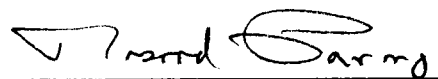


To the Graduate Council :

We are submitting herewith a dissertation written by Satish P. Ketkar entitled "Numerical and Experimental Investigation of Convection/Diffusion Solidification Processes Using Enthalpy Method." We have examined the final copy of this dissertation and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mechanical Engineering.

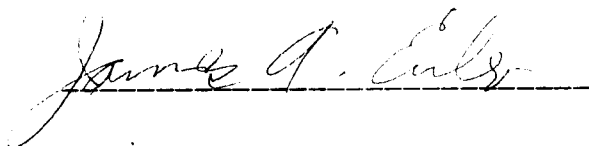


Masood Parang, Major Professor



Rao V. Arimilli, Major Professor

We have read this dissertation and
recommend its acceptance :



Accepted for the Council:



Vice Provost and Dean of The Graduate School

**NUMERICAL AND EXPERIMENTAL INVESTIGATION OF
CONVECTION/DIFFUSION SOLIDIFICATION PROCESSES USING AN ENTHALPY
METHOD**

**A Dissertation
Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville**

**Satish P. Ketkar
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ABSTRACT

Transient heat transfer problems involving solid-liquid phase change moving boundaries have attracted a great deal of interest in recent years. Applications of phase change moving boundary problems in wide range of technologies have given the impetus and motivation for research in this area for many years. The solution methodologies for these problems can be classified into three broad categories, Analytical, Numerical and Experimental. Analytical methods are applicable only to relatively simple problems and only in one dimension. Limitations of analytical methods compell researchers to seek solutions numerically and observe the phenomenon experimentally.

The most versatile method for moving boundary problems is the enthalpy method. There have been a few studies which use enthalpy method and consider convective effects in the liquid. The present study uses a formulation developed by Voller, Markatos & Cross. The main feature of the formulation is that the latent heat effects are isolated in the so called 'source term'. The governing equations so formulated have the same general form as the conventional conservation equations of mass, momentum, and energy. Standard algorithms such as SIMPLE or SIMPLER, therefore can be used. In the present paper the problem of solidification in a rectangular cavity, cooled from one vertical side with remaining sides kept insulated, is solved. The velocities in the solid need to be made zero. This was done using Darcy source technique, which adds a 'Darcy source' to the leading coefficient to the velocity discretization equation. This allows for a gradual slow down of the velocities in the solid region. This technique produced a physically realistic velocity field and interface location.

The numerical technique utilized here is relatively new. For this reason, one of the focusses of this study is the experimental verification of this numerical model. An experimental apparatus is built with one copper wall (cold wall) and other walls made of plexiglass (adiabatic walls). The liquid used for solidification experiments is Caprilic acid. Caprilic acid is used because of its less than ambient melting point 14°C

and low volume reduction upon solidification (3 - 4 %). Photographs of the interface location are presented at various times. The numerical solution is compared with the experimental data for the interface location and temperature. The numerical and experimental solutions are found to be in good agreement.

The numerical model is used to conduct a parametric study. The results are presented for a wide range of physical parameters. Low Prandtl number (0.01) signifying liquid metals (Aluminum, Iron, etc.) and high Prandtl numbers (10, 100) signifying paraffins are considered. Rayleigh number range of 10^4 to 10^6 , aspect ratios of 0.1 to 10, a range of cold wall temperatures, a range of initial superheat levels for the liquid are also considered. A simple corelation is presented for the time for complete solidification.

The results show that for Rayleigh number of 10^4 , when Prandtl number is 0.01 the interface is curved with solidification more advanced near the bottom than at the top of the enclosure. However, at Prandtl number of 100 the interface is essentially planar. Influence of aspect ratio on the volume fraction solidified is found to be weak. However, for lower aspect ratios (< 0.5) the interface is planar and for higher aspect ratios (> 1) the interface is curved.

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LIST OF SYMBOLS

AR	Aspect Ratio, Height/Length
c	Specific heat of solid and liquid
D/Dt	Substantial Derivative
Fo	Fourier number , $\alpha t/L^2$
Fo _{cs}	Fourier number for complete solidification
f(T)	Function defined by Equation 5
Gr*	Modified Grashoff number, $[gL^3\beta\lambda\rho^2/\mu k]$
H	Total enthalpy = h+ f(T); h=cT
Ht	Height of the enclosure
h _m	Sensible enthalpy at the melt temperature T _m
L	Length
k _s , k _l	Thermal conductivities of solid and liquid
P	Pressure
Pr	Prandtl number, $c\mu/k$
Ra*	Modified Rayleigh number, $[gL^3\beta\lambda\rho^2/\mu k]$ Pr
Ste	Stefan number, $c(T-T_m)/\lambda$
t	Time
T	Nondimensional temperature, $c(T-T_m)/\lambda$
T _c	Nondimensional cold wall temperature, $c(T_c-T_m)/\lambda$
T _i	Nondimensional initial superheat, $c(T_i-T_m)/\lambda$
T _m	Melt temperature
u,v	x,y velocities
x,y	Coordinate axis defined in Figure 2

GREEK SYMBOLS

α	Thermal diffusivity, k/c_p
β	Coefficient of thermal expansion
λ	Latent heat
ψ	Streamfunction
μ	Dynamic viscosity
ρ	Density of solid and liquid

CHAPTER 1

INTRODUCTION

Transient Heat transfer problems involving solid-liquid phase change moving boundary occur in many situations of engineering interest, such as casting of metals and glass, freeze drying of foods, storage of thermal energy, ice accretion on vehicles and structures, nuclear reactor safety, freezing or thawing of moist ground soil and many others. Applications of phase change moving boundary problems in wide range of technologies have given the impetus and motivation for research in this area for many years. Most of the early research on the problem was restricted to cases where the liquid phase is stagnant or the motion is entirely due to the moving boundary phenomenon itself, i.e., the diffusion problem.

The problem is highly nonlinear due to the movement of the interface. This nonlinearity has fascinated and challenged engineers and mathematicians for nearly a century since the pioneering work of Stefan[1] on ice growth.

The Phase Change Conduction Problem

At some instant of time t , there are two regions V_s and V_l adjoining each other. Each contains one phase of a pure substance. Consider only solid and liquid phases. The surface separating these phases is the interface and it moves with time. It is assumed that the total volume V , which is the sum of V_s and V_l does not change with time, that there is no convective motion within V and there is no expansion or contraction. The interface motion, temperature and enthalpy changes etc. are governed by the boundary conditions on the outside surface S of V , initial conditions and the properties of the material. The heat conduction equation for each of the two phases can be written as follows.

For the solid phase

$$\rho C_S [\delta T / \delta t] = \text{Div}(k_S \text{grad } T)$$

and for liquid

$$\rho C_L [\delta T / \delta t] = \text{Div}(k_L \text{grad } T)$$

Where

ρ = Densities of the material

T = Temperature

k_S, k_L = Thermal Conductivities of solid and liquid phases, respectively.

t = Time

Div = Divergence

As the interface location and hence the domain of applicability for the governing equations is unknown a priori, two conditions are required on the interface to completely define the problem. One is that the temperature on the interface should equal the equilibrium phase change temperature T_m and the second condition comes from the conservation of energy applied at the interface as follows

$$(k_S [\delta T / \delta n]) - (k_L [\delta T / \delta n]) = \rho \lambda \Sigma',$$

where n is the direction of the normal to Σ (the interface surface) and Σ' is the velocity of Σ along n . At the external boundary any of the three standard types of boundary conditions may apply.) 4

6 (Review of Analytical Methods)

Early analytic work on the solution of phase change moving boundary problem dates back to 1831 by Lamé' and Clapeyron [2] and Stefan [1] in 1891 in relation to ice formation. Only a few Stefan problems admit explicit solutions, all of which are

similarity solutions. Such problems form the backbone of our understanding of the melting-freezing processes and they are the only means of checking the accuracy of numerical codes as well as checking the accuracy of the approximate solutions. Explicit solutions are limited to semi-infinite regions subject to constant initial and boundary temperature and with physical properties constant in each phase. Well posedness of 1-D general Stefan problems was established only in the mid 1970's. Since explicit solutions exist for only very few realistic problems we need to look for approximate solutions.

Analytical approximations can be classified under the following broad categories [3].

1. Quasi-stationary approximations
2. Perturbation expansions.
3. Megerlin approximation.
4. Heat balance integral method.

The basic assumption of the quasi-stationary approximation is that the sensible heat is negligibly small compared to the latent heat. This approximation is applicable only to one phase problems (i.e. the problem needs to be solved only in one of the phases, the other phase being at the melt temperature of the material under consideration). With quasi-stationary approximation it is possible to have solutions for time variant boundary temperatures, boundary fluxes and convective boundary conditions (recall that explicit solutions were possible only for constant temperature conditions). Solomon, Alexiades, and Wilson[4] have proved that the solution of Stefan problem with convective boundary condition tends to quasi-stationary approximation as specific heat of the liquid tends to zero. With quasi-stationary approximation one can solve in closed form the melting and freezing problem in cylinders and spheres.

Another approximation method is the perturbation method. These methods utilize series expansions in small(or large)parameters to reduce the problem into a series of simpler problems which could be solved explicitly. Generally only the first few terms in the perturbation expansion can be found in practice due to increasing mathematical complications. In Stefan type problems there are few naturally

occurring small parameters. Researchers have applied expansions in Stefan number. Like other analytic approximation methods, perturbation methods can be applied only to relatively simple problems, serving as a rough guide indicating qualitative behavior rather than quantitative information. Unfortunately, there are no error estimates available for any of these approximate methods and the validation of any method must be performed by comparing it with other methods or experimental information. Perturbation solutions can be considered as corrections to the quasi-stationary solution and the zeroth-order perturbation solution should match the quasi-stationary solution. Generally the expansions are carried out in dimensionless variables with the interface immobilized by a change of variables. This approach is applicable to one-phase problems in slab, cylindrical, and spherical geometries with any of the standard boundary conditions and has been applied by many researchers[6-9]. The Perturbation method was applied to rapid freezing of dilute alloys by Alexiades[5]. The method has also been applied to some two-phase problems in finite domains when the initial temperature is not the melt temperature. These problems become complicated leading to singular perturbations since the initial condition can not be satisfied by the zeroth order solution. So, small time expansions are needed which must be matched asymptotically with the outer solution. This method has been used for problems in slab and annular domains by Weinbaum and Jiji [6]. Prusa and Yao [7] used perturbation expansions for the solution of melting around a horizontal heated cylinder for constant flux boundary condition. Stefan and Rayleigh numbers were used as parameters for expansion. Sen[8] used a perturbation method for solution for the shape of a solidification interface subjected to a spatially periodic heat flux. Perturbation expansions were also used by Milanez and Boldrini [9] for inward spherical solidification by convective cooling.

Other approximate methods are Megerlin's method and the Heat Balance Integral method. Megerlin's method tries to fit a parabolic profile for the temperature. In this method however, global energy balance can not be satisfied and so the heat equation is satisfied only on the front. Goodman[10] applied an integral method, which dates back

to Von Karman and Pohlhausen, to solve one-dimensional transient melting problems. In Goodman's method a parabolic temperature profile is used and overall heat balance is satisfied. Another version of heat balance integral method was applied by Poots[11] to investigate solidification inside a square prism. Tsai and Strieder[12] applied such a method for the solution of melting in a semi-infinite slab with initial subfreezing. Voller[13] developed Heat Balance Integral method based on an enthalpy formulation. In summary, one can say that analytical methods are applicable only to relatively simple problems and only in one dimension.

Review of Numerical Methods

The limitations of analytical and approximate methods compell researchers to apply numerical methods for the moving boundary problems. By far the largest number of available multidimensional solutions of phase change problems involve numerical schemes. Numerical methods have a wider range of applicability and do not require infinite mathematical wisdom as some of the analytical and semi-analytical methods do. Main drawback of numerical methods is that they sometimes fail to give physical insight into the problem. The treatment of latent heat is a major problem associated with phase-change solution methodologies. A comprehensive review of progress made until about 1980 is in Lunardini[14]. Other sources of review articles include Lewis, Morgan, and Habashi[15], Lewis and Morgan[16], Brody and Apelian[17], Dantzig and Berry[18], Voller and Cross[19], and Poirier and Salcudean[20].

Numerical methods can be classified into two broad classes based on the choice of dependent variable. One group takes temperature as the sole dependent variable. Several studies in this category commonly referred to as "front tracking methods" are reviewed here .

Springer & Olson [21] proposed a standard explicit finite difference approach to study freezing in the cylindrical annulus. The movement of the front within the annulus was demonstrated. Rathen & Jiji [22] used the explicit finite difference

method to verify the result of their semi-analytical solution in the corner region. Lazaridis [23] recast the jump condition by expressing $(\delta T/\delta n)$ in terms of $(\delta T/\delta x)$ and $(\delta T/\delta y)$ to overcome the difficulty of expressing normal derivative of temperature on the interface. He could then obtain solutions to several two and three dimensional phase change problems. Belinas & Jiji [24] solved a problem of phase change in the presence of fluid motion. An explicit finite difference formulation was used to investigate flow in a pipe with surface solidification.

In another class of methods based on temperature, the spatial variables are transformed so as to 'fix' or 'immobilize' the front. In the transformed space, the solid phase and the liquid phase each occupy a fixed volume and the parameters of the front location are transferred into the governing differential equation. The immobilization of the interface makes the problem geometrically simple, therefore allowing easy finite difference formulation; but the governing differential equation becomes highly nonlinear. Such a scheme was applied by Spaid et al. [25] Duda et al. [26] used the front fixing technique along with implicit difference formulation in their analysis of phase change in cylindrical containers.

In solving problems with constant temperature boundary conditions, the 'Isotherm Migration Method' is very appealing. In this formulation one of the spatial variables is exchanged with temperature making the exchanged spatial variable as dependent variable and temperature as independent variable. Consequently, if a uniform mesh is employed in the new variables, in the physical domain the corresponding mesh will be fine where there are large temperature gradients and coarse in the regions with small temperature gradients. Crank and Gupta[27] used this approach along with explicit difference formulation to solve a number of two dimensional problems. The authors have mentioned that it is difficult to use implicit formulation because of the nonlinearity of the transformed equations.

Some researchers have applied a Boundary Integral Equation Method (BIEM) for the solution of moving boundary problems. A major advantage of BIEM is that the

problem is formulated in terms of the unknowns on the boundary of the domain and therefore, only the boundary of the region of interest needs to be discretized. O'Neill[28] used BIEM for solution of two-dimensional phase-change problems. Convection can enter through boundary conditions but not within phase boundaries. A general formulation based on space-time Green's function was developed for the heat conduction equation. Sadegh et al.[29] applied BIEM technique for the solution of freezing around buried pipes. Coleman[30] applied BIEM for solidification of dilute alloys.

