.5.18}$$

we have from (6.5.15) and (6.5.17) that

$$\epsilon \sim \frac{97}{720}\gamma, \qquad (6.5.19)$$

which for large $\alpha$ is very small. Substituting (6.5.19) into (6.5.16), expanding the denominator, integrating and grouping terms of like powers of $\gamma$ yields

$$t \sim \frac{1}{\gamma \nu^2}\Big[(\cosh(y) - 1) - \frac{97\gamma}{720}\big((y^2 + 2)\cosh(y) - 2y\sinh(y) - 2\big)\Big], \qquad (6.5.20)$$

with $y$ as given by (6.5.1)$_2$. Furthermore, taking the limit as $\nu^2$ tends to zero (no heat lost) one can again recover the classical Neumann solution. Moreover, estimate (6.5.20) can easily be seen to satisfy the bounds given by (6.3.7), while setting $R = 0$ in (6.5.16) yields

$$t_c \approx \frac{1}{\gamma \nu^2} \int_0^\nu \frac{\sinh(\xi)}{1 + \epsilon \xi^2} d\xi, \qquad (6.5.21)$$

an accurate estimate for the time to complete melting.

## 6.6 Cylindrical melting

From (6.4.1), (6.4.2) and (6.4.4) with $\lambda = 1$, we have the new independent variables $x$ and $y$, given explicitly by

$$x = \frac{I_0(\nu r)K_0(\nu R) - I_0(\nu R)K_0(\nu r)}{I_0(\nu)K_0(\nu R) - I_0(\nu R)K_0(\nu)}, \quad y = \nu(1 - R), \qquad (6.6.1)$$

so that in terms of (6.4.1)$_3$ and (6.6.1) the system given by (6.2.1)-(6.2.3) with $\lambda = 1$ becomes

$$\left(\frac{\partial K_1}{\partial r}(r, R)\right)^2 \frac{\partial^2 \phi}{\partial x^2} + b^2 x \frac{\partial \phi}{\partial x} - b^2 \phi =$$
$$\frac{-\nu}{\alpha(\nu - y)}\frac{\partial \phi}{\partial x}(0, y)\left\{\left[\frac{\partial K_1}{\partial R}(r, R) - x\frac{\partial K_1}{\partial R}(1, R)\right]\frac{\partial \phi}{\partial x} - b\frac{\partial \phi}{\partial y}\right\}, \qquad (6.6.2)$$

subject to the boundary conditions

$$\phi(1, y) = 1, \qquad \phi(0, y) = 0, \qquad (6.6.3)$$

and the energy balance condition on the moving boundary becomes

$$\frac{\partial \phi}{\partial x}(0,y) = \frac{\alpha b}{\nu^2}\left(1 - \frac{y}{\nu}\right)\frac{dy}{dt}, \quad y(0) = 0, \tag{6.6.4}$$

with $b$ in (6.6.2) and (6.6.4) given by

$$b = \nu K_1(1,R). \tag{6.6.5}$$

In obtaining equations (6.6.2) and (6.6.5) we used the well known identity (see Gradshteyn and Ryzhik, 1980 p. 969)

$$I_1(z)K_0(z) + I_0(z)K_1(z) = \frac{1}{z}. \tag{6.6.6}$$

Substituting (6.4.3) into (6.6.2)-(6.6.4), equating coefficients of like powers of y, yields the same system of equations as given by (6.5.6). However, the $F_n(x)$ are different. For example, $F_1(x)$ is given by

$$F_1(x) = -\frac{A''_0}{\nu} - \frac{A'_1(0)}{\alpha}(x - 1)A'_0. \tag{6.6.7}$$

The boundary conditions on the $A_n$'s are as given by (6.5.8), while the energy balance condition (6.6.4) becomes

$$\sum_{n=0}^{\infty} A'_n(0)y^n = \frac{\alpha b}{\nu^2}\left(1 - \frac{y}{\nu}\right)\frac{dy}{dt}, \quad y(0) = 0. \tag{6.6.8}$$

Solving for $A_0(x)$ yields the same solution as given for the planar case by (6.5.11)-(6.5.12), while solving for $A_1(x)$ yields

$$A_1(x) = \frac{\alpha\gamma(x - 1)}{\nu(3 + \gamma)}\left[1 - e^{-\frac{\gamma}{2}[(1-x)^2 - 1]}\right]. \tag{6.6.9}$$

Differentiating (6.6.9) and setting $x = 0$ yields the desired result, namely

$$A'_1(0) = \frac{\alpha\gamma^2}{\nu(3 + \gamma)}. \tag{6.6.10}$$

Substituting results for $A'_0(0)$ and $A'_1(0)$ into (6.6.8), integrating and returning to original variables yields the following boundary motion estimate

$$t \approx \frac{1}{\gamma} \int_R^1 \frac{\xi K_1(1,\xi)d\xi}{1 + \epsilon(1 - \xi)}, \quad \text{with} \quad \epsilon = \frac{\gamma}{(3 + \gamma)}, \quad (6.6.11)$$

which is easily shown to satisfy the bounds (6.3.7), while setting $R = 0$ in (6.6.11) yields

$$t_c \approx \frac{1}{\gamma} \int_0^1 \frac{\xi K_1(1,\xi)d\xi}{1 + \epsilon(1 - \xi)}, \quad (6.6.12)$$

an estimate for the time to complete melting.

## 6.7 Spherical melting

For the spherical case the variables $x$, $y$, and $\phi$ are given by

$$x = \frac{\sinh[\nu(r - R)]}{\sinh[\nu(1 - R)]}, \quad y = \nu(1 - R), \quad \phi(x,y) = rT(r,t), \quad (6.7.1)$$

where we have chosen to simplify the governing equation (6.2.1) by the standard transformation $(6.7.1)_3$ before finding the pseudo-steady state solution required in defining $x$. Thus in terms of the new variables (6.7.1) the system (6.2.1)-(6.2.3) with $\lambda = 2$ becomes

$$\left[1 + b^2x^2\right]\frac{\partial^2\phi}{\partial x^2} + b^2x\frac{\partial\phi}{\partial x} - b^2\phi =$$
$$\frac{-\nu}{\alpha(\nu - y)}\frac{\partial\phi}{\partial x}(0,y)\left\{\left[ax - (1 + b^2x^2)^{1/2}\right]\frac{\partial\phi}{\partial x} - b\frac{\partial\phi}{\partial y}\right\}, \quad (6.7.2)$$

subject to the boundary conditions

$$\phi(1,y) = 1, \quad \phi(0,y) = 0, \quad (6.7.3)$$

and the energy balance condition on the moving boundary becomes

$$\frac{\partial\phi}{\partial x}(0,y) = \frac{\alpha b}{\nu^2}\left(1 - \frac{y}{\nu}\right)\frac{dy}{dt}, \quad y(0) = 0, \quad (6.7.4)$$

where again, for convenience we have introduced new variables $a$ and $b$ which are given by

$$a = \cosh(y), \quad b = \sinh(y). \quad (6.7.5)$$

Substituting (6.4.3) into (6.7.2)-(6.7.4), equating coefficients of like powers of $y$ yields the same system of equations as given by (6.5.6) with $F_1(x)$ identical to (6.6.7). The boundary conditions on the $A_n$'s are again as given by (6.5.8), while the energy balance condition (6.7.4) becomes

$$\sum_{n=0}^{\infty} A'_n(0)y^n = \frac{\alpha b}{\nu^2}\left(1 - \frac{y}{\nu}\right)\frac{dy}{dt}, \quad y(0) = 0, \qquad (6.7.6)$$

remembering that b is given by $(6.7.5)_2$.

Solving for $A_0(x)$ and $A_1(x)$ yields the same solutions as for the cylindrical case, so that $A'_0(0)$ and $A'_1(0)$ are given by

$$A'_0(0) = \alpha\gamma, \qquad A'_1(0) = \frac{\alpha\gamma^2}{\nu(3 + \gamma)}. \qquad (6.7.7)$$

However, we note here that on returning to the original variables the cylindrical and spherical temperature estimates, $T_1$ and $T_2$, will in fact be different because of the fact that the variables $x$, $y$, and $\phi$ are different for the two cases. Furthermore, the remaining $A_n(x)$ would be different for the two geometries.

Substituting results (6.7.7) into (6.7.6), integrating and returning to original variables yields the following boundary motion estimate

$$t \approx \frac{1}{\gamma\nu}\int_R^1 \frac{\xi\sinh[\nu(1 - \xi)]d\xi}{1 + \epsilon(1 - \xi)}, \qquad (6.7.8)$$

where $\epsilon$ is given by $(6.6.11)_2$, while setting $R = 0$ yields

$$t_c \approx \frac{1}{\gamma\nu}\int_0^1 \frac{\xi\sinh[\nu(1 - \xi)]d\xi}{1 + \epsilon(1 - \xi)}, \qquad (6.7.9)$$

the estimate for the time to complete melting.

## 6.8 Numerical results and discussion

In this final section we present a detailed numerical comparison between the theoretical bounds and the boundary fixing estimates for the boundary motions for

all the three geometries. In particular, we look at the two extreme cases, namely for large and small $\nu$. In closing, a short discussion is given pertaining to the choice of boundary fixing transformation.

Figures 6.1 and 6.2 compare the upper and lower bounds on the boundary motion, as given by equations (6.3.3) and (6.3.7), with the series approximation (6.5.16), for the plane with $\alpha = 1.0$, and $\nu = 1.0$ and 5.0 respectively. As hoped, the series approximation neatly fits between the theoretical bounds. Furthermore, for increasing $\alpha$, the two bounds are shown to tighten and converge to the series estimate. Figures 6.3 and 6.4, and 6.5 and 6.6 illustrate the same features for the cylindrical and spherical cases respectively.

In Table 6.1 the boundary fixing series estimates are tabulated together against the theoretical bounds for the times to complete melting $t_c$, for $\alpha = 1.0$ and a large range of $\nu$ values. For small values of $\nu$, namely $\nu < 1.0$ there is seen to be relatively little or no change in the estimates on the times to complete melting. This is not surprising remembering that $\nu^2$ is a measure of the amount of heat being lost. However, for large $\nu$, that is, for $\nu > 1.0$ the change in the melting times can be orders of magnitude, so changing the nature of the melting. In Table 6.2 $\nu$ is fixed while $\alpha$ is allowed to take on a large range of values. Not surprising, for large $\alpha$ the bounds and the series estimate are seen to be in very close agreement.