The difficulty with temperature based formulations is that one must assume a priori the existence and smoothness of a sharp interfacial surface to even formulate the problem. It is possible to treat the Stefan-type problems through 'weak formulations', discussed in References 31-35, 86, and 87. In the weak formulations of moving boundary problems no a priori assumptions regarding the interface(s) need be made and interface conditions are not to be imposed explicitly, since they are absorbed as natural interface conditions in the formulation. Solid and liquid regions need not be treated separately. Instead the conservation laws are imposed globally, irrespective of phase (see [86, 87] for mathematical justifications). The phases and the location of the interface are determined later from the solution. Thus, more general process, involving possibly complicated interfaces and/or 'mushy zones' can be modelled with equal ease, in any number of dimensions. Their computational advantage is that they lead to 'fixed domain' numerical schemes, without front-tracking.

One of the popular weak formulations is the 'ENTHALPY METHOD'. It was introduced in the mathematical literature by Kamenomostskaja [31] and Oleinik [32], and as a practical numerical method by Rose [33] and Solomon [34]. The enthalpy formulation enjoys widespread applications. The energy balance is made between conduction heat flux and the rate of change of enthalpy, not temperature. Meyer[35] described a fully implicit two-dimensional finite difference scheme for studying problems where the change of phase takes place over a range of temperatures.

Shamsunder and Sparrow [36] modified Meyer's method and described a discrete version of enthalpy method. Some researchers [37] studied the effect of density change on the multidimensional conduction phase change. The most attractive feature of the enthalpy model is that the interface is completely eliminated from the calculations and it is absorbed as a natural boundary condition. Voller and Cross [38-41] have investigated the Enthalpy method and have developed some powerful algorithms for the solution of phase change problems.

So far the methods which solve diffusion dominated phase change problems have been discussed. Experimental studies [42-45], have shown that in some situations the effects of convection are important. One approach in accounting for convective effects is to use empirical relationships for liquid phase convective heat transfer. This approach has been used with moderate success in metallurgical applications [46,47]. A general approach is to take full account of the convection effects in the governing equations of the problem and develop numerical schemes to efficiently and effectively solve these equations. Kroeger & Ostrach [48] used a stream function formulation to estimate the steady state position of the melt profile in an analysis of continuous casting. Sparrow et al [49] also use a stream function formulation in developing a finite difference numerical procedure for the analysis of a pure material in a cylindrical region. This work was extended by Ramachandran et al [50] for melting in a rectangular cavity with adiabatic top and bottom boundaries. A coordinate transformation is used to conform the mesh to the solid-liquid interface. The density variation causing the natural convective flow is dealt through the Boussinesq approximation. Desai et al.[51] and Desai and Kim [52] used a finite element method with the stream-function-vorticity technique to model the advancing liquid metal front in runner channels and the free convection in molds. The Stream-function-vorticity approach was also used by Okada[53] for the analysis of heat transfer during melting from a vertical wall and by Ho and Chen[54] for numerical simulation of melting of ice around a horizontal cylinder. The main advantage of the stream-function-vorticity approach is that iterations to correct the pressure field are not required and the continuity equation is satisfied implicitly. A

major disadvantage is that the formulation is applicable only in two dimensions. Webb and Viskanta[55] and Bernard et al.[56] have used primitive variables with a front tracking scheme for the solution of melting driven by natural convection in a rectangular enclosure. Prasad and Sengupta[57] also used primitive variables for numerical investigation of melting inside a horizontal cylinder including effects of natural convection.

A major consideration in these schemes for convection/diffusion phase change is the position and shape of the interface. At the interface , temperature, velocity , heat removal conditions have to be satisfied. This approach limits the application of the methods. As mentioned before, by introduction of the enthalpy method the interface calculation is no longer needed and the boundary conditions to be satisfied at the interface are absorbed as natural interface conditions in the formulation. This results in fixed grid solutions. Enthalpy techniques have also been applied successfully in convection/diffusion moving boundary problems. Morgan [58] developed a finite element enthalpy technique in conducting a numerical analysis of solidification with natural convection. In this scheme the interface is placed on the surface of elements undergoing phase change. Schneider [59] presented an enthalpy model with natural convection in the melt for solid-liquid phase-change processes. For further detailed literature survey on numerical modelling of heat transfer during solid-liquid phase-change processes the reader is referred to Salcudean and Abdullahn [60]. Voller et al.[61] developed an enthalpy method for convection/diffusion phase change. They use the SIMPLE algorithm of Patankar [62] to solve the governing equations. Various methods of treating the moving interface in the fixed grid formulation are also described. The formulation was applied by Prakash, Symonds, and Singhal[63] for phase-change processes involving welding processes. Brent, Voller, and Reid[64] applied the formulation for melting of a pure metal from the vertical wall.

The essential feature of the scheme developed by Voller et al. [61] is that the latent heat effects are isolated in the source term. The formulation is valid for isothermal

evolution of latent heat as well as over a temperature range. Three schemes for ensuring that the velocities actually take a zero value in the solid phase are suggested. The method assumes constant properties. The above study was limited to a test problem which had a Rayleigh number of 3000 and the Prandtl number of 100. In most of the practical situations of interest the range of Rayleigh numbers is very

high (of the order of 10^4 to 10^7) and the Prandtl numbers vary from 0.01 for molten metals like aluminum to 50 for wax. So there seems to be a need to study the problem of convection/diffusion phase change for various values of Rayleigh and Prandtl numbers and their influence on the solidification times, nature and shape of interface.

Review of Experimental Studies

Experimental data is essential to verify the validity of numerical and analytical approaches. Many researchers have performed experiments in the area of solid-liquid phase-change problems. Hale, Jr. and Viskanta[65] have studied experimentally solid-liquid interface motion during freezing and melting from above as well as from below. They concluded that natural convection in the liquid must be accounted for in the prediction of the phase-change boundary motion for unstable situations which arise during melting from below and solidification from above.

Gau and Viskanta[66] have reported flow visualization for freezing from above with a hot bottom wall. The phase-change -material(PCM) used in these experiments is n-octadecane. Aluminum powder is used as a flow tracer. The results indicate that natural convection in the melt decreases the rate of solidification from above. The motion of the melt caused the solid-liquid interface to become concave facing the liquid at later stages of freezing. Natural convection gradually retarded and in the end completely terminated the motion of the interface. Two persistent horizontal convection rolls were observed. Gau, Viskanta, and Ho[67] have reported flow

visualization results for melting from below in a rectangular cavity. Again, the PCM used is n-octadecane and Aluminum powder is used as a flow tracer. Similar experiments have been performed by Diaz and Viskanta[68]. Their experiments revealed Benard-like three dimensional convection cells, which increased in size and merged with the neighboring ones and formed nearly two-dimensional rolls as melting progressed. Van Buren and Viskanta[69] conducted experiments for freezing from a vertical plate. They used a Mark-Zehnder interferometer to observe the isotherms patterns. Hale,jr. and Viskanta [44] reported photographic observations of the solid-liquid interface motion during melting of n-octadecane heated from an isothermal vertical wall. They concluded from the melt shapes and temperature in the paraffin (n-octadecane) that natural convection plays an important role in the heat transfer process. Ho and Viskanta[70] also studied the problem of heat transfer during melting from an isothermal vertical wall. They used a shadowgraph technique to obtain the heat transfer data. Experimental results clearly indicated that, except in the very early stages of melting, the rates of melting and the heat transfer were greatly affected by buoyancy driven convection in the liquid. It was also observed that initial subcooling of the solid substantially impeded the phase-change process. They also performed numerical simulations of the problem. A front-tracking scheme was employed for this purpose. Gau and Viskanta[71] performed experiments to determine the role of natural convection during melting and solidification of a pure metal(Gallium) on a vertical wall. Due to anisotropy in the thermal conductivity of Gallium and crystallographic effects, the interface is found to be highly irregular. Gau and Viskanta[45] also performed experiments for melting and solidification in a rectangular cavity using Lipowitz metal($T_m=70$) as a working substance. Gau and Viskanta[72] also studied the effect of natural convection on solidification from above and melting from below of a pure metal(Gallium).

Sparrow, Schmidt, and Ramsey [42]conducted experiments for melting of solid due to an embedded heat source. A horizontal cylinder was taken as the heat source, which was embedded in solid at its fusion temperature. The experiments were performed with a eutectic mixture of sodium nitrate and sodium hydroxide(melting

temperature, 244°C). White et al.[73] observed photographically the variation with time of size and shape of melt region around horizontal cylinder embedded in a solid paraffin. An array of cylindrical heaters is used by some investigators [74]. Regularly arranged Benard convection cells were observed early in the process and flow in these cells produced a solid-liquid interface with many hemispherical capped cells. These cells grew in size and joined the neighboring ones as the melting progressed. Ramsey et al. [75] performed photographic study of melting about an embedded horizontal heating cylinder. Bathelt and Viskanta[76] reported heat transfer experiments during melting from a horizontal cylindrical heat source with a uniform surface heat flux and uniform surface temperature embedded in n-heptadecane and n-octadecane. They recorded the instantaneous shape of the melt volume photographically.

Webb, Moallemi, and Viskanta[77] studied melting of ice in a horizontal cylindrical capsule. Brewster and Gebhart[78] performed measurements of natural convection in downward freezing of pure water. Souza Mendes et al.[79] performed experimental study of melting of solid around a vertical cylinder embedded in it. They observed that conduction heat transfer prevails initially, and the time at which natural convection becomes important is a function of Rayleigh number. For high values of Rayleigh number($Ra = 10^6$) convection takes over soon. Chaboki and Sparrow[80] conducted experimental studies in which melting of a phase-change material occurred in a closed vertical tube which was rotated about the vertical axis colinear with that of the tube. It was found that rotation gave rise to considerably more rapid melting than for no rotation, with time required to achieve a given amount of melting being halved due to rotation.

Wolff and Viskanta [81] studied melting of a pure metal from a vertical wall. Tin was used as the phase-change material. Experiments were performed in a rectangular enclosure. Wolff and Viskanta [82] also performed solidification experiments with pure tin in a rectangular cavity. They performed numerical study to match the experimental results. A primitive variable-based front tracking scheme was used in

the numerical model. The numerical predictions of the solidification interface was reported to be disappointing. Webb and Viskanta[83] studied natural convection dominated melting heat transfer in an inclined enclosure. It was observed that the effect of the enclosure inclination was to establish three-dimensional convective motion which intensified as the inclination angle from the vertical was increased. The three dimensionality of the flow field resulted in nonuniform melting of the solid. The flow patterns were found to be dependent on the angle of inclination and the initial subcooling. For further survey of experimental literature the reader is referred to Reference 84.

Objectives and Scope of Study

The focus of the present study is a parametric study using an enthalpy method for solidification problem and experimental validation of the numerical solution. In the present study the author has developed a computer code incorporating the technique proposed by Voller et al.[61] in conjunction with the SIMPLER-like algorithm (Appendix A) for the solution of solid-liquid phase-change problem in a rectangular enclosure. The validity of the formulation and the computer code developed is tested with experimental data for both solidification and melting. The experimental melting data is taken from Wollf and Viskanta[81] for melting of pure tin. As usable experimental solidification data were not found in the literature the author designed and performed experiments using 98% pure Caprillic acid(melting point 14°C). The data obtained on temperature history and phase-change front location in these experiments are used to verify the numerical results. The validity of the analysis is presented and discussed.

To the author's knowledge, Ramchandran et al.[50] are the only researchers who have presented a parametric investigation of solidification in a two-dimensional rectangular cavity. The lowest Prandtl number considered was 0.1 and the highest Rayleigh number considered was of the order of 10^5 . They used a stream-function-vorticity approach to generate their numerical solution. However,

parametric investigation of solid-liquid moving boundary problems using an enthalpy method does not exist. In the present study results are presented for a range of Rayleigh and Prandtl numbers. Low Prandtl numbers(0.01) signifying liquid metals (Aluminum,Tin,Iron, etc.) and high Prandtl numbers(10,100) signifying paraffins are considered. For various parameters, volume fraction solidified (extent of solidification), isotherms, and interface locations are presented. The effect of cold wall temperature and initial superheat on the extent of solidification and the effect of aspect ratio are also examined and discussed.

CHAPTER 2

NUMERICAL MODEL

The following assumptions are used in conservation equations for the melt and the solid region. 1) The thermophysical properties of solid and liquid are assumed constant and equal 2) The melt is assumed to be an incompressible laminar Newtonian fluid and the Boussinesq approximation is presumed to be valid. Using the following non-dimensionalization

$$x^* = \frac{x}{L}; y^* = \frac{y}{L}; u^* = \frac{u}{(\alpha/L)}; v^* = \frac{v}{(\alpha/L)}; \quad (1)$$

$$P^* = \frac{P}{\rho(\alpha/L)^2}; Fo = \frac{\alpha t}{L^2}; T^* = \frac{T - T_m}{\lambda/c}; H^* = \frac{H}{\lambda}$$

and dropping the superscript (*) the governing dimensionless equations for continuity and momentum reduce to (see Appendix A)

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (2)$$

$$\frac{Du}{D(Fo)} = Pr[\nabla^2 u] - \frac{\partial P}{\partial x} \quad (3)$$

$$\frac{Dv}{D(Fo)} = Pr[\nabla^2 v] - \frac{\partial P}{\partial y} + Ra^* T. \quad (4)$$

For the energy equation, we follow the approach of Voller et al.[61].The main feature of the methodology developed by Voller is to split the enthalpy into sensible enthalpy h (= dimensionless T) and a function $f(T)$, which represents the liquid fraction,

$$f(T) = \begin{cases} 1 & T > T_m \\ 0 < f(T) < 1 & T = T_m \\ 0 & T < T_m \end{cases} \quad (5)$$

Substituting $H=h+f(T)$ into the energy equation(A-11, see Appendix A) and assuming phase-change at a fixed temperature and a sharp interface, the convective velocity at the interface is zero(implying divergence of $f(T)$ is zero), the dimensionless energy equation reduces to

$$\frac{\partial h}{\partial (Fo)} + \left[u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} \right] - \nabla^2 h + \frac{\partial f(T)}{\partial (Fo)} = 0 \quad (6)$$

The governing equations (1)-(6) are solved for a solidification problem in a two-dimensional rectangular enclosure with three adiabatic walls ($dT/dx=0$), one cold vertical wall($T=T_c$ for $x=0$), and zero velocities(u and v) on all the walls. The phase (solid,liquid,or two-phase) is determined by the value of $f(T)$. If the value of $f(T)$ is less than or equal to 0 in a control volume ,then the control volume is solid, while an $f(T)$ value of greater than or equal to 1 implies a control volume in liquid phase. All control volumes with $f(T)$ between 0 and 1 are phase changing control volumes.

This equation is similar to the general differential equation(A-15) discussed in Appendix A, described by Patankar and can be solved by methods described in reference 62.It is necessary to make the velocities approach zero in the control

volumes undergoing phase change. Voller [61] has proposed the addition of a large term S in the leading coefficient a_p (see Appendix A) of the momentum equations, of the form

$$S = \text{large term} \cdot (1 - f(T)).$$

In the liquid $f(T) = 1$ so the value of S is zero. In the solid, $f(T) = 0$ and the large source term will drive the velocity to zero there. For control volumes changing phase, $0 < f(T) < 1$ and S is between 0 and the large term. This ensures gradual slowdown of velocities in the control volumes changing phase and ensures that the velocities are very close to zero in the solid and the velocity solution is unaffected in the liquid region.

The method for dealing with the source term during the solution iterations of the SIMPLER algorithm, as outlined by Voller is as follows: (see Appendix A) On commencement of SIMPLER algorithm over one time step, initial values for current nodal latent heats are taken to be the values at previous time level. After solution of nodal enthalpies at the i^{th} iteration, $f(T)$ is updated as follows

$$[f(T)]_{i+1} = f(T)_i + (h)_i, \text{ and}$$

$$\text{if } [f(T)]_{i+1} > 1 \text{ then set } [f(T)]_{i+1} = 1, \quad (7)$$

$$\text{if } [f(T)]_{i+1} < 0 \text{ then set } [f(T)]_{i+1} = 0.$$

Upon completion of the i^{th} iteration of SIMPLER, the front is within those control volumes for which $0 < f(T) < 1$ and its precise location can be found from the value of $f(T)$. For example, if $f(T) = 0.6$ in a particular control volume implies that the control volume is 60% liquid. The major advantage of the enthalpy approach is that a fixed grid numerical formulation can be employed and the energy balance condition at

the interface is automatically satisfied[86,87]. The above algorithm of Voller et al. [61] can be applied only if the properties in the solid and liquid region are constant and equal. A more detailed discussion of the method used can be found in Appendix A.

Equations (2) through (6) are solved by a SIMPLER-like algorithm of Patanker in conjunction with the enthalpy-porosity technique of Voller et al. [61] for the solution of the two-dimensional continuity, momentum and energy (enthalpy) equations. In order to avoid difficulties arising from decaying convection and melting at small times, the following algorithm is used(see Appendix A for more details).

- 1.The solution is started with a guessed value of the velocity field and a value of $f(T)$, depending on phase.
2. The energy equation is solved to generate temperatures($T=h$).
3. The coefficients of the pressure equation are calculated and the pressure field is obtained.
4. The momentum equations are then solved using this pressure field.
5. If conservation of mass is satisfied within the tolerance limit(taken to be 0.001 in this study), go to the the next time step.
6. If mass conservation is not satisfied then the pressure correction equation is solved.
7. The velocity field is then corrected using the pressure corrections.
8. The nodal latent heat values are updated according to Equation 7.
9. With the newly corrected velocity field, the energy equation is solved.
10. Go to step 3.
11. The algorithm is then advanced in time.

Grid refinement studies were conducted. Table 1 illustrates the effect of grid size on volume fraction, temperature,time step necessary for convergence, and CPU time, for the case of $Pr = 1$, $Ra^* = 10^5$, $Fo = 0.063$, $T_c = -0.5$, $T_i = 0.5$. It is observed that as a finer grid is used the time step needs to be reduced to achieve convergence. Therefore, in addition to the

TABLE 1

Influence of grid size on computed results for
 $Pr = 1$, $Ra^* = 10^5$, $Fo = 0.063$, $T_c = -0.5$, $T_i = 0.5$

Grid	Volume fraction solidification	Temperature $X = 1, Y = 1.0$	ΔFo	CPU
8 x 8	0.114	0.31	0.01	1 min
15 x 15	0.121	0.41	0.001	7 min
20 x 20	0.129	0.435	0.001	20 min
30 x 30	0.137	0.4499	0.0001	1.5 hr
40 x 40	0.136	0.4553	0.0001	3 hrs

increased computation due to the greater number of points, the number of time steps needed to reach a certain Fourier number is also substantially increased. The time step needed to achieve convergence was determined by trial and error. Figure 1 shows the flow chart of the numerical computations.

Similar results were obtained for higher Prandtl and Rayleigh number (10 and 5.17×10^9 , respectively, with $AR = 2.3$, and $Fo = 0.01$). In general, it was found that for a given Rayleigh number and time step, reducing the Prandtl number results in slower convergence. Similarly, increasing the Rayleigh number given a Prandtl number and time step, increases the required CPU time. In addition, convergence is not achieved beyond a certain Rayleigh number for each case without reducing the time step.

The prohibitive cost of computational time (up to 2 orders of magnitude more) and the greatly reduced improvement in computational accuracy (limited to 10%) with increase in grid refinement, suggested a 12×22 grid size choice for the freezing case and a 15×15 grid for the melting case.

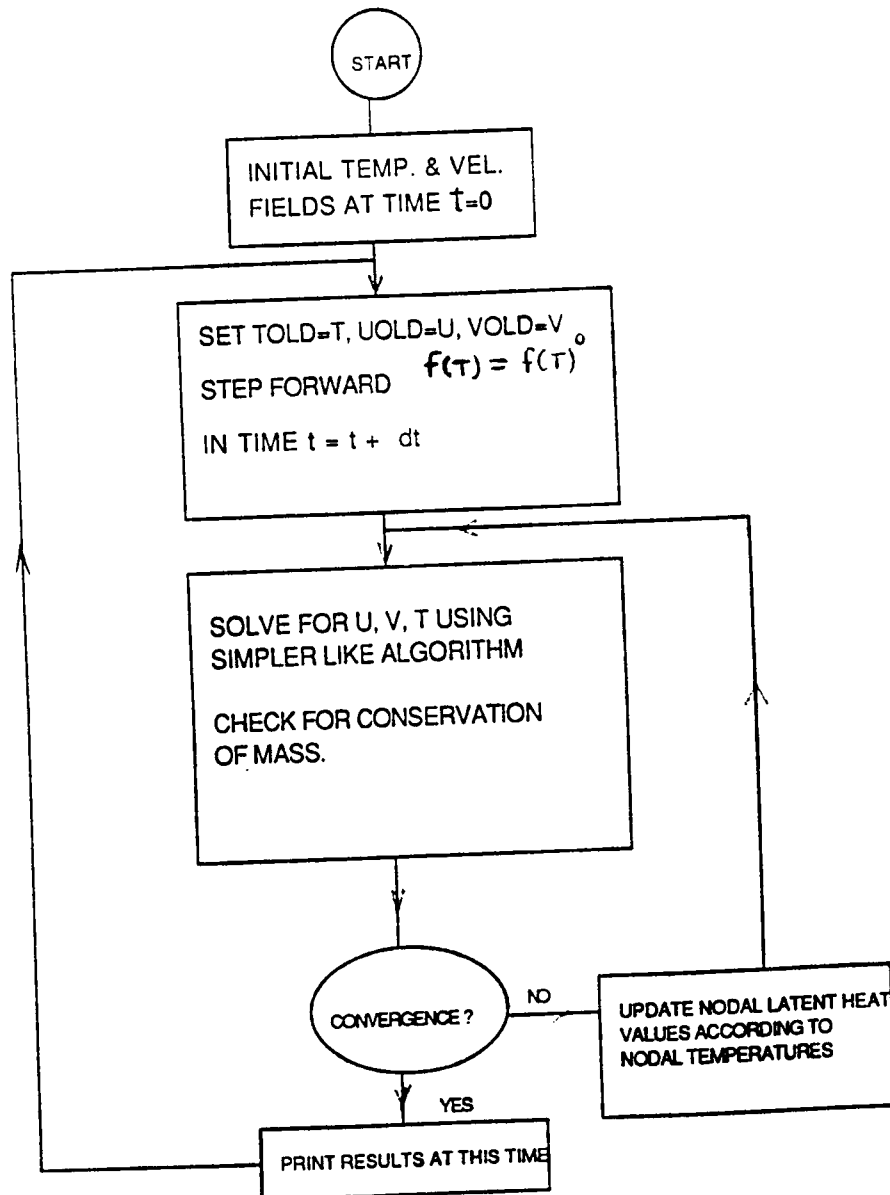


Figure 1 Flow chart of the numerical computation

CHAPTER 3

EXPERIMENTS

The purpose of conducting the experimental investigation was to validate the numerical scheme used and the computer code developed. The solidification experiments were conducted in a rectangular enclosure to simulate two-dimensional freezing. One wall of the experimental test cell is made out of two 1/4 " copper plates with internally milled passages which are joined together with screws. Cold water from the ice-water solution is circulated through the milled passages using a pump. This simulates a constant temperature cold wall. In this study the copper wall is maintained at a constant temperature of 3° C, which is 11° C below the freezing temperature of the working fluid Caprillic acid. In addition to the copper wall(cold wall) the enclosure is comprised of five walls made of 3/4" plexiglass(adiabatic walls) Figure 2-4 show the sketch of the enclosure designed and built for this study. Figure 5 shows the schematic of the experimental setup used. Plexiglass is used because of its low thermal conductivity and also to facilitate visualization of the freezing phase-front.

The experimental apparatus was 6.25" long, 5.75" high, and 4" wide making the aspect ratio (height/length)0.88. The observed results that will be discussed shortly confirmed that within the experimental uncertainty the solidification process remained two-dimensional. Caprillic acid was chosen as the working fluid in the experiments because it has a melting point of 14° C and a small volume change when solidified (3-4%). The main advantage of caprillic acid is that its melting point is only a few degrees below the ambient room conditions which provides convenience in the design of the experimental setup. The thermophysical properties of Caprillic acid are well established and can be found in chapter 4 and Reference 85.