At this point we must note that basically no other boundary fixing transformation can lead to consistent and accurate estimates. The requirements being that, for large $\alpha$ the pseudo-steady state approximation must be recovered, and that for all $\alpha$ and $\nu$ the estimate must lie between the theoretical bounds eliminates almost all other boundary fixing transformations.

| $\alpha = 1$ | Plane | | | Cylinder | | | Sphere | | |
|---|---|---|---|---|---|---|---|---|---|
| $\nu$ | Low. | (6.5.16) | Upp. | Low. | (6.6.12) | Upp. | Low. | (6.7.9) | Upp. |
| 0.01 | 0.500 | 0.628 | 1.000 | 0.250 | 0.293 | 0.500 | 0.167 | 0.197 | 0.333 |
| 0.10 | 0.500 | 0.629 | 1.001 | 0.250 | 0.293 | 0.500 | 0.167 | 0.197 | 0.334 |
| 0.30 | 0.504 | 0.633 | 1.008 | 0.251 | 0.294 | 0.503 | 0.167 | 0.198 | 0.335 |
| 0.50 | 0.511 | 0.641 | 1.021 | 0.254 | 0.297 | 0.508 | 0.170 | 0.199 | 0.338 |
| 0.70 | 0.521 | 0.654 | 1.042 | 0.258 | 0.301 | 0.516 | 0.171 | 0.202 | 0.342 |
| 1.00 | 0.543 | 0.682 | 1.086 | 0.266 | 0.311 | 0.532 | 0.175 | 0.207 | 0.350 |
| 2.00 | 0.691 | 0.865 | 1.381 | 0.320 | 0.372 | 0.640 | 0.203 | 0.239 | 0.407 |
| 3.00 | 1.008 | 1.257 | 2.015 | 0.431 | 0.498 | 0.862 | 0.260 | 0.304 | 0.520 |
| 4.00 | 1.644 | 2.045 | 3.289 | 0.644 | 0.737 | 1.288 | 0.364 | 0.422 | 0.728 |
| 5.00 | 2.928 | 3.631 | 5.857 | 1.050 | 1.193 | 2.099 | 0.554 | 0.637 | 1.107 |

Table 6.1  Boundary fixing estimate and bounds on the time to complete melting for the three geometries with $\alpha = 1.0$ and various values of $\nu$

| $\nu = 1$ | Plane | | | Cylinder | | | Sphere | | |
|---|---|---|---|---|---|---|---|---|---|
| $\alpha$ | Low. | (6.5.16) | Upp. | Low. | (6.6.12) | Upp. | Low. | (6.7.9) | Upp. |
| 0.01 | 0.005 | 0.074 | 0.549 | 0.003 | 0.028 | 0.267 | 0.002 | 0.019 | 0.177 |
| 0.02 | 0.011 | 0.089 | 0.554 | 0.005 | 0.035 | 0.271 | 0.004 | 0.023 | 0.179 |
| 0.05 | 0.027 | 0.121 | 0.570 | 0.013 | 0.048 | 0.279 | 0.009 | 0.033 | 0.184 |
| 0.10 | 0.054 | 0.161 | 0.597 | 0.027 | 0.066 | 0.293 | 0.018 | 0.044 | 0.193 |
| 0.20 | 0.109 | 0.228 | 0.652 | 0.053 | 0.096 | 0.319 | 0.035 | 0.064 | 0.210 |
| 0.50 | 0.272 | 0.404 | 0.815 | 0.133 | 0.178 | 0.399 | 0.088 | 0.119 | 0.263 |
| 1.00 | 0.543 | 0.682 | 1.086 | 0.266 | 0.311 | 0.532 | 0.175 | 0.207 | 0.350 |
| 2.00 | 1.086 | 1.228 | 1.629 | 0.532 | 0.575 | 0.798 | 0.350 | 0.381 | 0.526 |
| 5.00 | 2.715 | 2.858 | 3.258 | 1.330 | 1.371 | 1.596 | 0.876 | 0.906 | 1.051 |
| 10.00 | 5.431 | 5.574 | 5.974 | 2.661 | 2.701 | 2.929 | 1.752 | 1.781 | 1.927 |

Table 6.2  Boundary fixing estimates and upper and lower bounds on the time to complete melting for the three geometries with $\nu = 1.0$ and various values of $\alpha$

**Figure 6.1**     Boundary motion estimate for the plane with $\alpha = 1.0$ and $\nu = 1.0$, upper and lower

bounds( —————— ), series estimate( — · — · — )



**Figure 6.2**     Boundary motion estimate for the plane with $\alpha = 1.0$ and $\nu = 5.0$, upper and lower

bounds( —————— ), series estimate( — · — · — )
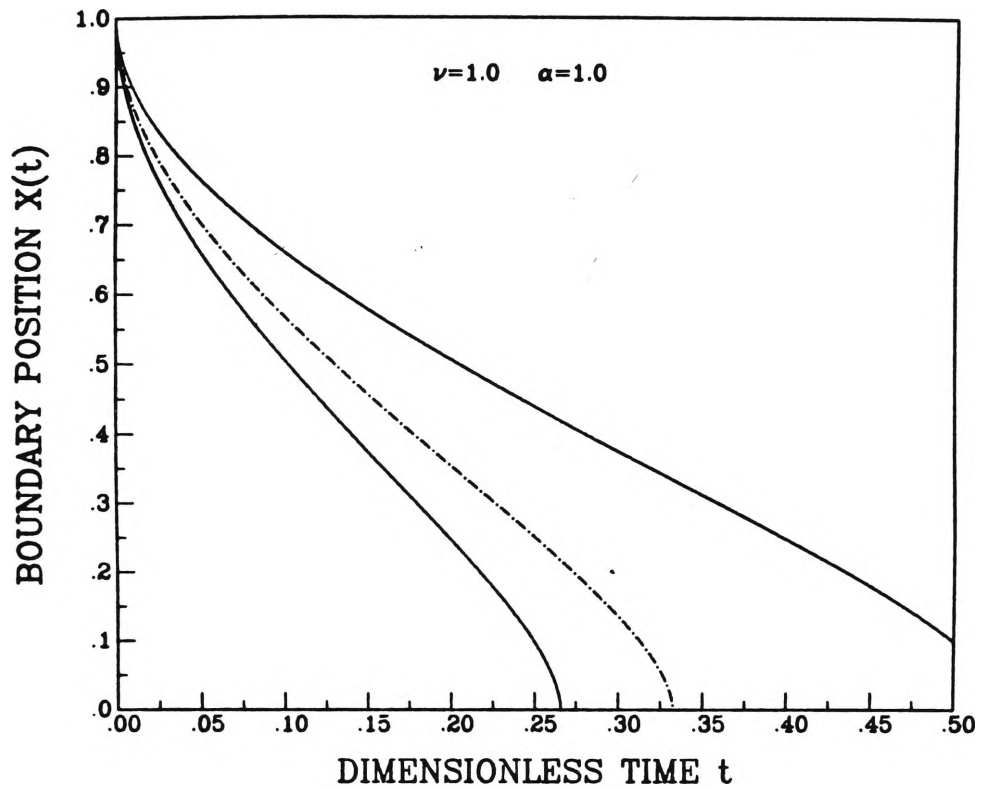
Figure 6.3     Boundary motion estimate for the cylinder with $\alpha = 1.0$ and $\nu = 1.0$, upper and lower

bounds( ———— ), series estimate( — · — · — )



Figure 6.4     Boundary motion estimate for the cylinder with $\alpha = 1.0$ and $\nu = 5.0$, upper and lower

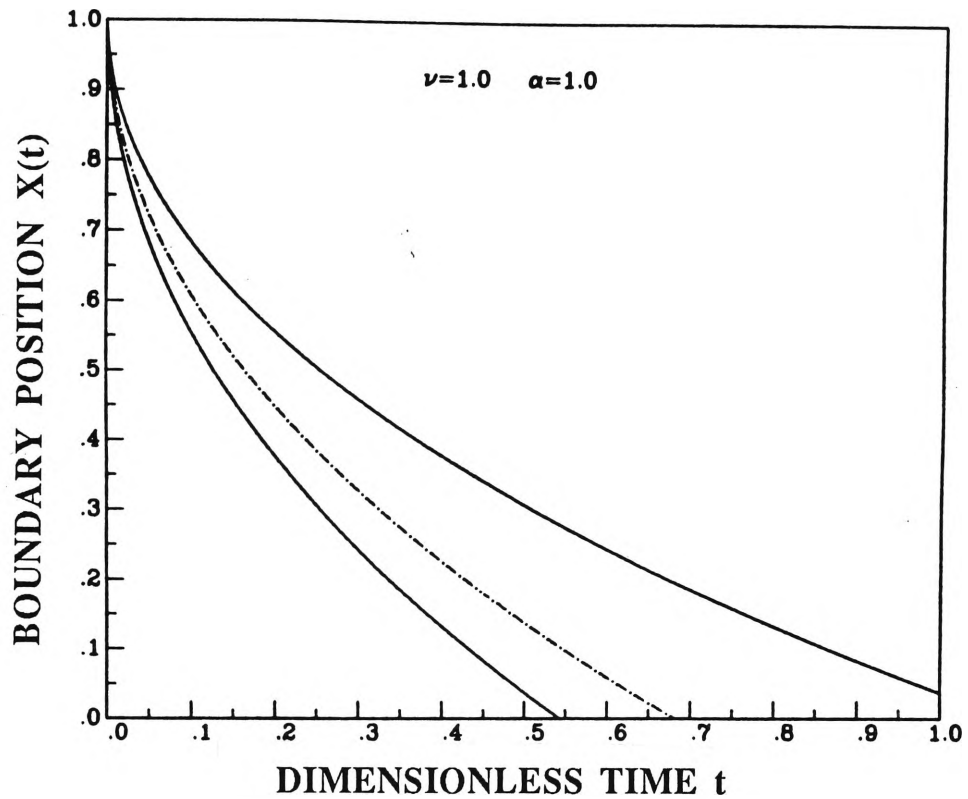bounds( ———— ), series estimate( — · — · — )

Figure 6.5    Boundary motion estimate for the sphere with $\alpha = 1.0$ and $\nu = 1.0$, upper and lower bounds( ———— ), series estimate( — · — · — )
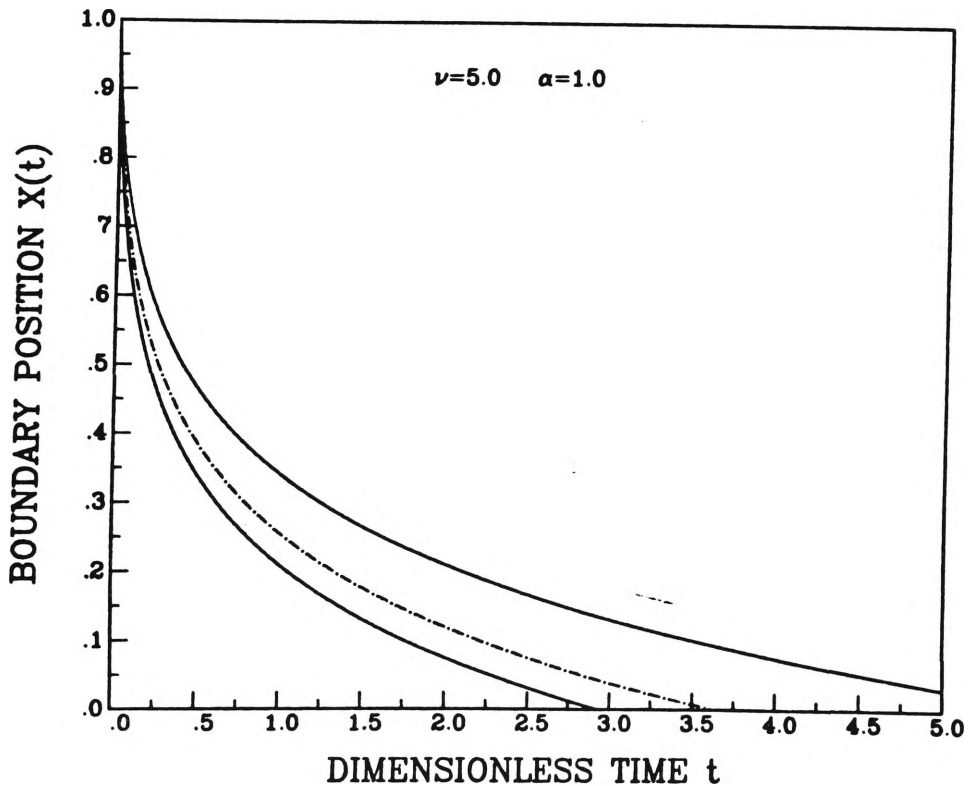


Figure 6.6    Boundary motion estimate for the sphere with $\alpha = 1.0$ and $\nu = 5.0$, upper and lower bounds( ———— ), series estimate( — · — · — )
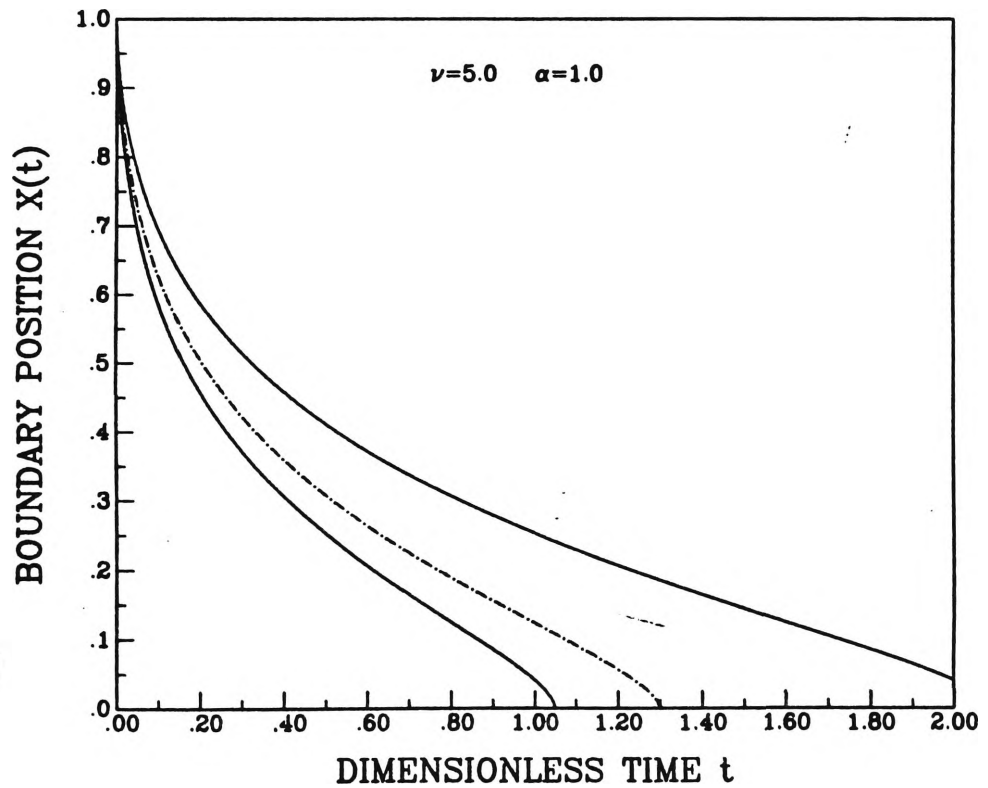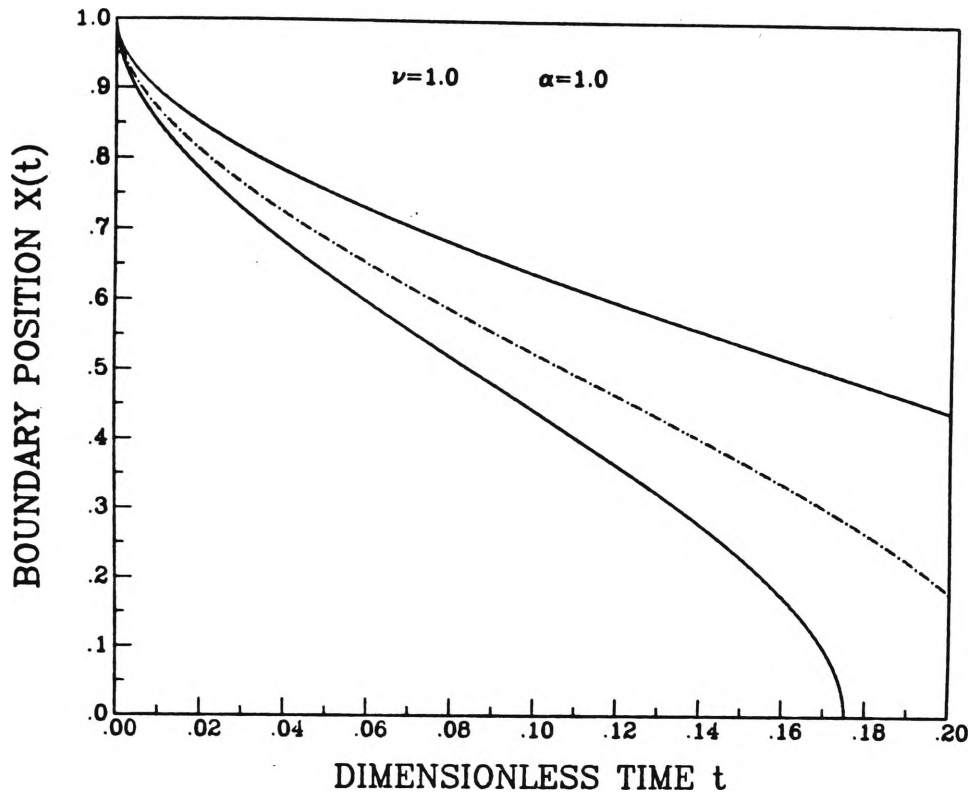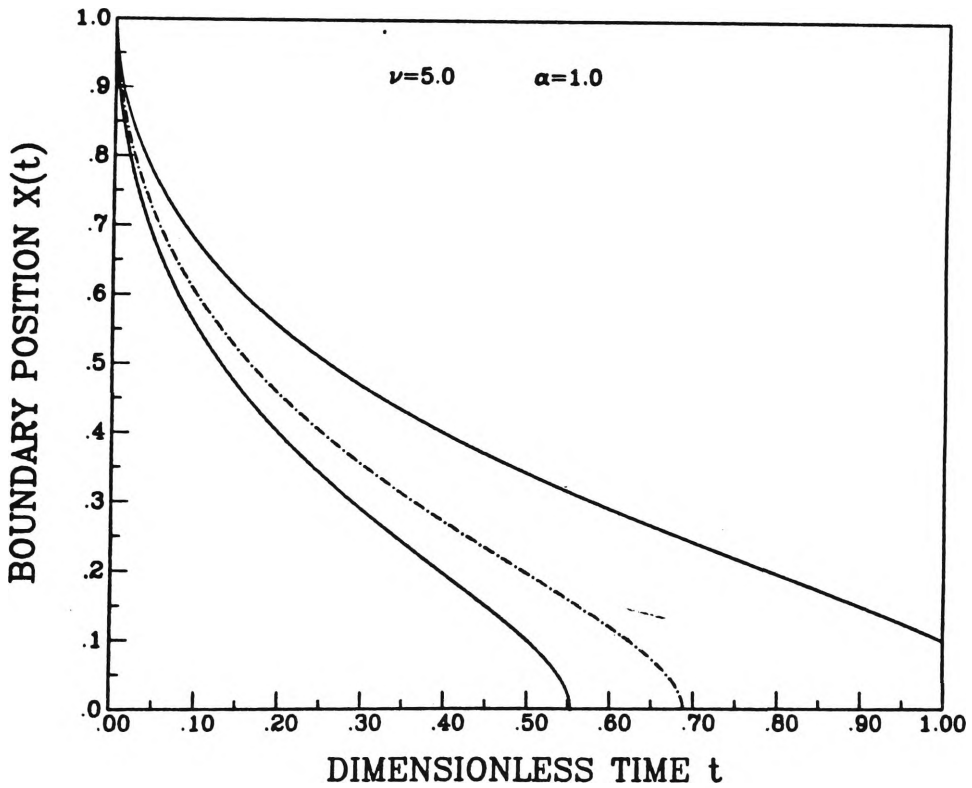
# CHAPTER SEVEN

# Diffusion Controlled Growth and Collapse of Spherical Bubbles

## 7.1 Introduction

In this chapter we consider the classical problem of the heat transfer controlled growth and collapse of an isolated spherical bubble in a fluid of infinite extent. The problem involves determining the time variation of the radius of the bubble immersed in an outer phase which is initially at a uniform temperature. In Section 7.2 we describe the physical problem in detail and formulate equations in dimensionless form. In Section 7.3 we describe the one known exact solution for the bubble of zero initial radius. In Section 7.4 we apply the formal boundary fixing series technique to the problem of the collapsing bubble, and derive the first two terms which are subsequently used to generate temperature and boundary motion estimates. In Section 7.5 we apply the same technique, however with a different boundary fixing transformation, to the case of the growing bubble. The leading term and the two successive approximations to the second term of the series are explicitly derived. Again, as in the collapsing bubble case, the two terms are used to generate temperature and boundary motion estimates. In Section 7.6, the effects of varying physical parameters have on both the temperature profiles and boundary motions are investigated. Furthermore, numerical comparisons between existing perturbation estimates, the exact similarity solution, and our approximations are presented.