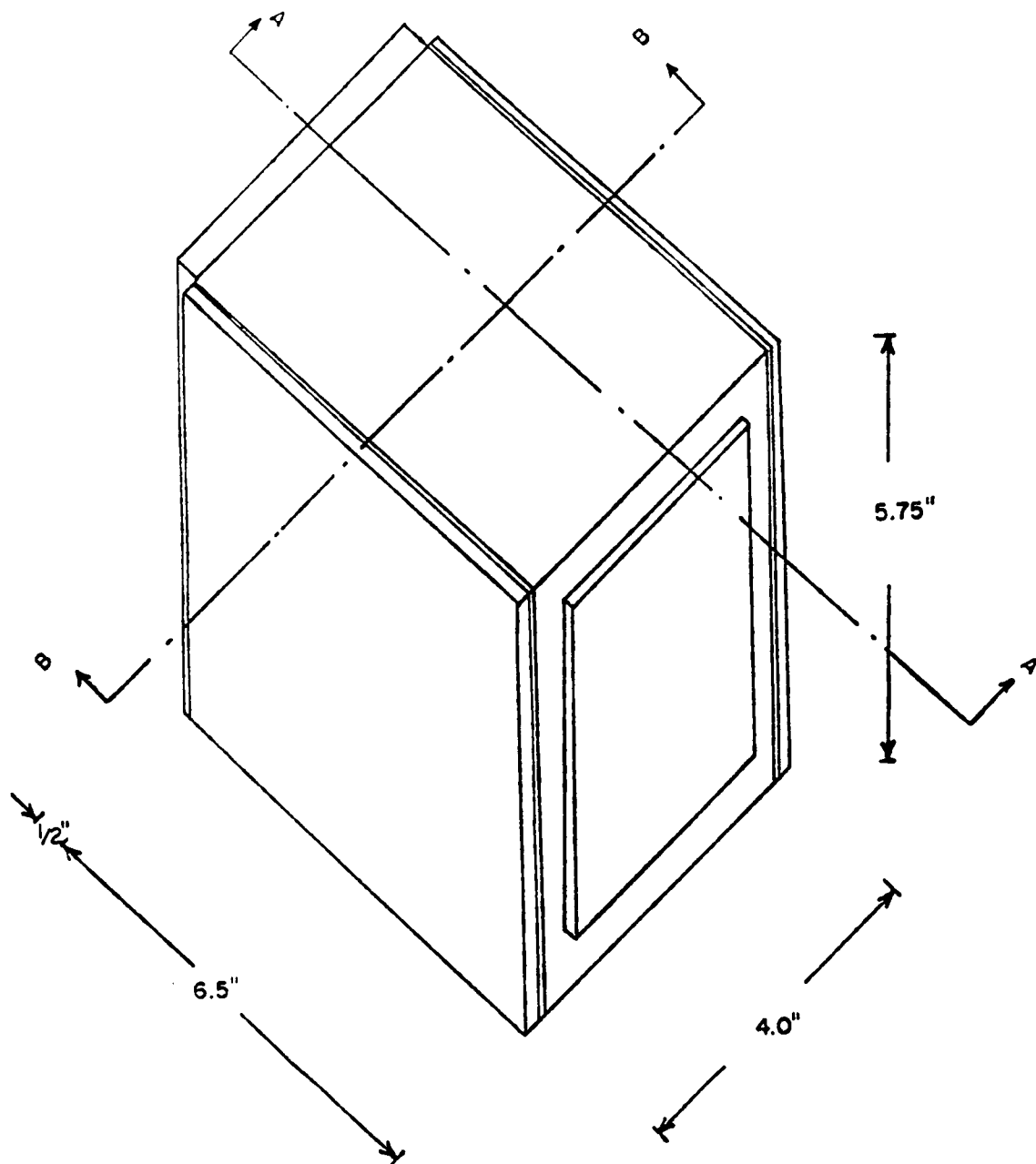


Figure 2 Isometric of the experimental apparatus

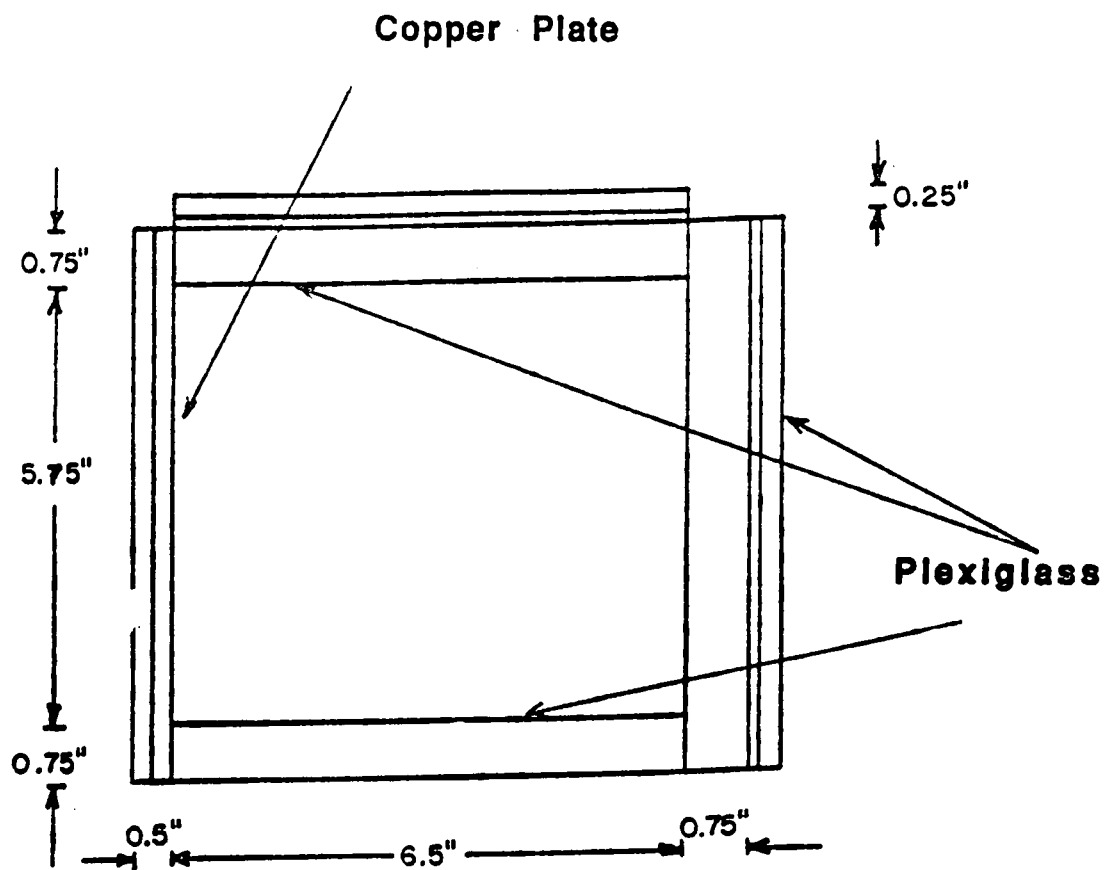


Figure 3 Section A-A of the experimental apparatus

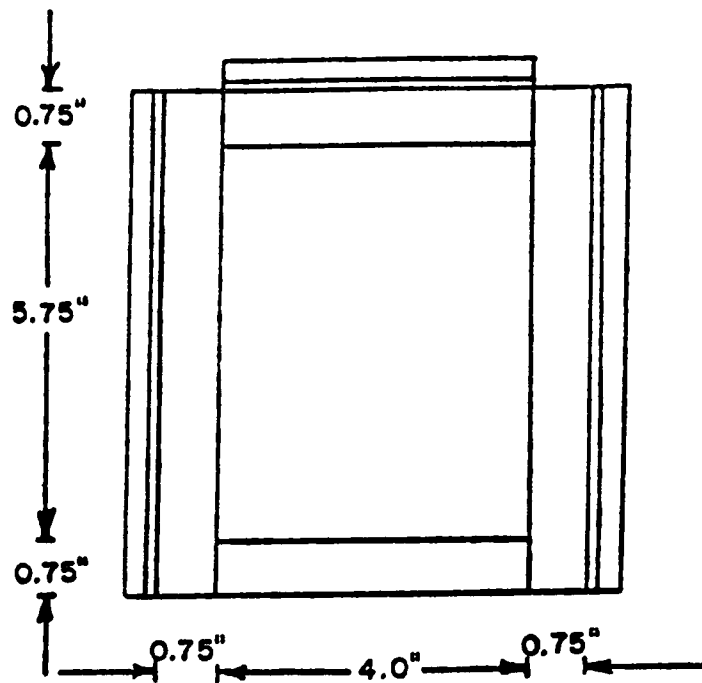


Figure 4 Section B-B of the experimental apparatus

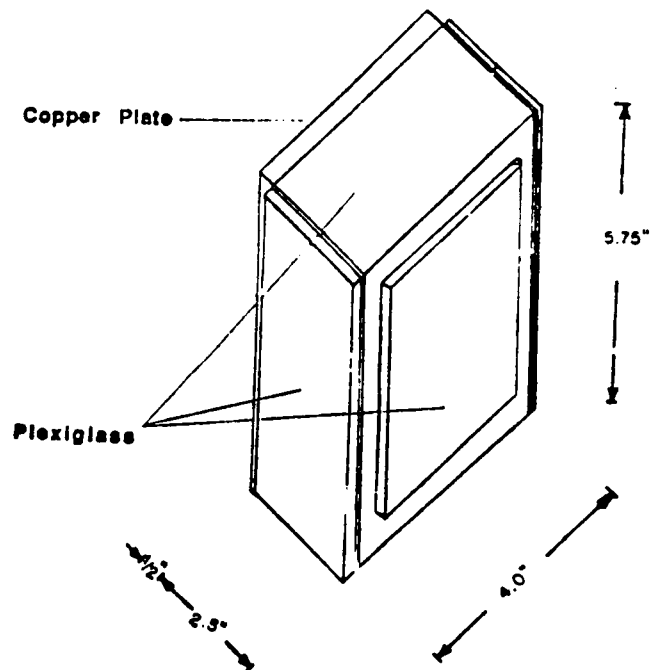
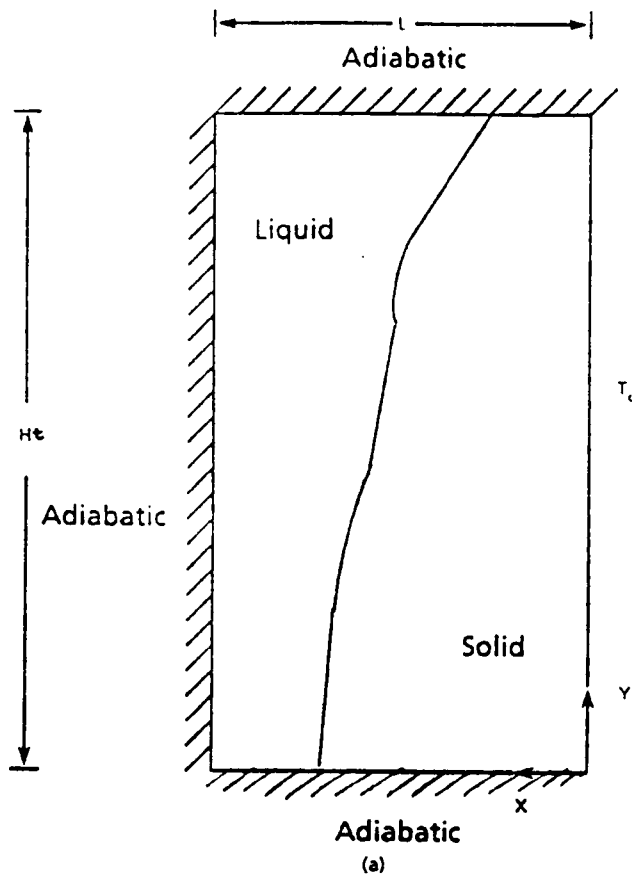


Figure 5 Coordinate system and boundary conditions and schematic of the experimental set-up

The phase-front is easily visualized through the plexiglass side walls and its advancement is directly measured (with an uncertainty of 1 mm) and at the same time photographed using an SLR camera. It was observed that, except in a region very close to the side walls (within 2% of the enclosure width), the remaining middle section of the enclosure show no three dimensional variations within experimental uncertainty (4%). These photographs are presented in Figure 6-7. The material used has a small impurity of 2%. However, no dendritic structure was observed and the phase-front remained sharp indicating that the phase change occurs at a fixed temperature within the experimental uncertainties.

It was felt that the length of the enclosure (6.25") was too long which resulted in very slow front advancement and a Rayleigh number too high for numerical computations. Therefore, the experimental enclosure was rebuilt with length of 2.5", height of 5.75", and width of 4", making the aspect ratio (height/length) 2.3. The experiments for phase-front location were run with this modified apparatus. The photographs of the front advancement are presented in Figure 8. The shape of the solid-liquid interface confirmed the excellent two-dimensionality of the experimental set up. Care was taken to avoid occurrence of air bubbles at the top of the enclosure.

Temperature measurement were carried out at two locations. One was at $x=0.4"$ and $y=3"$ and the other at $x=2"$ and $y=3"$. The latter location remained in the liquid state throughout the experimental run of 3.5 hours. The thermocouple used to measure the temperature was mounted on a 2mm diameter low thermal conductivity ceramic rod and was inserted in the experimental setup through a small aperture at the top of the enclosure.

Flow visualization was attempted using Aluminum powder. Aluminum powder when introduced into Caprillic acid rapidly settled to the bottom of the enclosure. Therefore it was discarded as the flow tracer. Next an attempt was made to make dyes with Caprillic acid as the base solvent. Methyl blue(blue), India ink (black), eosine

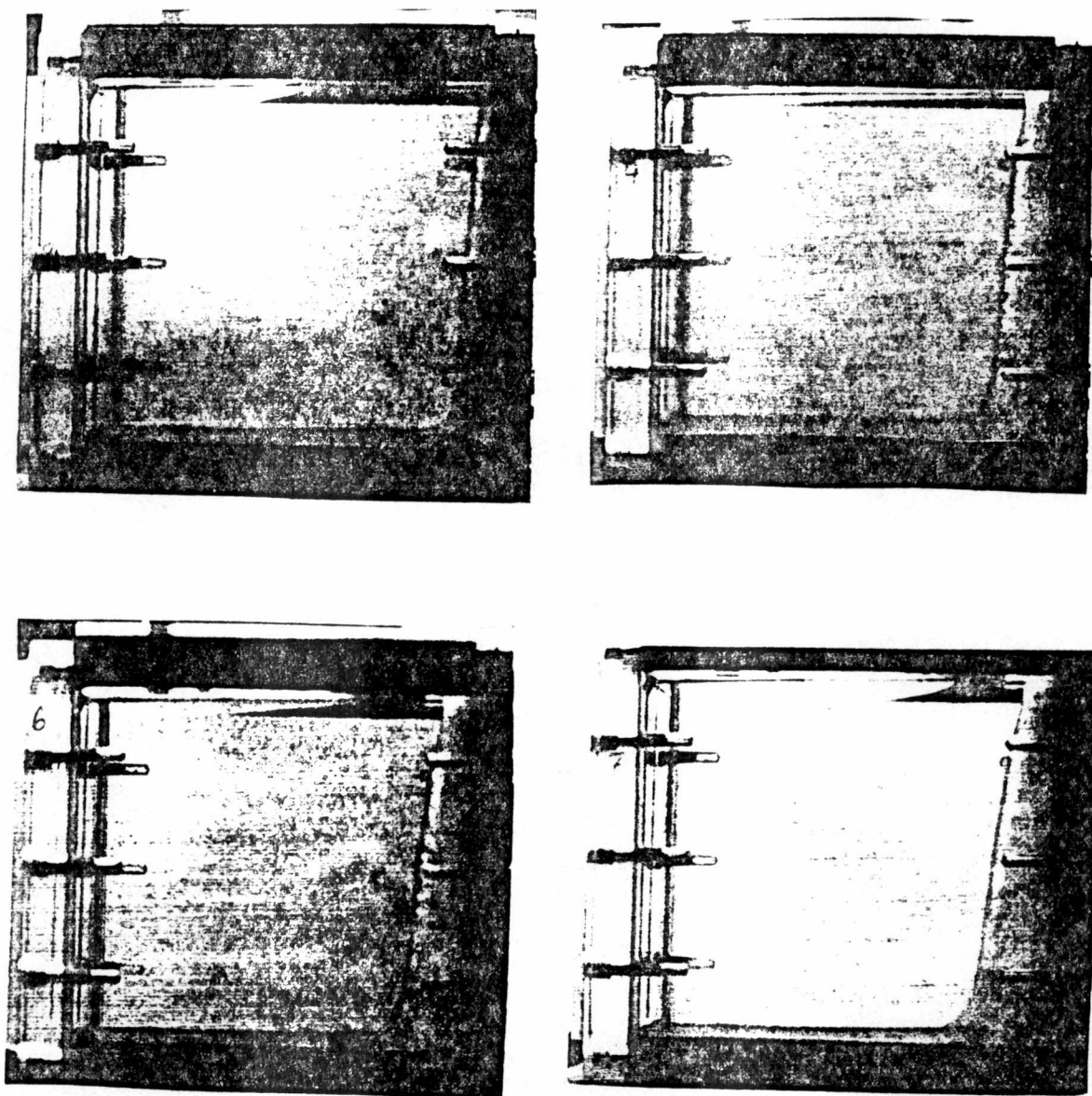


Figure 6 Solid-liquid interface location for the experimental set-up with $AR=0.88$ at a)2hr.b)4hr.c)6hr.d)7hr.

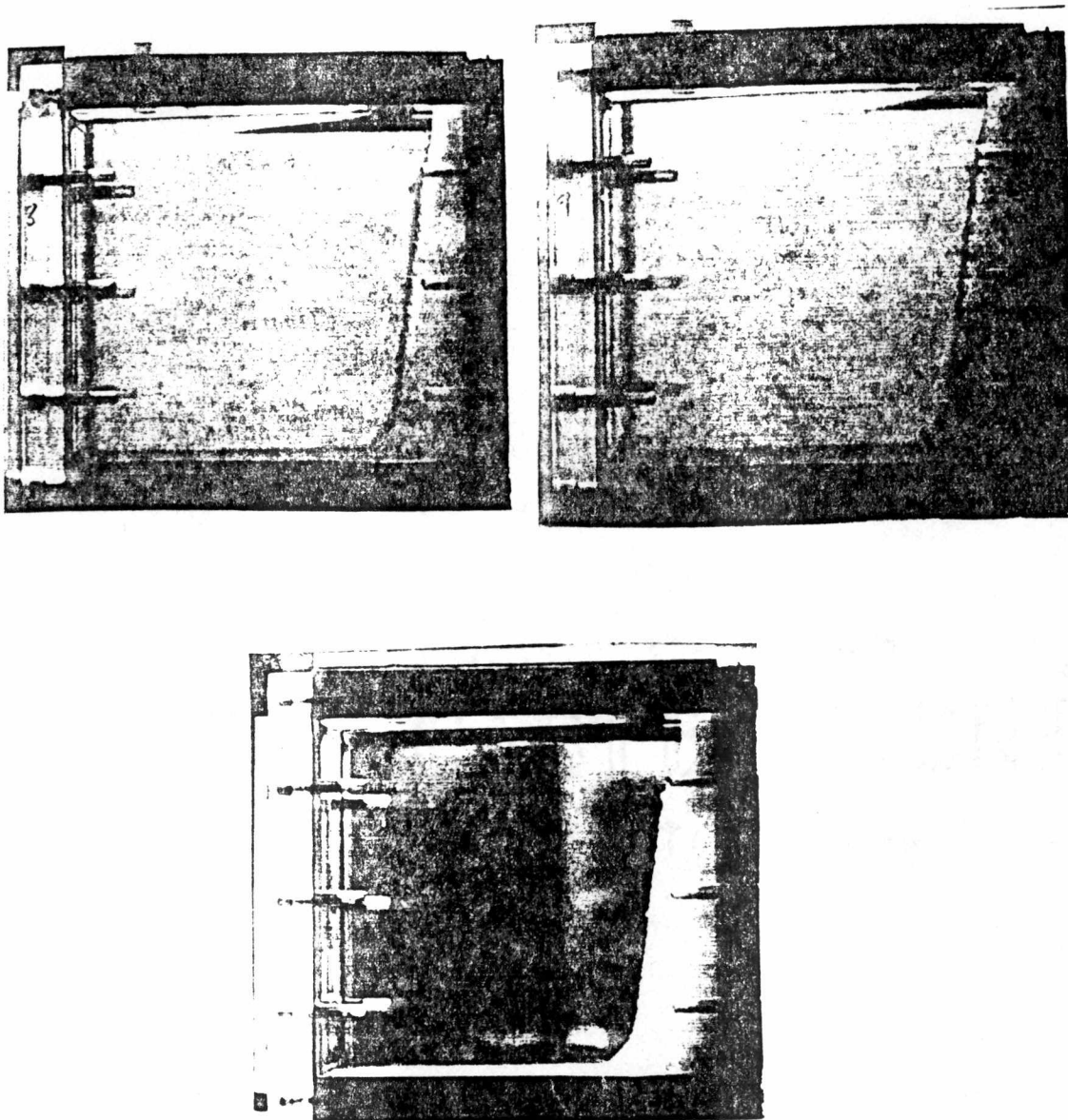
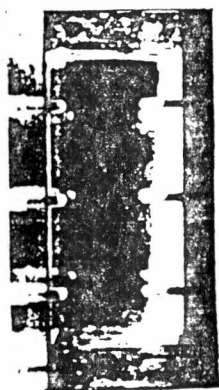
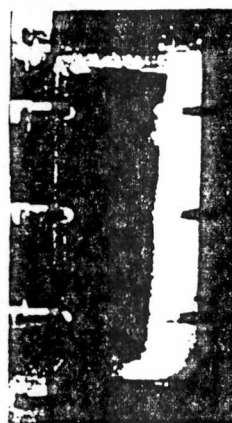