## 7.2 Governing equations

In this section we describe the equations governing heat controlled growth and collapse of an isolated, stationary bubble immersed in an infinite fluid and initially of radius $a$. The analysis is limited to the case where both the initial temperature distribution, $T_\infty$, and the interfacial temperature, $T_R$, are constant. To further simplify the analysis, the thermal properties of the system are assumed temperature independent and gravitational, viscous, inertial, or surface effects are all neglected. Based on these assumptions the governing equation can be written in non-dimensional form as

$$\frac{\partial T}{\partial t} + \left(1 - \frac{\beta}{\alpha}\right)\left(\frac{R}{r}\right)^2 \frac{dR}{dt}\frac{\partial T}{\partial r} = \frac{\partial^2 T}{\partial r^2} + \frac{2}{r}\frac{\partial T}{\partial r}, \quad R(t) < r < \infty, \quad (7.2.1)$$

subject to boundary and initial conditions

$$T(R(t),t) = 1, \quad T(\infty,t) = 0, \quad t > 0, \quad (7.2.2)$$

$$T(r,0) = 0, \quad r > 1, \quad (7.2.3)$$

and the energy balance condition on the moving interface

$$\frac{dR}{dt} = \alpha\frac{\partial T}{\partial r}(R(t),t), \quad R(0) = 1, \quad (7.2.4)$$

where $T(r,t)$ is the dimensionless temperature, $r$ and $t$ are position and time variables and $R(t)$ is the position of the moving boundary separating the two phases. These variables and the parameters $\alpha$ and $\beta$ are given in terms of the starred physical quantities by

$$T = \frac{T^* - T_\infty}{T_R - T_\infty}, \quad r = \frac{r^*}{a}, \quad t = \frac{kt^*}{\rho_0 c_v a},$$

$$(7.2.5)$$

$$R(t) = \frac{R^*(t^*)}{a}, \quad \alpha = \frac{\rho_0}{\rho_i}\frac{(T_R - T_\infty)c_v}{\Delta H}, \quad \beta = \frac{(T_R - T_\infty)c_v}{\Delta H},$$

where $\rho_i$ and $\rho_0$ are the inner and outer phase densities respectively, $c_v$ is the heat capacity at constant volume for the outer phase, $k$ is the thermal diffusivity of the

outer phase, and $\Delta H$ is the specific enthalpy of the phase change. The parameter $\alpha$, being the ratio of the velocity of the boundary to the heat flux at the boundary, controls the motion of the boundary $R(t)$ and the larger the value of $|\alpha|$ the faster the boundary moves. Furthermore, from equations (7.2.4) and (7.2.5) it is clear that for bubble growth both $\alpha$ and $\beta$ are negative, while for bubble collapse, they are both positive. In the special case when $\alpha = \beta$, the densities in the two phases are equal, the convective term in equation (7.2.1) disappears and the system is driven solely by unsteady diffusion. However, for many practical cases of interest, such as vapour bubble formation in superheated liquids, one has $|\alpha| >> |\beta|$ and as expected, convection has a significant influence on both the temperature distribution and on the motion of the boundary.

## 7.3 Exact solution

For a bubble of zero initial radius (that is $R(0) = 0$) the above equations admit the exact solution

$$T(r,t) = \frac{-\Gamma}{\alpha} \int_0^{R(t)/r} e^{\Gamma\left[(1-\xi^{-2})+2\delta(1-\xi)\right]/2} d\xi , \tag{7.3.1}$$

where $\delta$ is defined by

$$\delta = 1 - \beta/\alpha , \tag{7.3.2}$$

and $\Gamma$ is the positive root of the transcendental equation

$$\frac{-\Gamma}{\alpha} \int_0^1 e^{\Gamma\left[(1-\xi^{-2})+2\delta(1-\xi)\right]/2} d\xi = 1 . \tag{7.3.3}$$

Substituting (7.3.1) with (7.3.3) into the energy balance condition on the moving interface (7.2.4) yields

$$t = \frac{1}{2\Gamma} R^2 , \tag{7.3.4}$$

the typical quadratic relationship between the position of the moving interface $R(t)$ and time $t$.

In the following two sections we obtain approximate solutions for collapsing and expanding spherical bubbles which are initially of finite radius. It will be shown that equation (7.3.1) essentially arises as the leading term in our approximation for diffusion controlled growth. Furthermore, it is intuitively obvious that equation (7.3.4) constitutes an upper bound for the time $t$ for an initially non zero radius bubble.

## 7.4 Diffusion controlled collapse

For a collapsing spherical bubble we fix the boundary by means of the transformations

$$x = \frac{1 - r}{1 - R}, \quad y = 1 - R, \quad T(r,t) = \phi(x,y), \tag{7.4.1}$$

so that $-\infty \le x \le 1$, $0 \le y \le 1$ and equations (7.2.1)-(7.2.4) becomes

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{2y}{(1 - xy)} \frac{\partial \phi}{\partial x} = \alpha \frac{\partial \phi}{\partial x}(1,y) \left\{ \delta \left( \frac{1 - y}{1 - xy} \right)^2 \frac{\partial \phi}{\partial x} - \left[ x \frac{\partial \phi}{\partial x} - y \frac{\partial \phi}{\partial y} \right] \right\}, \tag{7.4.2}$$

$$\phi(1,y) = 1, \quad \phi(-\infty,y) = 0, \tag{7.4.3}$$

$$y \frac{dy}{dt} = \alpha \frac{\partial \phi}{\partial x}(1,y), \quad y(0) = 0. \tag{7.4.4}$$

On assuming a formal series solution of the form

$$\phi(x,y) = \sum_{n=0}^{\infty} a_n(x) y^n, \tag{7.4.5}$$

and substituting into (7.4.2) we obtain the following system of ordinary differential equations

$$a''_0 + \gamma [(x - \delta) a'_0] = 0, \tag{7.4.7}$$

$$a''_n + \gamma [(x - \delta) a'_n - n a_n] = f_n(x), \quad n = 1, 2, 3 \ldots \tag{7.4.7}$$

where primes denote differentiation with respect to $x$ and the arguments of the functions $a_n$ are understood to be $x$ unless otherwise indicated. The functions $f_n(x)$

are easily determined, for example $f_1(x)$ is given by

$$f_1(x) = [2[1 + \gamma\delta(x - 1)] + \alpha a'_1(1)(\delta - x)]a'_0(x), \qquad (7.4.8)$$

where $\gamma$ is defined by

$$\gamma = \alpha a'_0(1). \qquad (7.4.9)$$

Further the boundary conditions become

$$a_0(-\infty) = 0, \quad a_0(1) = 1, \qquad (7.4.10)$$

$$a_n(-\infty) = 0, \quad a_n(1) = 0, \quad n = 1,2,3\ldots \qquad (7.4.11)$$

while the energy balance condition (7.4.4) becomes

$$y\frac{dy}{dt} = \alpha \sum_{n=0}^{\infty} a'_n(1)y^n, \quad y(0) = 0. \qquad (7.4.12)$$

It is apparent from this equation that only the $a'_n(1)$ are required to determine the motion of the boundary.

On solving (7.4.6) subject to (7.4.10) we obtain

$$a_0(x) = \frac{\gamma}{\alpha} \int_{-\infty}^{x} e^{\gamma\left[(1-\delta)^2 - (\xi-\delta)^2\right]/2} d\xi, \qquad (7.4.13)$$

where $\gamma$ is the positive root of the transcendental equation

$$\frac{\gamma}{\alpha} \int_{-\infty}^{1} e^{\gamma\left[(1-\delta)^2 - (\xi-\delta)^2\right]/2} d\xi = 1. \qquad (7.4.14)$$

Further on solving equation (7.4.7) with boundary conditions (7.4.11) for $n = 1$ yields

$$a_1(x) = \frac{\gamma}{\alpha}\{(x - \delta)c_1 \int_{-\infty}^{x} e^{\gamma\left[(1-\delta)^2 - (\xi-\delta)^2\right]/2} d\xi$$

$$+ [(x - \delta)c_2 + c_3]e^{\gamma\left[(1-\delta)^2 - (x-\delta)^2\right]/2}\}, \qquad (7.4.15)$$

where the constants $c_1$, $c_2$ and $c_3$ are given by

$$c_1 = 1 - \gamma\delta(1 - \delta) + \frac{\gamma(1 - \delta)}{[1 + \alpha(1 - \delta)]}\left[\alpha\delta(1 - \delta) + \frac{2\delta}{3} - \frac{\alpha}{\gamma} - \frac{\alpha}{3\gamma}a'_1(1)\right], \quad (7.4.16)$$

$$c_2 = \frac{1}{3}\left[\frac{\alpha}{\gamma}a'_1(1) - 2\delta\right], \quad (7.4.17)$$

$$c_3 = \frac{(1 - \delta)}{[1 + \alpha(1 - \delta)]}\left[\alpha\delta(1 - \delta) + \frac{2\delta}{3} - \frac{\alpha}{\gamma} - \frac{\alpha}{3\gamma}a'_1(1)\right], \quad (7.4.18)$$

while the constant $a'_1(1)$ is found to be given by

$$a'_1(1) = \frac{\beta\gamma}{\alpha^2} + \frac{3}{\beta} - \frac{\gamma}{\alpha} - \frac{6}{\beta^2}\left[\frac{\beta\gamma}{\alpha^2} + \frac{2}{\beta} + \frac{1}{(\beta + 1)}\right]^{-1}. \quad (7.4.19)$$

Including only the first two terms of (7.4.12) and integrating we obtain the following estimate for the boundary motion

$$t \approx \frac{1}{\gamma}\left[\frac{\gamma(1 - R)}{\alpha a'_1(1)} - \left(\frac{\gamma}{\alpha a'_1(1)}\right)^2 log|1 + \alpha a'_1(1)(1 - R)/\gamma|\right], \quad (7.4.20)$$

so that we obtain the following estimate for the collapse time $t_c$ ($R(t_c) = 0$),

$$t_c \approx \frac{1}{\gamma}\left[\frac{\gamma}{\alpha a'_1(1)} - \left(\frac{\gamma}{\alpha a'_1(1)}\right)^2 log|1 + \alpha a'_1(1)/\gamma|\right]. \quad (7.4.21)$$

Expanding the boundary motion estimate (7.4.20) for small times (i.e. $R(t) \approx 1.0$), the remaining leading term is

$$t \sim \frac{1}{2\gamma}(1 - R)^2 \quad \text{or} \quad R \sim 1 - \sqrt{2\gamma t}, \quad (7.4.22)$$

the expected quadratic relationship. For very fast collapsing bubbles, (7.4.22) can be expected to yield reliable estimates even for total collapse times $t_c$.