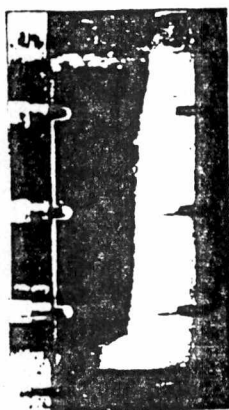
Figure 7 Solid-liquid interface location for the experimental set-up with $AR=0.88$ at a) 8hr. b) 9 hr. c) 11 hr.



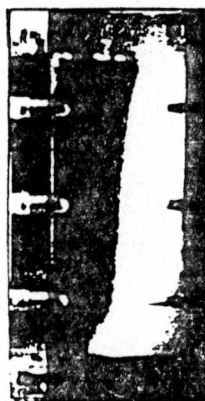
(a)



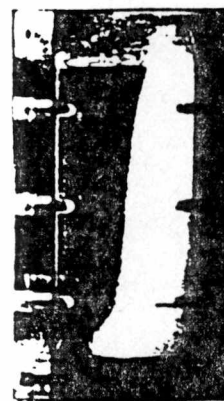
(b)



(c)



(d)



(e)

Figure 8 Solid-liquid interface location for the experimental set-up with $AR=2.3$ at a) 1hr. b) 2hr. c) 4hr. d) 6hr. e) 7 hr.

red (red) were tried. A few drops of these dyes were mixed with Caprillic acid in a plastic test tube which was put on a shaker to mix it thoroughly with Caprillic acid. This mixture was then mounted on a cetrifuge machine. India ink and eosine red proved inappropriate because it precipitated to the bottom of the test tube leaving Caprillic acid (colorless) on the top. Therefore India ink and eosine red were also rejected. Methyl blue did not precipitate to the bottom in the cetrifuge and it formed a dark blue dye in Caprillic acid. This dye was introduced into the experimental setup from the top of the enclosure. The dye traced the flow for a short time and then diffused with the working fluid. However, photographs of the flow field do not show the flow patterns very clearly.

CHAPTER 4

RESULTS AND DISCUSSION

Freezing Case

The numerical code developed in this study is compared with Caprillic acid solidification experiments conducted for this specific purpose and discussed in Chapter 3. Caprillic acid properties used in the model are: thermal conductivity 0.148 W/m-K, coefficient of thermal expansion 9.0×10^{-4} 1/K, density of 910 kg/m³, dynamic viscosity 5.74×10^{-3} kg/m-s, specific heat 2093 J/kg-K, latent heat 1.49×10^5 J/kg, and melt temperature of 287 K. The initial temperature was 295 K and the cold wall temperature was 276 K. The parameters for this experiment are $Ra^* = 5.17 \times 10^9$, $Ste = 0.187$, $Pr = 81.17$, $A = 2.3$. A numerical grid of 12 x 22 is employed. The high modified Rayleigh number required a time step of 10^{-4} to achieve convergence. A more refined grid would have required at least an order of magnitude smaller time step and therefore was tried but not used for the computational run.

For the melting experiments there is a characteristic temperature difference which can be used for normalizing the temperature field. For these solidification experiments (one cold wall and all other walls insulated) there is no characteristic temperature difference driving the natural convection flow, and therefore, a ratio of latent heat to specific heat (as described in Equation 1) is used. The phase-front location computed numerically and measured experimentally is shown in Figure 9. Both the observed and computed phase-fronts are tilted providing conclusive evidence of the effect of natural convection on this heat transfer process. The fluid in the vicinity of the vertical insulated wall, opposite the cold wall, rises and its temperature increases. When the liquid reaches the top of the enclosure it turns 90° and flows toward the solid-liquid interface, impinging onto the solid-liquid interface.

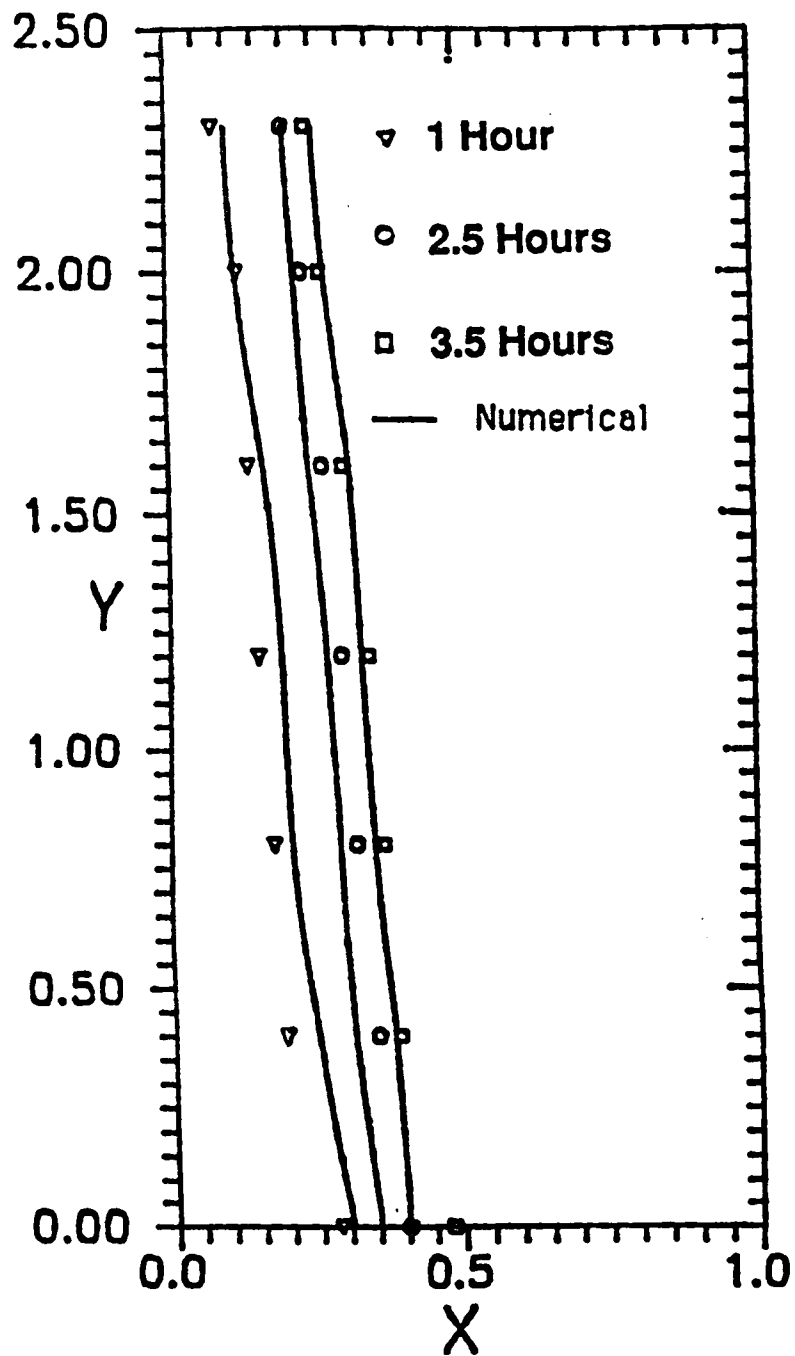


Figure 9 Comparison of numerical and experimental solidification fronts of Caprillic acid. ($T_w=3^{\circ}\text{C}$, $Ra^*=5.17 \times 10^9$)

The flow is again deflected and it descends down the phase-front and its temperature decreases. The local solidification rate is the lowest at the top of the enclosure due to higher temperature of the liquid there. The liquid descending down the interface again turns at the bottom of the enclosure and flows back up the insulated wall facing the cold wall. As the driving potential for the flow decreases with time, the problem becomes one of decaying convection and the velocities in the liquid region decrease with time.

The numerical solution and experimental results are in good agreement. There is a discrepancy between the solutions near the bottom of the enclosure. Specifically the experiments show a "toe" at the bottom of the phase-front profile. This may be due to the insignificant but present heat loss through the bottom wall which is ignored in the numerical model. In addition, conduction along the walls (ignored in the numerical model) may, when coupled with the direction of the convection cell in the melt, be responsible for the observed toe near the bottom wall. Figure 10 shows numerical and experimental comparison of temperature solutions at two locations. One of these points goes through the change of phase while the other stays in the liquid region for the duration of this particular experimental run of 3.5 hours. The experimental and numerical solutions agree well at later times. At earlier times the numerical solution appears to predict a weaker natural convection than shown by the experimental data. This is believed to cause the discrepancy in the experimental and the numerical temperature results at smaller times. The CPU time for the longest solidification run was 2.05 hours(on a VAX-8800).

Melting Case

The numerical code developed is run to generate results for the interface locations for melting of pure(99.99%) metal tin in a rectangular enclosure and the results are compared with the experimental data of Wolff and Viskanta [82]. The thermophysical properties of pure tin (99.99%) are: density of $6.98 \times 10^3 \text{ Kg/m}^3$, specific heat $2.57 \times 10^2 \text{ J/ Kg K}$, thermal conductivity 32.2 W/ m K ,

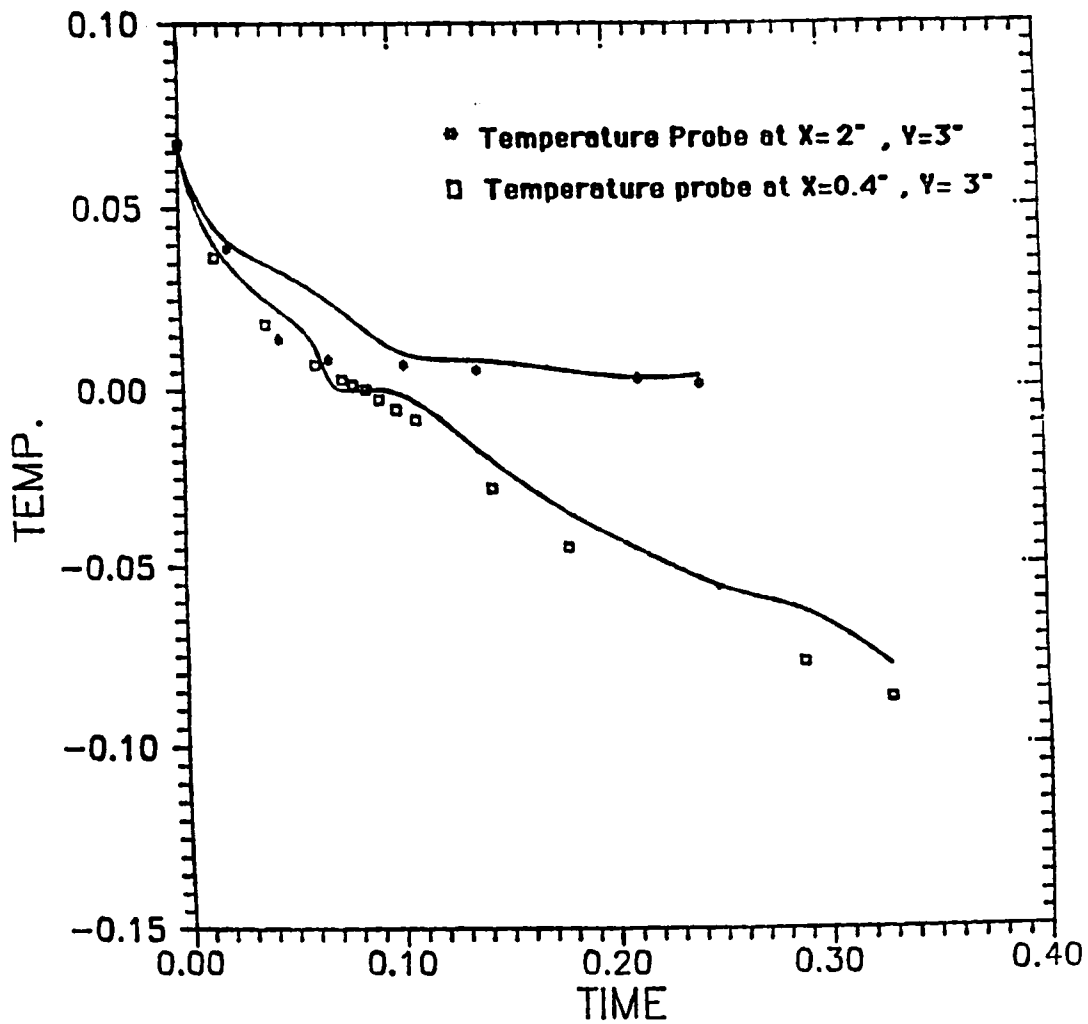


Figure10 Numerical and experimental temperature results for solidification of Caprillic acid. ($T_w = 3^\circ \text{C}$, $Ra^* = 5.17 \times 10^9$)

kinematic viscosity $2.81 \times 10^{-7} \text{ m}^2/\text{s}$, latent heat of fusion $60.6 \times 10^3 \text{ J/Kg}$, coefficient of thermal expansion $1.06 \times 10^{-4} \text{ 1/K}$, the melt temperature of 231.9°C . The initial temperature of tin was 2°C below the melt temperature. The parameters for this run are Rayleigh number = 2.91×10^5 , Stefan number = 8.48×10^{-3} , Prandtl number = .0089, and aspect ratio = 0.75. The numerical solution was continued up to a real time of 2.089 hours ($Fo = 16.75$). The numerical results are compared with the experimental data for 0.579, 1.012, and 2.079 hours. As discussed in Chapter 2 , to save computational costs without sacrificing accuracy, a 15×15 grid was used to run this melting case on a Vax 8800 computer. The CPU time for this run, with a time step of 10^{-3} , was 15 minutes.