## 7.5 Diffusion controlled growth

For an expanding spherical bubble we fix the boundary by means of the transformations

$$X = \frac{R - 1}{r - 1}, \quad Y = \frac{1}{R - 1}, \quad T(r, t) = \Phi(X, Y), \quad (7.5.1)$$

so that $0 \leq X \leq 1$, $0 \leq Y \leq \infty$ and equations (7.2.1) – (7.2.4) become

$$X^4 \frac{\partial^2 \Phi}{\partial X^2} + \frac{2X^4 Y}{(1 + XY)} \frac{\partial \Phi}{\partial X} = \alpha \frac{\partial \Phi}{\partial X}(1, Y)\left\{\delta X^4 \left(\frac{1 + Y}{1 + XY}\right)^2 \frac{\partial \Phi}{\partial X} - \left[X \frac{\partial \Phi}{\partial X} - Y \frac{\partial \Phi}{\partial Y}\right]\right\},$$

$$(7.5.2)$$

$$\Phi(1, Y) = 1, \quad \Phi(0, Y) = 0, \quad 0 \leq Y \leq \infty, \tag{7.5.3}$$

$$\frac{dY}{dt} = \alpha Y^3 \frac{\partial \Phi}{\partial X}(1, Y), \quad Y(0) = \infty, \tag{7.5.4}$$

and $\delta$ is defined by (7.2.7). Again on assuming a formal series solution of the form

$$\Phi(X, Y) = \sum_{n=0}^{\infty} A_n(X) Y^n, \tag{7.5.5}$$

substituting into (7.5.2) and equating coefficients of like powers of $Y$ we obtain a system of ordinary linear differential equations given by

$$X^4 A''_0 - \Gamma\left[(X - \delta X^4)A'_0\right] = 0, \tag{7.5.6}$$

$$X^4 A''_n - \Gamma\left[(X - \delta X^4)A'_n - nA_n\right] = F_n(X), \quad n = 1, 2, 3, \ldots \tag{7.5.7}$$

where primes denote differentiation with respect to $X$ while the arguments of $A_n$ are understood to be $X$ unless otherwise indicated. The functions $F_n(X)$ can be obtained in a straightforward manner. For example $F_1(X)$ is given by

$$F_1(X) = \frac{\Gamma}{\alpha}\left[2\Gamma\delta X^4(1 - X) + 2X^4 + \alpha A'_1(1)(X - \delta X^4)\right]e^{\Gamma[(1 - X^{-2}) + 2\delta(1 - X)]/2}.$$

$$(7.5.8)$$

The constant $\Gamma$ is defined by

$$\Gamma = -\alpha A'_0(1), \tag{7.5.9}$$

while the boundary conditions on the $A_n$ are

$$A_0(0) = 0, \quad A_0(1) = 1, \tag{7.5.10}$$

$$A_n(0) = 0, \quad A_n(1) = 0, \quad n = 1, 2, 3, \ldots, \tag{7.5.11}$$

and the energy balance condition (7.5.4) becomes

$$\frac{dY}{dt} = \alpha Y^3 \sum_{n=0}^{\infty} A'_n(1) Y^n, \quad Y(0) = \infty. \tag{7.5.12}$$

On solving equation (7.5.6) subject to boundary conditions (7.5.10) we obtain

$$A_0(X) = \frac{-\Gamma}{\alpha} \int_0^X e^{\Gamma\left[(1-\xi^{-2})+2\delta(1-\xi)\right]/2} d\xi ,$$  (7.5.13)

where $\Gamma$ is a positive root of the transcendental equation (7.5.5). Unfortunately on attempting to solve (7.5.7) for $n = 1$, the homogeneous equation, namely

$$X^4 A'' - \Gamma[(X - \delta X^4)A' - A] = 0 ,$$  (7.5.14)

does not readily admit a simple solution for $\delta$ non-zero. Moreover we have been unable to reduce this equation to one of standard form by means of transformation of either the independent or dependent variables. Since $A_1(X)$ is analytic at $X = 1$ and $0 \leq X \leq 1$ we obtain an approximate solution of (7.5.7) and (7.5.11) with $n = 1$ by assuming a Taylor series

$$A_1(X) = \sum_{n=0}^{\infty} \frac{A_1^{(n)}(1)}{n!}(X - 1)^n ,$$  (7.5.15)

where the values of the derivatives $A_1^{(n)}(1)$ for $n \geq 2$ in terms of $A'_1(1)$ are deduced by repeated differentiation of (7.5.7) with $n = 1$. On using $A_1(1) = 0$ we obtain the following results for $n = 2$ and $n = 3$,

$$A''_1(1) = 2\Gamma[1 + \alpha(1 - \delta)A'_1(1)]/\alpha ,$$  (7.5.16)

$$A'''_1(1) = \Gamma\left\{2\Gamma(2 - 3\delta) + \alpha[3\Gamma(1 - \delta)^2 - 7]A'_1(1)\right\}/\alpha .$$  (7.5.17)

Thus from $A_1(0) = 0$ and including two and three non-zero terms respectively of (7.5.15) we may deduce the following estimates of $A'_1(1)$, thus

$$A'_1(1) \approx \frac{\Gamma}{\alpha}\left(1 - \frac{\beta\Gamma}{\alpha}\right)^{-1}, \text{ or}$$

$$A'_1(1) \approx \frac{\Gamma}{\alpha}\left[1 + \Gamma\left(\frac{1}{3} - \frac{\beta}{\alpha}\right)\right]\left[\left(1 - \frac{\beta\Gamma}{\alpha}\right) + \frac{\Gamma}{6}\left(\frac{3\beta^2\Gamma}{\alpha^2} - 7\right)\right]^{-1}$$  (7.5.18)

On including only the first two terms of (7.5.4) and integrating we obtain the following estimate for the boundary motion

$$t \approx \frac{1}{\Gamma}\left\{\frac{(R-1)^2}{2}\right\}, \qquad (7.5.19)$$

$$t \approx \frac{1}{\Gamma}\left\{\frac{(R-1)^2}{2} + \frac{\alpha A'_1(1)}{\Gamma}(R-1) + \left(\frac{\alpha A'_1(1)}{\Gamma}\right)^2 \log|R - 1 - \alpha A'_1(1)/\Gamma|\right\}, \qquad (7.5.20)$$

where the constant $A'_1(1)$ is estimated from either $(7.5.18)_1$ or $(7.5.18)_2$. From (7.5.20) the expected quadratic behaviour is apparent for large times.

## 7.6 Numerical results and discussion

In this final section we address a number of issues. Firstly, we investigate the effects of varying the parameters $\alpha$ and $\beta$ has on both the temperature profiles and boundary motions. In particular, how the temperature profiles change in shape and the effect on boundary velocities. Secondly, we present a numerical comparison between existing perturbation estimates, the exact similarity solution, and our two series approximations. Finally, we finish with a short discussion on the perturbation technique of Vrentas and Shih (1980b) and comment on possible further work that still could be done with the series method.

Figures 7.1 and 7.2 illustrate the effect of varying the parameter $\alpha$ has on both the temperature profiles and boundary motions for the growing bubble of zero initial radius. It is clear from Figure 7.1 that the velocity of the boundary increases as $|\alpha|$ decreases while less heat diffuses out into the outer phase. Figures 7.3 and 7.4 show the temperature profiles for the collapsing bubble of initial unit radius. The surprising feature being the invariant temperature point at $r = 1$ as seen in both Figures. Figure 7.5 illustrates the $\alpha$ dependence of the invariant temperature point for selected values of $\beta$, while Figure 7.6 is the contour graph of the $\alpha\beta$-plane with the solid lines being the indicated fixed isotherms. Figures 7.7 and 7.8 show the

boundary motion estimates for selected values of $\alpha$ and $\beta$. As expected, the shifted exact similarity solution forms an upper bound on the actual boundary motion estimate.

Tables 7.1 and 7.2 contain tabulated roots of the transcendental equations (7.3.3) and (7.4.14) respectively for a representative selection of parameters $\alpha$ and $\beta$. In both cases, the roots $\Gamma$ and $\gamma$ increase as $|\alpha|$ increases, reflecting the fact that the velocity of the boundary position increases as $|\alpha|$ increases for both collapsing and growing bubbles.

In Tables 7.3, 7.4 and 7.5 are tabulated estimates for the time $t$ as a function of the boundary position $R(t)$. In all the cases $\beta$ was chosen to be zero to enable comparisons with existing perturbation solutions (Vrentas and Shih, 1980b). With $\alpha = -1.0$ for all four estimates, namely; perturbations, (7.5.19), (7.5.20) and (7.3.4) are seen to yield reasonable estimates. However, the perturbation estimates do appear to be somewhat lower than one might expect. For such large times ($t > 100$) it would be reasonable to expect the true solution to lie between the shifted similarity solution (7.5.19) and the actual similarity solution (7.3.4). For $\alpha = -10.0$, and $\alpha = -100$ (intermediate and short times) the perturbation estimates are seen to be considerably inconsistent with the other estimates.

In all the three cases (i.e. $\alpha = -1.0$, $-10.0$, and $-100.0$)) the two-term series approximation (7.5.20) is seen to consistently yield estimates slightly higher than the established upper bound given by the similarity solution (7.3.4) (having started at zero and not one). The error is probably due to the second approximation introduced by estimates (7.5.18) for $A'_1(1)$. Furthermore, from Tables 7.3, 7.4, and 7.5 it would appear that the one term series approximation (7.5.19) constitutes a lower bound on time $t$.