The numerical and experimental results for front locations in melting experiments is shown in Figure 11. The solid lines represent the numerical solution from Reference 82. The numerical results of the present study compare better than that of Reference 78 with the experimental data at large times (e.g., 2.079 hours). At 0.579 and 1.012 hours the numerical solution overpredicts the experimental observations. The discrepancy at 0.579 hours is 10% at $Y = .75$ and 12% at $Y = 0$ for the present study while it is about 8.6 % at $Y = 0.75$ and 22 % at $Y = 0$ for the numerical study of wolff and Viskanta [82]. The numerical result of Reference 78 compare better than the present study at shorter times (e.g., 1.012 hours) in the middle and at the top of the enclosure while a large (20%) discrepancy is observed for both numerical solutions at the bottom ($Y = 0$) of the enclosure. The present computed solution compares well with the experimental data at 2.079 hours although a difference of 12 % is observed near the bottom of the enclosure. The discrepancy between the numerical and experimental data at earlier times may be explained by the thermal inertia of the experimental system [82]. Wolff and Viskanta have used a method described by Webb and Viskanta [83] to generate the numerical solution. The method employs a front tracking scheme with temperature as the independent variable. This method suffers all the inherent limitations of the front tracking schemes discussed in Chapter 1, such as a solution in ever changing domain in space and time, and satisfying the Stefan condition at each time step. The use of enthalpy

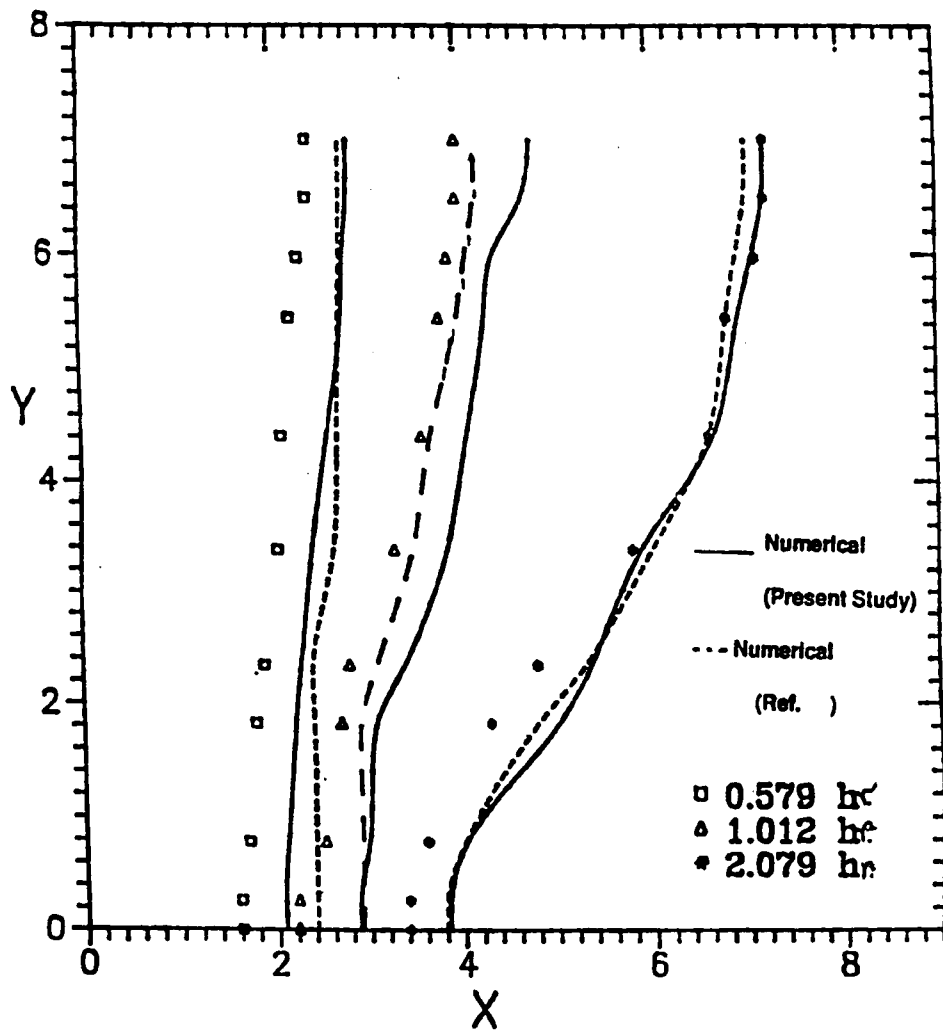


Figure 11 Comparison of numerical and experimental interface locations for melting of tin at 0.579 hr., 1.012 hr., 2.079 hr.
 ($T_w = 233.9^\circ\text{C}$, $\Delta T = 2^\circ\text{C}$, $Ra = 2.91 \times 10^5$)

method in the present study eliminates the need to track the phase-front which is recovered from the nodal latent heat value.

Numerical and experimental results for temperature at a real time of 2.079 hours in the melting experiment is shown in Figure 12 for $Y/Ht = 0.9$ and $Y/Ht = 0.1$. The solid line represents the numerical solution of the present study while the dashed lines represent the numerical solution of Reference 82. The computed solutions at the top of the enclosure ($Y/Ht = 0.9$) shows a large discrepancy with the experimental data. The experimental and numerical solutions, however, are in better agreement near the bottom of the enclosure ($Y/Ht = 0.1$).

Convection is pronounced in the positive X direction at the top of the enclosure for the melting problem and it transports the thermal energy up to the melt front where the non-dimensional temperature is 0. This results in high temperature gradients in the vicinity of the melt-front which is confirmed by the experimental data. The numerical model used in this study seems to overpredict this behavior.

The comparison of the numerical and experimental solution adds confidence to the formulation used in this numerical model and the computer code developed. The numerical code was run to investigate the influence of parameters such as Rayleigh and Prandtl numbers, cold wall temperature, initial superheat, and aspect ratio on the nature and position of the phase-front and the volume fraction solidified (extent of solidification).

Parametric Studies

Figures 13-20 show isotherms and streamlines exhibiting flow patterns for Prandtl numbers of .01, 10, and 100 and Rayleigh numbers of 10^4 , 10^5 , 10^6 . All the computational runs are conducted with a 20×20 grid unless specified otherwise. It can be seen from these results that the maximum value of the stream function ϕ decreases with time depicting a decaying convective flow pattern. For example ϕ_{max}

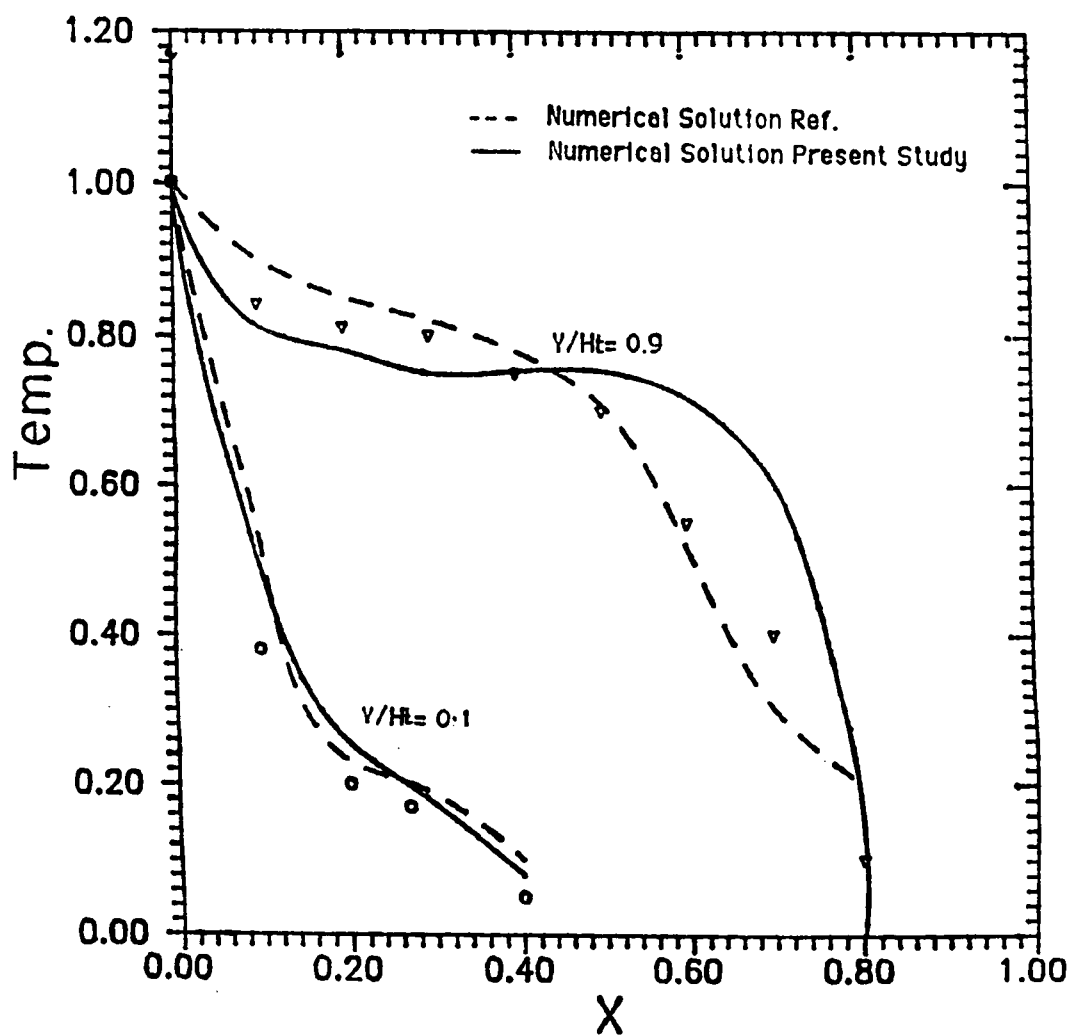


Figure12 Comparison of numerical and experimental temperature measurement for melting of pure tin
 ($T_w = 233.9^{\circ}\text{C}$, $\Delta T = 2^{\circ}\text{C}$, $t = 2.079\text{ hr.}$)

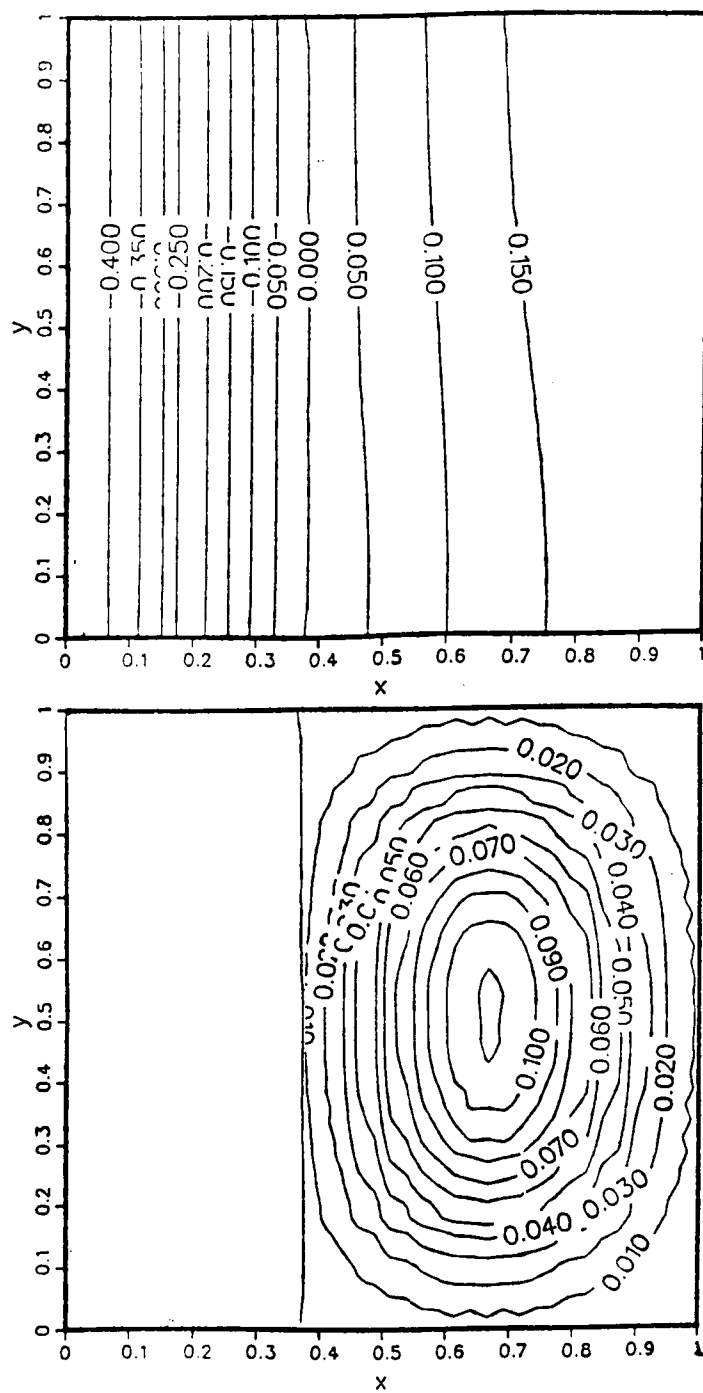


Figure13 Isotherms and streamlines ($Pr=10$, $Ra^*=10^4$, $T_c = -0.5$, $T_i = 0.5$, $Fo=0.3$, $AR=1.0$)

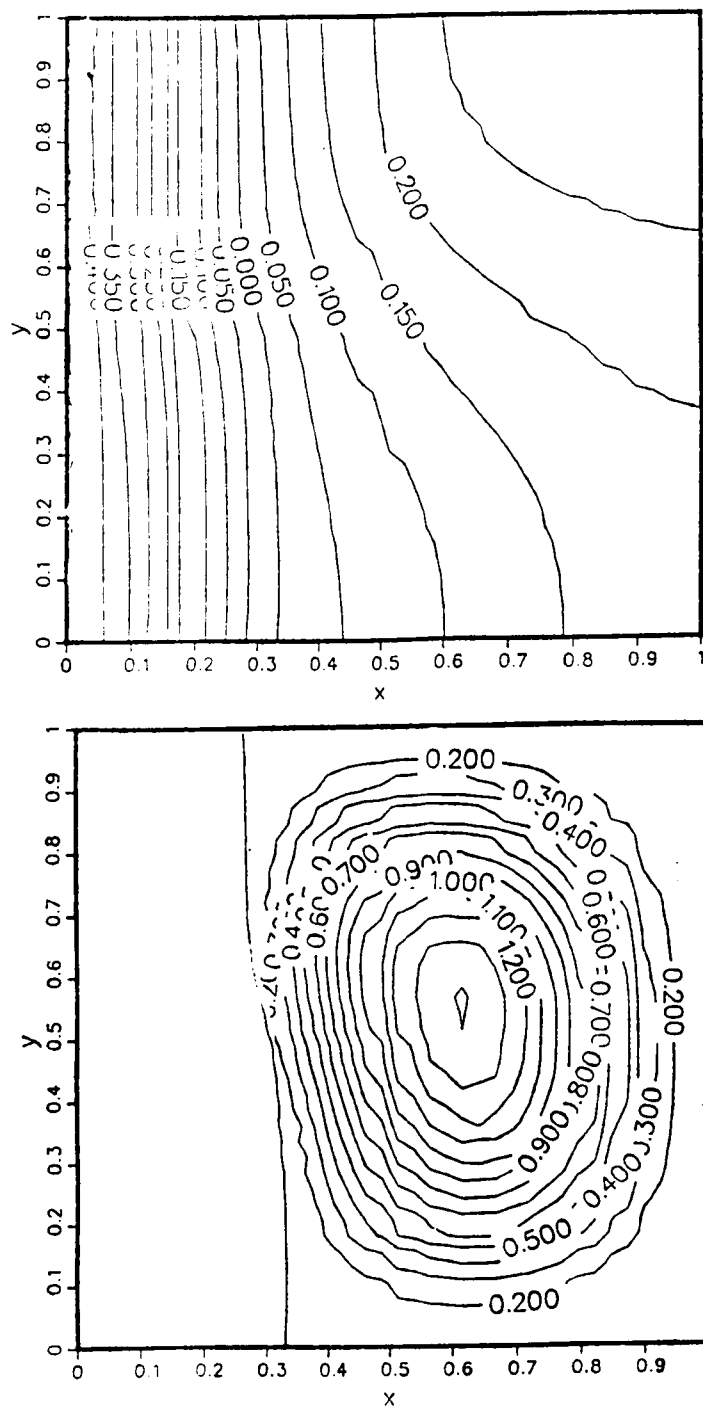


Figure14 Isotherms and streamlines ($Pr=10$, $Ra^*=10^5$, $T_c = -0.5$,
 $T_i = 0.5$, $Fo=0.2$, $AR= 1.0$)

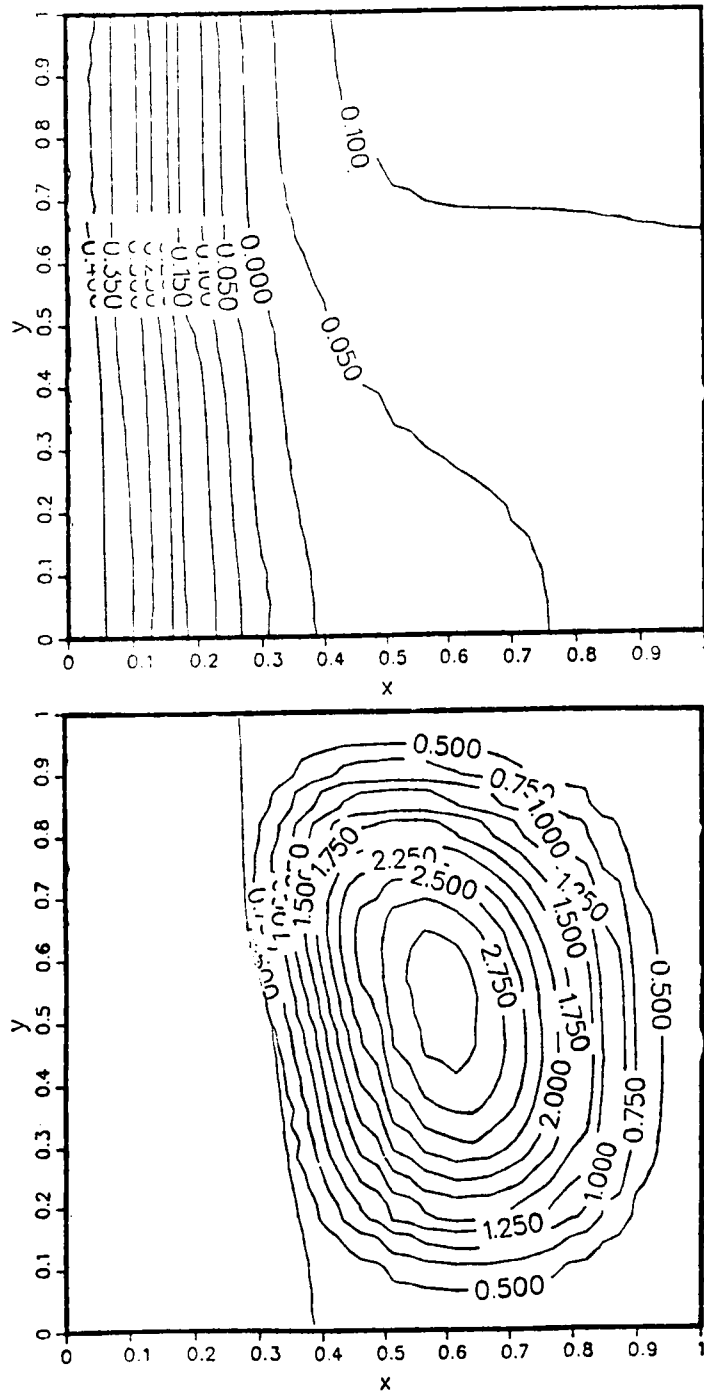


Figure15 Isotherms and streamlines ($Pr=10$, $Ra^*=10^6$, $T_c = -0.5$, $T_i=0.5$, $Fo=0.2$, $AR=1.0$)

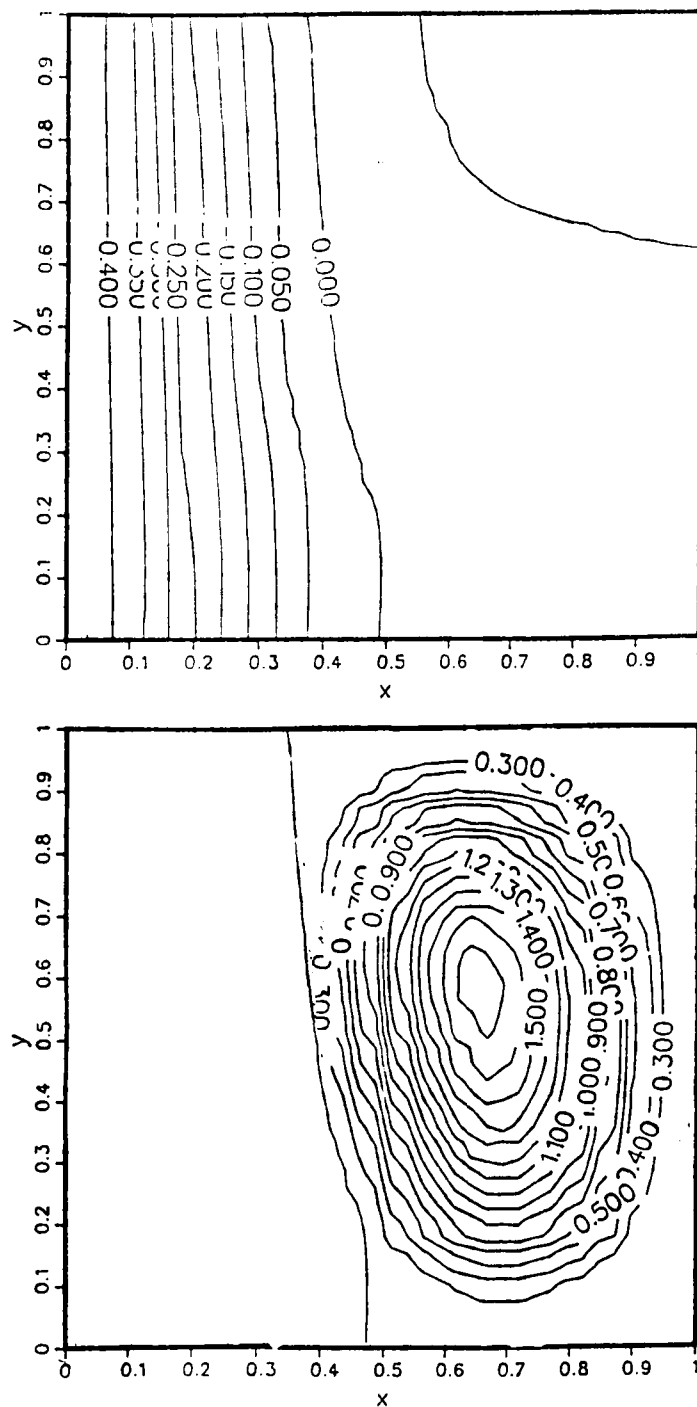


Figure16 Isotherms and streamlines ($Pr=10$, $Ra^*=10^6$, $T_c=-0.5$, $T_i=0.5$, $Fo=0.3$, $AR=1.0$)

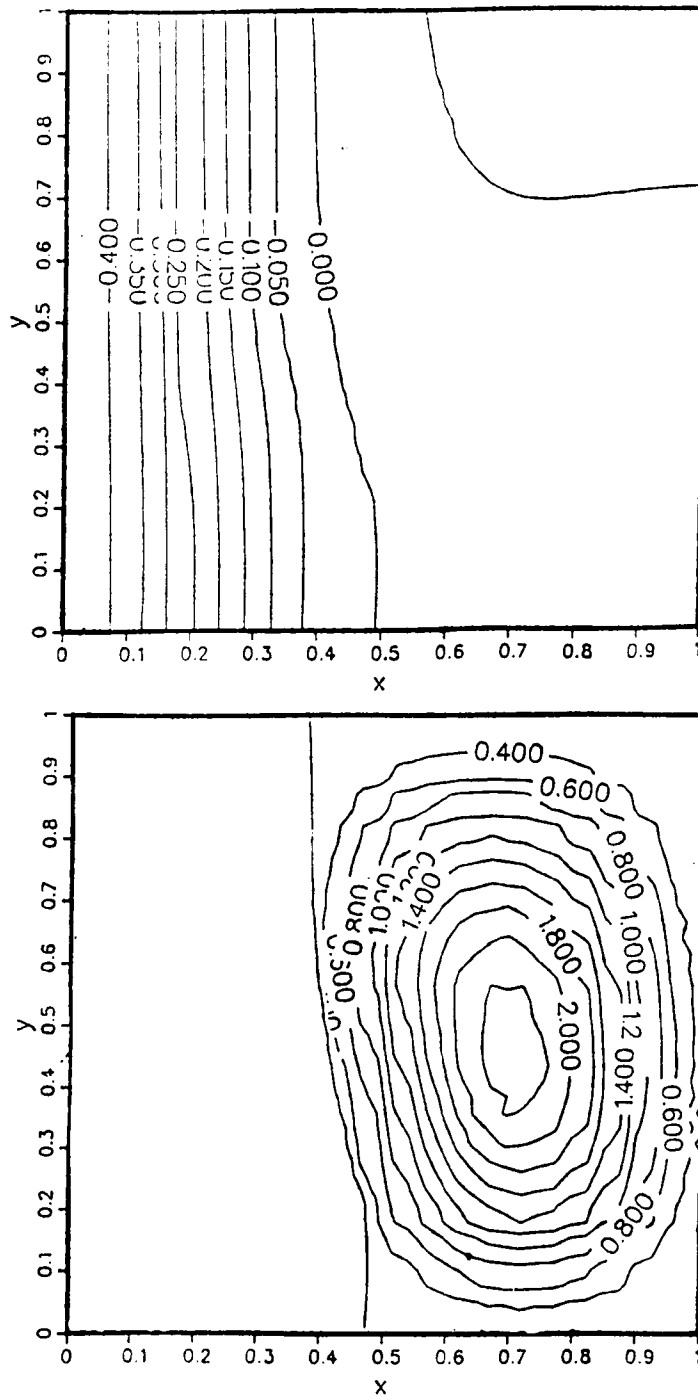


Figure17 Isotherms and streamlines ($Pr=0.01$, $Ra^*=10^4$, $T_c=-0.5$, $T_i=0.5$, $Fo=0.3$, $AR=1.0$)

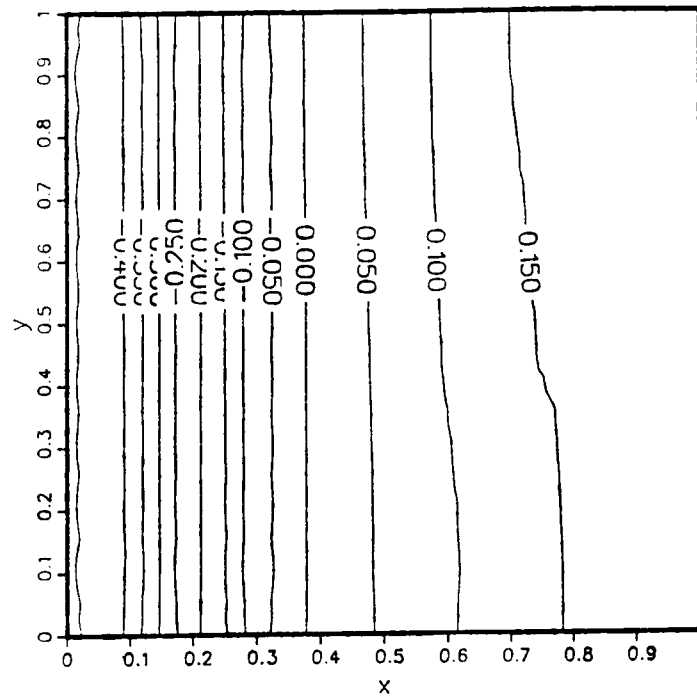


Figure 18 Isotherms ($Pr=100$, $Ra^*=10^5$, $T_c=-0.5$, $T_i=0.5$, $Fo=0.3$, $AR=1.0$)