In conclusion, we note that the perturbation scheme of Vrentas and Shih has a number of difficulties associated with it. Firstly, the singular behavior in both space and time, requires a complex space-time inner-outer matching scheme in order to obtain a uniformly valid composite approximation, for both the temperature and boundary motion. Secondly, their solutions appear to be valid for strictly small values of $\beta$ (less than 0.01). Thirdly, their solutions are in a very awkward parametric form, where the free parameter, in general, can not be eliminated between the equations. Finally, the parametric equations for $t$ and $R(t)$ are given in terms of complicated double integrals with singular integrands making numerical evaluations extremely expensive. In comparison to the perturbation technique of Vrentas and Shih (1980b), our series solutions appear much simpler and applicable to a larger range of parameter values. For completeness, it would be very nice to be able to solve equation (7.5.14), thereby allowing us to find $A_1{}'(1)$ exactly.
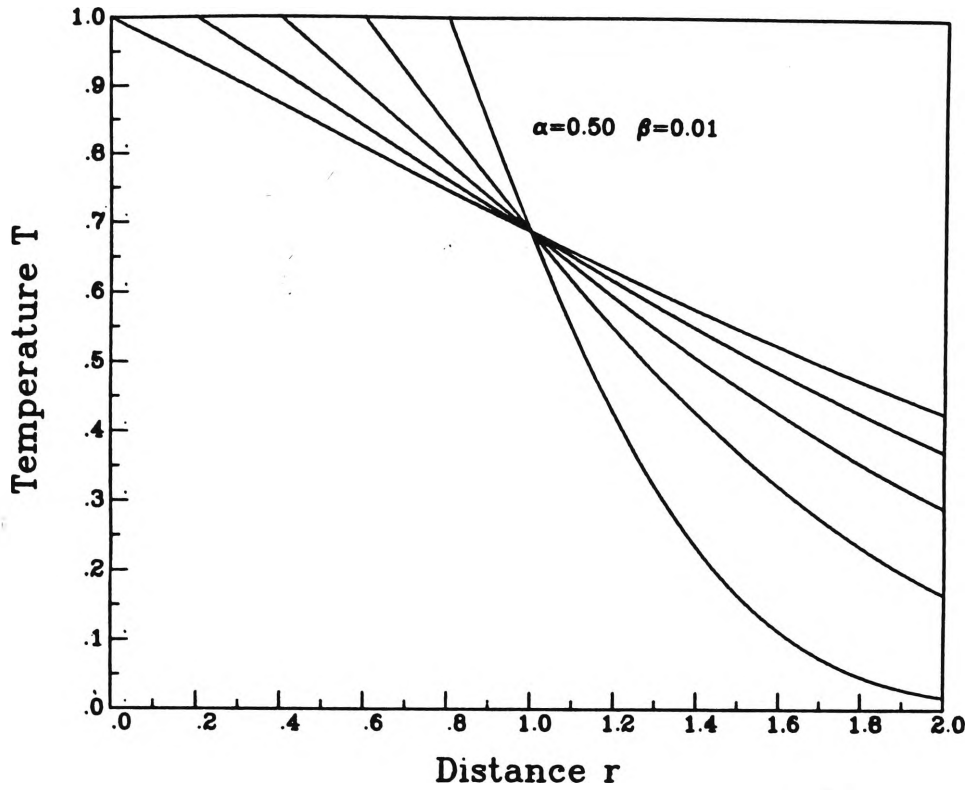
Figure 7.3    Temperature profiles for the collapsing bubble with $\alpha = 0.5$ and $\beta = 0.01$ for equally spaced boundary positions (i.e. $R(t) = 0.8, 0.6, 0.4, 0.2,$ and $0.0$)
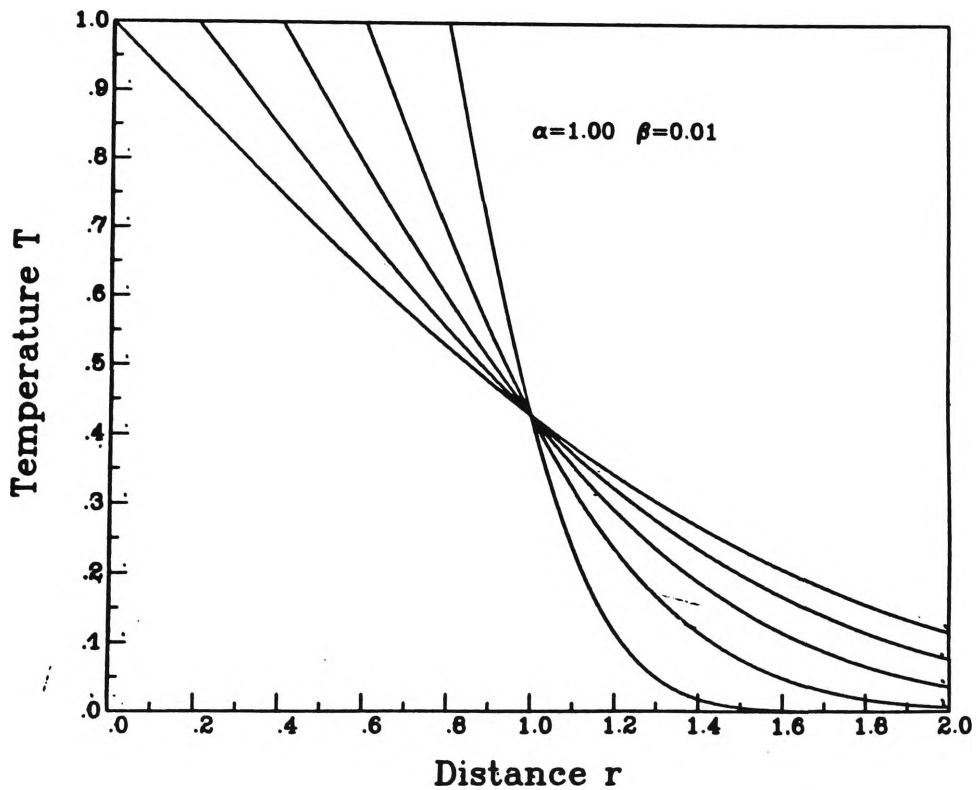


Figure 7.4    Temperature profiles for the collapsing bubble with $\alpha = 1.0$ and $\beta = 0.01$ for equally spaced boundary positions (i.e. $R(t) = 0.8, 0.6, 0.4, 0.2,$ and $0.0$)
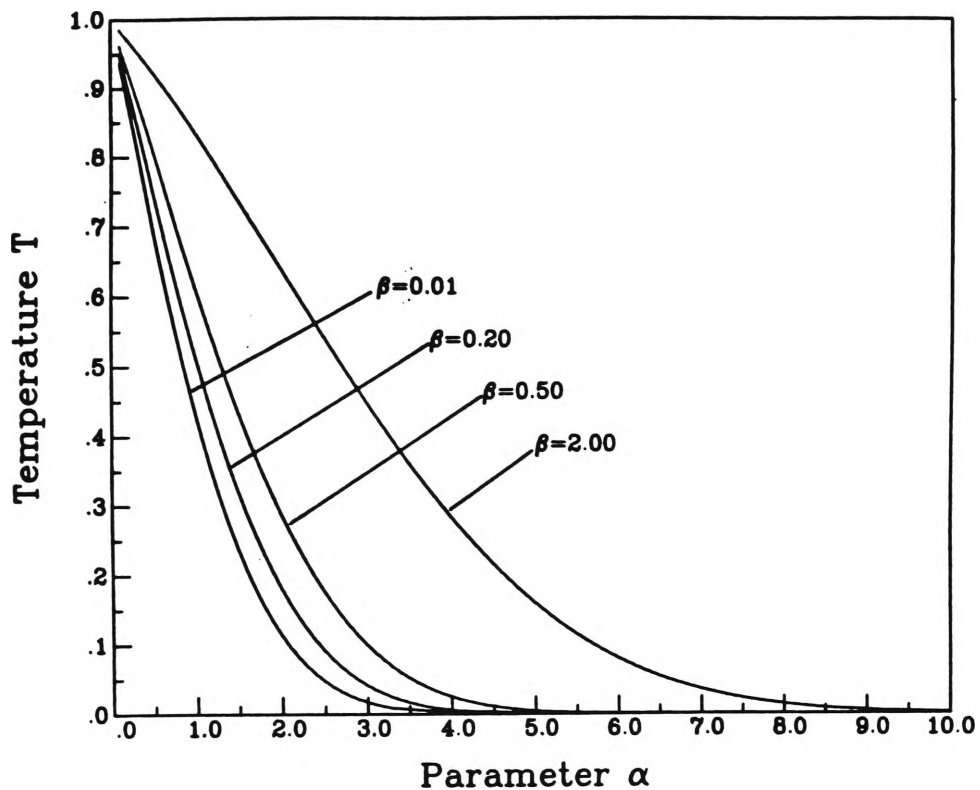
Figure 7.5    Temperature at $r = 1.0$ for the collapsing bubble with $\beta = 0.01, 0.20, 0.50$, and $2.00$ as a function of increasing $\alpha$
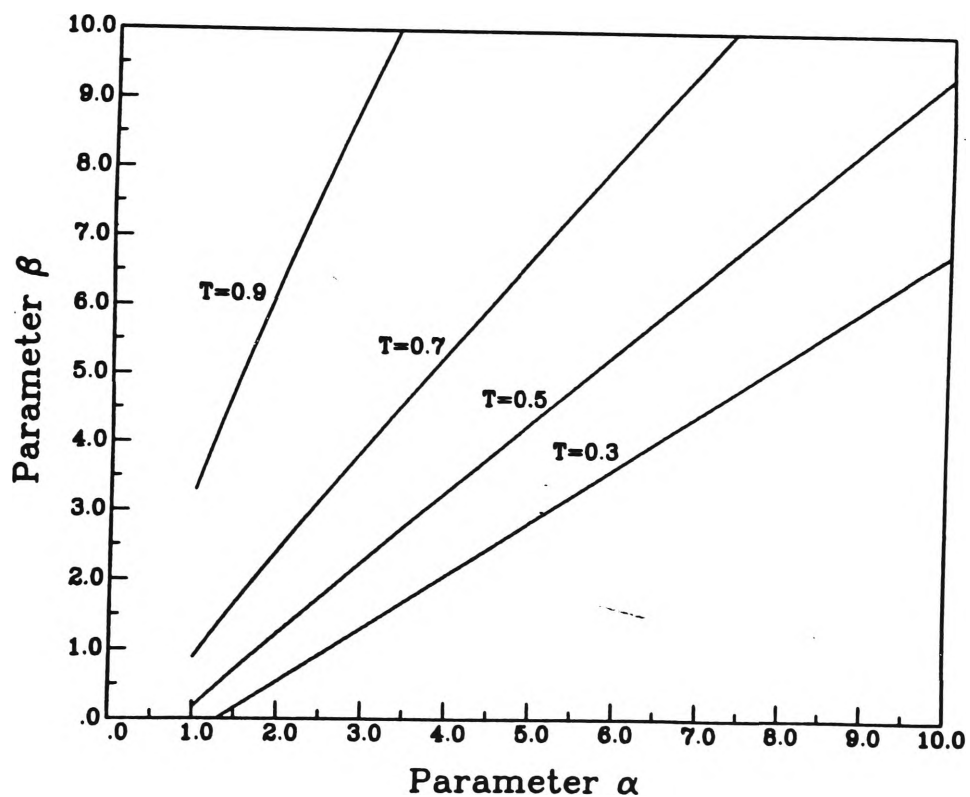


Figure 7. 5    The invariant temperature at $r = 1.0$ as a function of the two parameters $\alpha$ and $\beta$ for selected values of $T$.
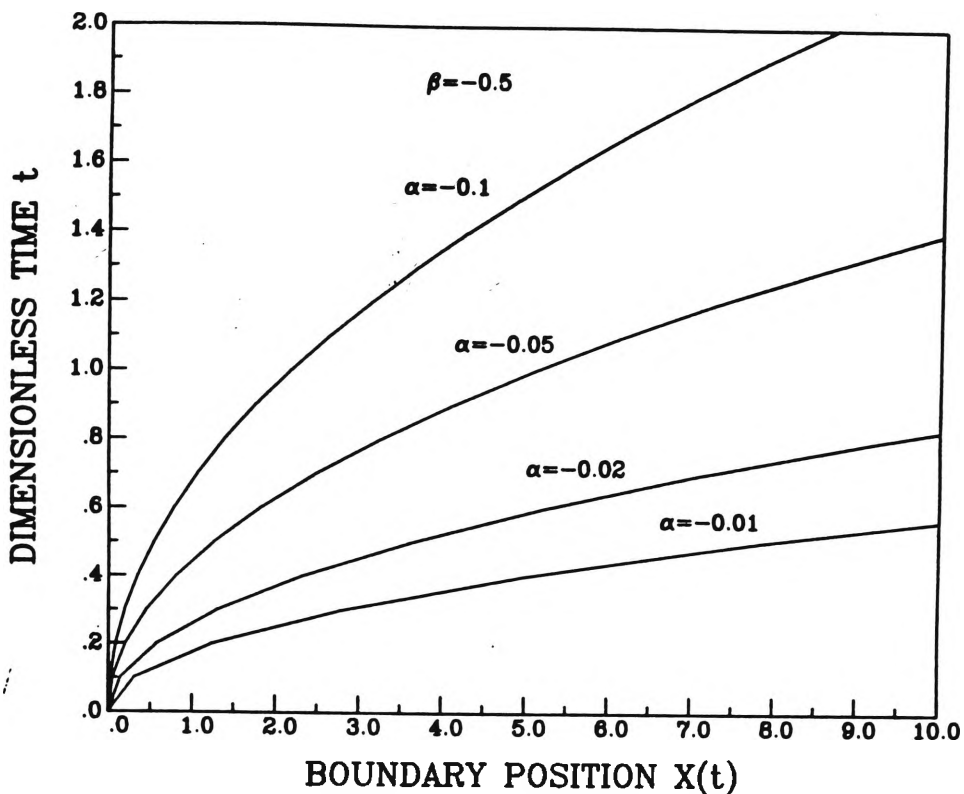
**Figure 7.1**    Exact boundary motion for the growing bubble of zero initial radius with $\beta = -0.5$ and selected values of $\alpha$
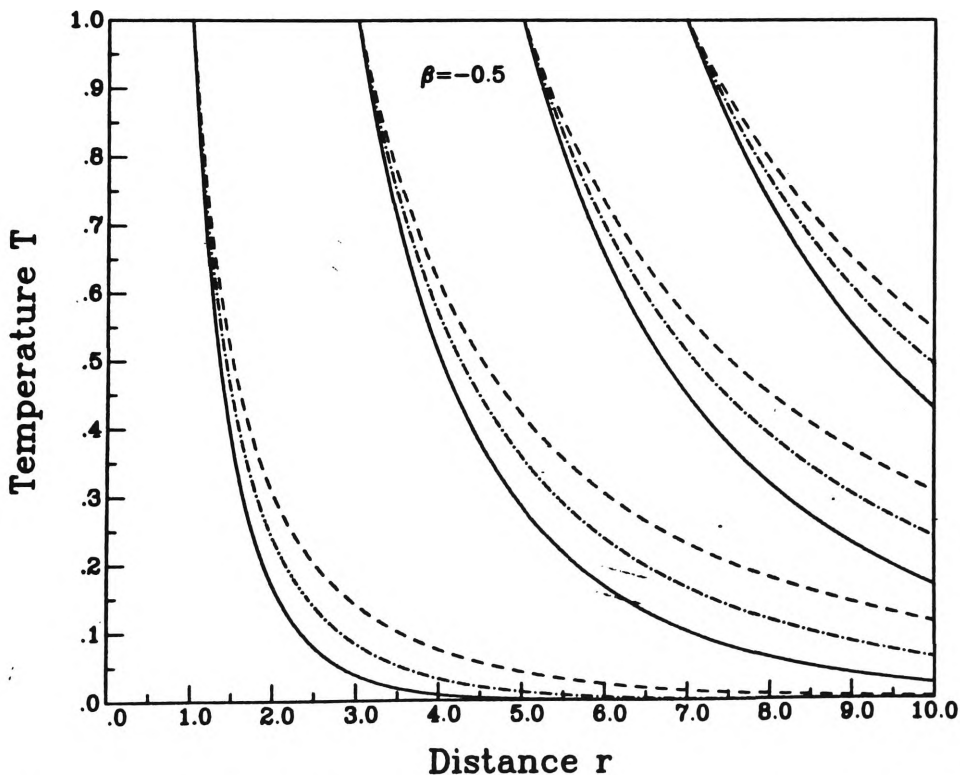


**Figure 7.2**    Exact temperature profiles for the growing bubble of zero initial radius with $\beta = -0.5$ and $\alpha = -0.1(----), \alpha = -0.05(-\cdot-\cdot-)$, and $\alpha = -0.02(\underline{\hspace{1cm}})$
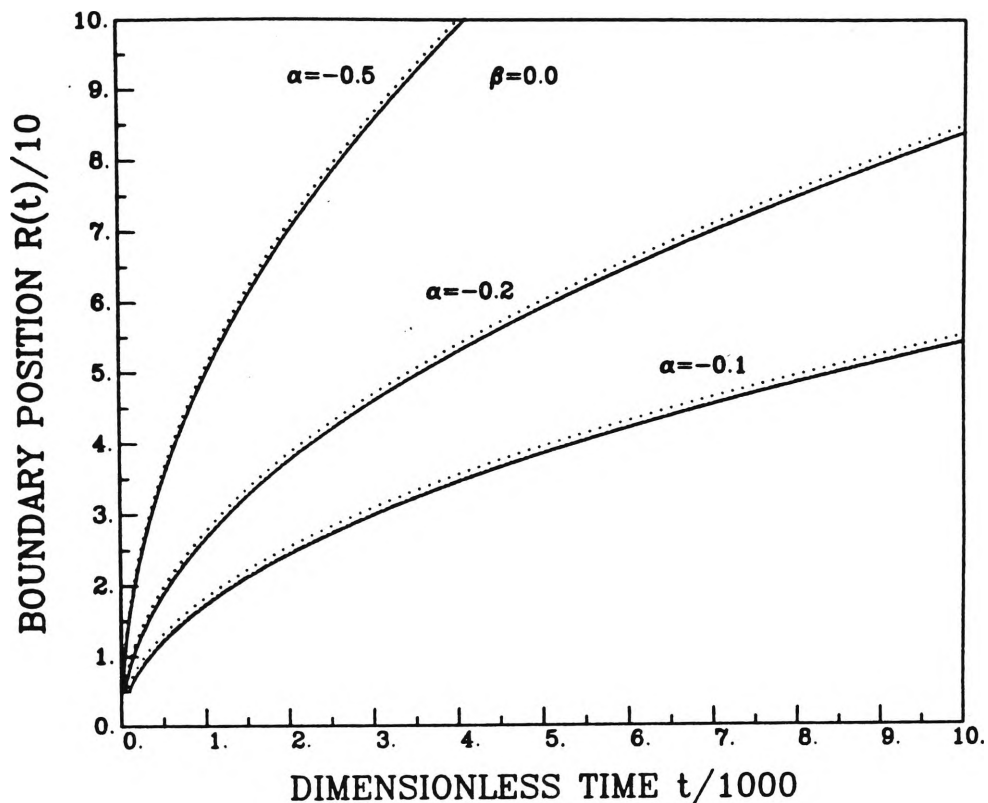
Figure 7.7    Various boundary motion estimates, shifted similarity solution $(7.5.19)(\cdots)$, with linear term$(---)$, and two term estimate $(7.5.20)(\text{---})$, for $\beta = 0.0$ and selected values of $\alpha$
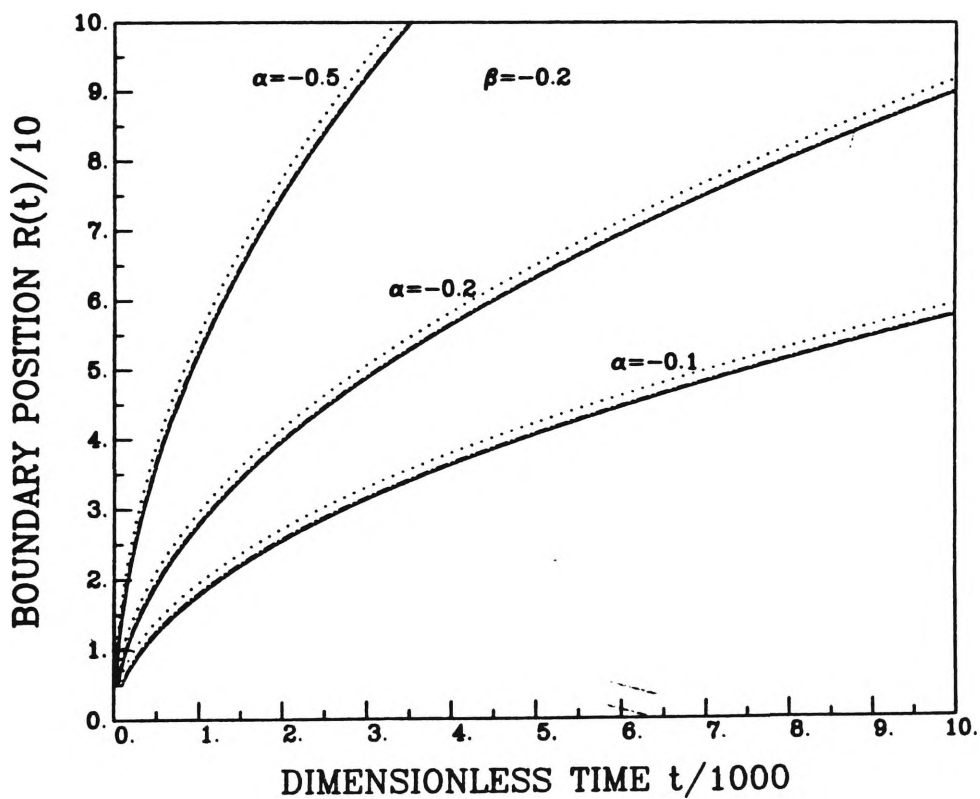


Figure 7.8    Various boundary motion estimates, shifted similarity solution $(7.5.19)(\cdots)$, with linear term $(---)$, and two term estimate $(7.5.20)(\text{---})$, for $\beta = -0.2$ and selected values of $\alpha$

| β | $\alpha$ | | | | | |
|---|---|---|---|---|---|---|
| | -0.1 | -0.5 | -1.0 | -5.0 | -10.0 | -50.0 |
| 0.00 | 0.149 | 1.226 | 3.479 | 56.07 | 207.8 | 4368. |
| -0.05 | 0.154 | 1.278 | 3.647 | 59.47 | 221.1 | 4518. |
| -0.10 | 0.160 | 1.335 | 3.833 | 63.27 | 236.0 | 4681. |
| -0.15 | 0.166 | 1.398 | 4.041 | 67.55 | 252.9 | 4860. |
| -0.20 | 0.172 | 1.469 | 4.273 | 72.40 | 271.9 | 5060. |
| -0.25 | 0.179 | 1.548 | 4.536 | 77.93 | 293.6 | 5287. |
| -0.30 | 0.187 | 1.637 | 4.836 | 84.29 | 318.4 | 5550. |
| -0.35 | 0.195 | 1.739 | 5.180 | 91.69 | 347.0 | 5865. |
| -0.40 | 0.206 | 1.856 | 5.580 | 100.4 | 380.3 | 6259. |
| -0.45 | 0.217 | 1.993 | 6.052 | 110.7 | 419.9 | 6789. |
| -0.50 | 0.230 | 2.155 | 6.616 | 123.2 | 468.5 | 7619. |

Table 7.1    Positive roots ($\Gamma$) of the transcendental equation $(7.3.3)$ for various combination of parameters $\alpha$ and $\beta$

| β | $\alpha$ | | | | | |
|---|---|---|---|---|---|---|
| | 0.1 | 0.5 | 1.0 | 5.0 | 10.0 | 50.0 |
| 0.0 | .0064 | 0.159 | 0.637 | 15.92 | 63.66 | 1592. |
| 0.1 | .0056 | 0.141 | 0.564 | 14.09 | 56.36 | 1409. |
| 0.2 | .0050 | 0.126 | 0.504 | 12.59 | 50.38 | 1259. |
| 0.3 | .0045 | 0.114 | 0.454 | 11.35 | 45.40 | 1135. |
| 0.4 | .0041 | 0.103 | 0.412 | 10.30 | 41.21 | 1030. |
| 0.5 | .0038 | 0.094 | 0.376 | 9.41 | 37.63 | 940. |
| 0.6 | .0035 | 0.086 | 0.345 | 8.64 | 34.55 | 863. |
| 0.7 | .0032 | 0.080 | 0.319 | 7.79 | 31.87 | 797. |
| 0.8 | .0030 | 0.074 | 0.295 | 7.38 | 29.52 | 738. |
| 0.9 | .0027 | 0.069 | 0.274 | 6.86 | 27.45 | 686. |
| 1.0 | .0026 | 0.064 | 0.256 | 6.40 | 25.61 | 640. |

Table 7.2    Positive roots ($\gamma$) of the transcendental equation $(7.4.14)$ for various combination of parameters $\alpha$ and $\beta$

| $\alpha = -1.0$<br>$\beta = 0.0$<br>$R(t)$ | Perturbation<br>estimate | One-Term<br>series<br>(7.5.19) | Two-Term<br>series<br>(7.5.20) | Similarity<br>solution<br>(7.3.4) |
|---|---|---|---|---|
| 5.0 | 3.13 | 2.30 | 3.76 | 3.59 |
| 10.0 | 12.55 | 11.64 | 14.82 | 14.37 |
| 15.0 | 28.23 | 28.17 | 32.93 | 32.33 |
| 20.0 | 50.19 | 51.88 | 58.17 | 57.48 |
| 25.0 | 78.42 | 82.77 | 90.57 | 89.81 |
| 30.0 | 112.93 | 120.86 | 130.15 | 129.33 |
| 35.0 | 153.71 | 166.12 | 176.90 | 176.03 |
| 40.0 | 200.76 | 218.58 | 230.83 | 229.93 |
| 45.0 | 254.09 | 278.21 | 291.94 | 291.00 |
| 50.0 | 313.70 | 345.03 | 360.23 | 359.26 |

Table 7.3     Various estimates for the time $t$ for increasing values of $R(t)$ with $\alpha = -1.0$ and $\beta = 0.0$

| $\alpha = -10.0$<br>$\beta = 0.0$<br>$R(t)$ | Perturbation<br>estimate | One-Term<br>series<br>(7.5.19) | Two-Term<br>series<br>(7.5.20) | Similarity<br>solution<br>(7.3.4) |
|---|---|---|---|---|
| 5.0 | .0600 | .0385 | .0630 | .0602 |
| 10.0 | .2400 | .1949 | .2483 | .2407 |
| 15.0 | .5400 | .4717 | .5514 | .5415 |
| 20.0 | .9600 | .8688 | .9742 | .9627 |
| 25.0 | 1.5000 | 1.3863 | 1.5169 | 1.5042 |
| 30.0 | 2.1599 | 2.0240 | 2.1979 | 2.1660 |
| 35.0 | 2.9399 | 2.7821 | 2.9626 | 2.9482 |
| 40.0 | 3.8399 | 3.6606 | 3.8658 | 3.8507 |
| 45.0 | 4.8599 | 4.6594 | 4.8893 | 4.8736 |
| 50.0 | 5.9998 | 5.7785 | 6.0330 | 6.0167 |

Table 7.4     Various estimates for the time $t$ for increasing values of $R(t)$ with $\alpha = -10.0$ and $\beta = 0.0$

| $\alpha = -100.0$<br>$\beta = 0.0$<br>$R(t)$ | Perturbation<br>estimate | One-Term<br>series<br>(7.5.19) | Two-Term<br>series<br>(7.5.20) | Similarity<br>solution<br>(7.3.4) |
|---|---|---|---|---|
| 5.0 | .0006 | .0006 | .0010 | .0010 |
| 10.0 | .0026 | .0032 | .0041 | .0040 |
| 15.0 | .0058 | .0078 | .0091 | .0090 |
| 20.0 | .0104 | .0144 | .0161 | .0161 |
| 25.0 | .0162 | .0230 | .0251 | .0249 |
| 30.0 | .0234 | .0335 | .0361 | .0359 |
| 35.0 | .0318 | .0461 | .0491 | .0489 |
| 40.0 | .0415 | .0607 | .0641 | .0638 |
| 45.0 | .0525 | .0772 | .0810 | .0808 |
| 50.0 | .0649 | .0958 | .1000 | .0997 |

Table 7.5   Various estimates for the time $t$ for increasing values of $R(t)$ with $\alpha = -100.0$ and $\beta = 0.0$

# APPENDIX

## Calculations for $A'_2(0)$

From equations $(6.5.6)_2$ and $(6.5.8)_2$ with $n = 2$ we have that $A_2(x)$ satisfies

$$A''_2 + \gamma[(x - 1)A'_2 - 2A_2] = F_2(x), \qquad (A.1)$$

subject to the boundary conditions

$$A_2(1) = 0, \qquad A_2(0) = 0. \qquad (A.2)$$

Substituting results $(6.5.11)$, $(6.5.12)$, $(6.5.13)$ and $(6.5.14)$ into $(6.5.7)_2$ we have that $F_2(x)$ is explicitly given by

$$F_2(x) = \alpha\gamma\left\{R(x)e^{-\frac{\gamma}{2}[(1-x)^2-1]} + \int_0^x e^{-\frac{\gamma}{2}[(1-\xi)^2-1]}d\xi\right\}, \qquad (A.3)$$

where $R(x)$ is given by

$$R(x) = \left[\gamma(x - 1)^3 + \frac{5\gamma}{2}(x - 1)^2 + \left(\frac{3\gamma}{2} - \frac{A'_2(0)}{\alpha}\right)(x - 1) - 1\right]. \qquad (A.4)$$

Using variation of parameters we know that $A_2(x)$ must have the form

$$A_2(x) = c_1 A_{21}(x) + c_2 A_{22}(x) - \int_x^1 \frac{F_2(\xi)}{W(\xi)}\{A_{21}(x)A_{22}(\xi) - A_{21}(\xi)A_{22}(x)\}d\xi, \qquad (A.5)$$

where the functions $A_{21}(x)$ and $A_{22}(x)$ are the two linearly independent solutions of $(A.1)$ and are given by

$$A_{21}(x) = 1 + \gamma(1 - x)^2,$$

$$A_{22}(x) = \frac{\alpha\gamma}{2}\left\{(x - 1)e^{-\frac{\gamma}{2}[(1-x)^2-1]} + [1 + \gamma(x - 1)^2]\int_1^x e^{-\frac{\gamma}{2}[(1-\xi)^2-1]}d\xi\right\}, \qquad (A.6)$$

and the Wronskian $W(x)$ is

$$W(x) = -\alpha\gamma e^{-\frac{\gamma}{2}[(1-x)^2 - 1]}.$$

(A.7)

Differentiating equation (A.5) with respect to x, using boundary conditions (A.2) and the fact that $A_{22}(1) = 0$ yields on setting $x = 0$

$$A'_2(0) = -\frac{W(0)}{A_{22}(0)} \int_0^1 \frac{F_2(\xi)}{W(\xi)} A_{22}(\xi) d\xi.$$

(A.8)

Evaluating the integral in (A.8) yields

$$A'_2(0) = \frac{\alpha\gamma}{1 + \gamma + \alpha\gamma}[K_1 - A'_2(0)K_2],$$

(A.9)

where the constants $K_1$ and $K_2$ are given by

$$K_1 = \frac{1}{2\gamma}(1 - \gamma - \alpha\gamma) + \left(\frac{1}{3} + \frac{7\gamma}{24} + \frac{\gamma^2}{24}\right), \qquad K_2 = \frac{1}{4\alpha}(3 + \gamma),$$

(A.10)

from which equation (6.5.15) follows directly.

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