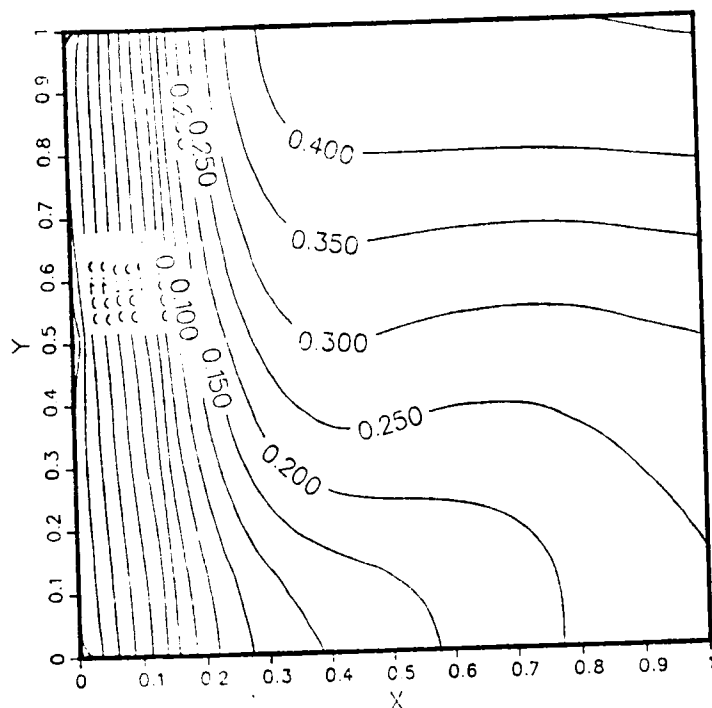


Figure19. Isotherms ($Pr=1, Ra^*=10^5, T_c=-.5, T_i=.5, Fo=.0624,$
 $AR=1$, grid size 40×40)

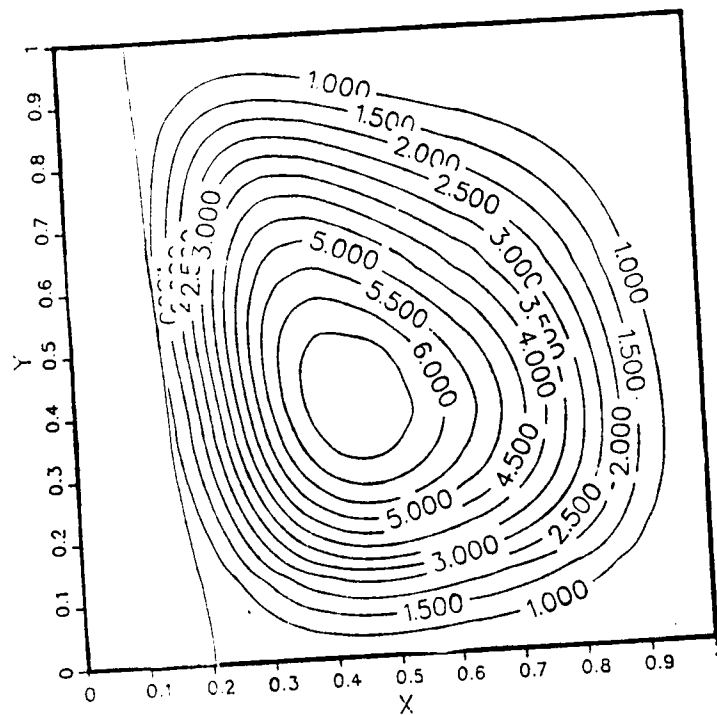


Figure 20. Streamlines ($Pr=1$, $Ra^*=10^5$, $T_c=-.5$, $T_i=.5$, $Fo=.0624$, $AR=1$, grid 40×40)

is 5.0 at $Fo=0.1$ and it is 2.2 at $Fo=0.3$ for $Pr=.01$, $Ra^*=10^4$, $T_i=0.5$, and $T_c=-0.5$. The ϕ_{max} value also decreases with the increasing Prandtl number, all other parameters being the same. For example at $Ra^*=10^4$, $T_c=-0.5$, $T_i=0.5$, for $Pr=10$. $\phi_{max}=.375$ at $Fo=0.1$ and it is equal to 0.11 at $Fo=0.3$, while $\phi_{max}=5.0$ at $Fo=0.1$ and $\phi_{max}=2.2$ at $Fo=0.3$ for $Pr=0.01$.

For a given Prandtl number the value of stream function increases with the increasing Rayleigh number. The CPU time increases with decreasing Prandtl number, all other parameters being the same. For example at $Ra^*=10^5$ for $Pr=10$, CPU is 1.26:96 minutes whereas for $Pr=.01$ it is 1.59 minutes. The CPU time also increases with the Rayleigh number all other parameters being the same(including the time step). For example at $Pr=10$, for $Ra^*=10^4$, CPU is 52.06 seconds, for $Ra^*=10^5$ CPU is 1.25:05 minutes, and for $Ra^*=10^6$ CPU time is 2.38:76 minutes. Some researchers [50,83] who have used temperature as a dependent variable in a front tracking scheme, with a streamfunction formulation for the flow, have observed recirculating flow patterns at the four corners in the melt region. In this study, with primitive variables for the flow and the enthalpy formulation for the phase change, no such cells were observed.

Figure 21 shows isotherms for $Pr=.01$, 10, and 100 when $Ra^*=10^4$. The phase-front for $Pr=10$ and 100 with $Ra^*=10^4$ is flat and the isotherms approach those of a conduction dominated heat transfer process. However for the case of $Pr=.01$ and $Ra^*=10^4$, the phase-front is tilted(more solidified at the bottom than at the top of the enclosure) and the isotherms in the liquid region suggest a strong flow dominated heat transfer. Further it was found that for Prandtl numbers of 10 and 100, the total solidification times are within 1% of each other for modified Rayleigh numbers of 10^4 and 10^5 . Recall that the modified Rayleigh number (Ra^*) is the product of Prandtl number and modified Grashoff number (Gr^*). Figure 22 shows isotherms for $Pr=.01$ and $Ra^*=10^3$. It can be seen that the isotherms indicate that convection is important. Figure 23 shows isotherms for $Pr=.001$ and

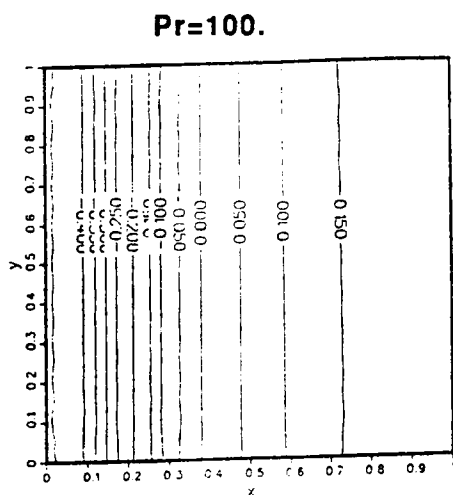
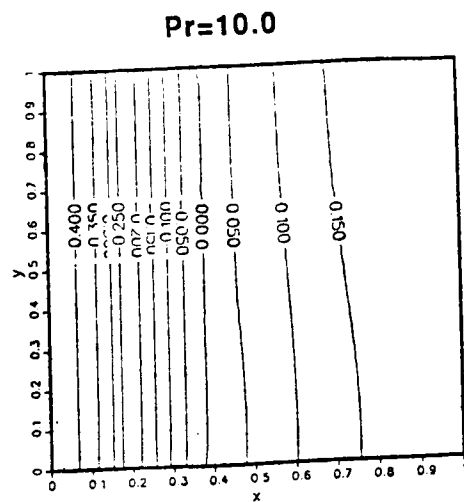
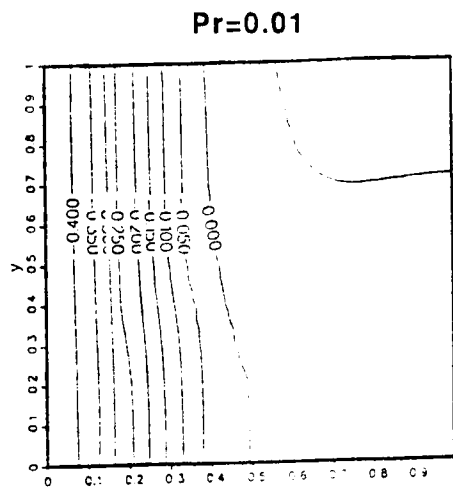


Figure 21 Effect of Prandtl number, Isotherms ($Pr=0.01, 10, 100$, $Ra^*=10^4$, $Fo=0.3$, $T_c=-0.5$, $T_i=0.5$, $AR=1.0$)

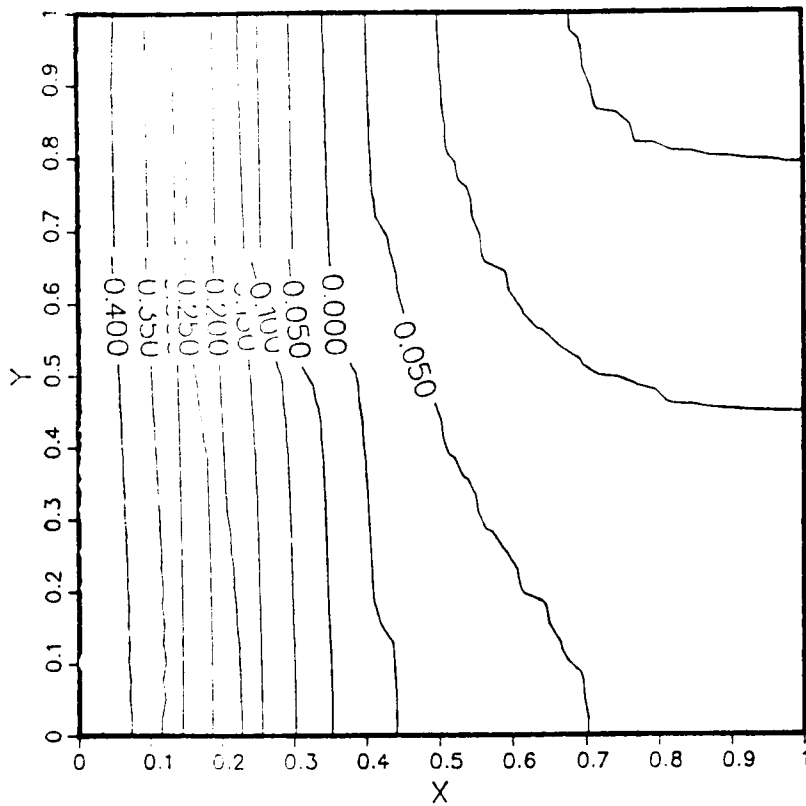


Figure22 Isotherms ($Pr=.01$, $Ra^*=10^3$, $Fo=0.2$, $T_c=-.5$, $T_i=0.5$, $AR=1$)

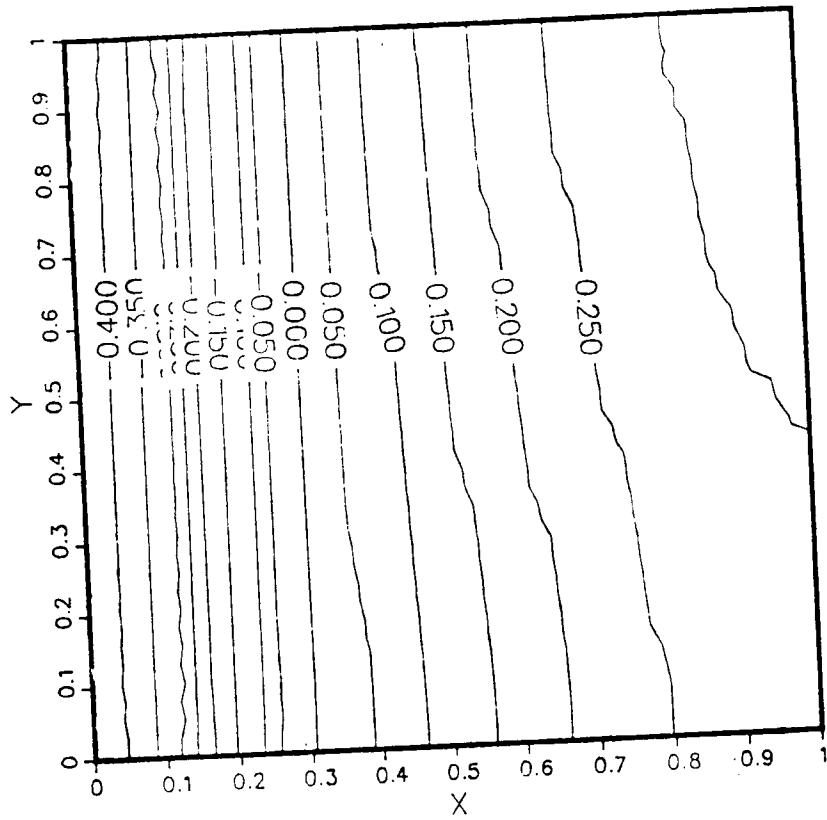


Figure23 Isotherms ($Pr=.001$, $Ra^*=10^2$, $Fo=0.2$, $T_c=-.5$, $T_i=0.5$, $AR=1$)

$Ra^* = 10^2$, $Gr^* = 10^5$. It can be observed that the process is conduction dominated. It was observed that for $Ra^* \geq 10^3$, the modified Grashoff number is the parameter that determines whether convection is important mode of heat transfer. For $Gr^* \geq 10^4$ convection plays an important role in the solidification process. For $Ra^* < 10^3$ solidification process is conduction dominated, irrespective of Gr^* or Pr . Figure 24 shows the effect of initial superheat on the extent of solidification for cold wall temperature $T_c = -1.0$, $Pr = 100$, $Ra^* = 10^6$, and $AR = 1.0$. The time for complete solidification is presented in Table 2. Figure 25 depicts the effect of cold wall temperature on the extent of solidification. The cases presented are for $Pr = 0.01$ and 100 , and $T_i = 0.6$, $Ra^* = 10^6$, and $AR = 1.0$. The cold wall temperatures considered are -1.0 , -0.8 , and -0.5 . It can be observed that as the initial superheat increases the extent of solidification decreases and the time for complete solidification increases. The extent of solidification increases as the cold wall temperature is decreased. In both cases the solidification is more rapid in the beginning as is evident by the slope of the volume fraction curves. It can be seen that at $Pr = 100$, the volume fraction (extent of solidification) curves have a higher slope at earlier times and there is a large reduction in slope at about $Fo = 0.17$, whereas at $Pr = 0.01$, the change in slope is gradual over the entire duration of solidification. At earlier times convection brings in liquid at higher temperature to the front and therefore inhibits solidification. At later times convection helps solidification while conduction offers progressively higher resistance. $Pr = 100$ and 0.01 result in $Gr^* = 10^4$ and 10^8 , respectively. In the former case convection is much weaker relative to the later case. Therefore, for $Pr = 100$, the weaker convection results in distinctly lower slope of volume fraction curves at later times.

Figures 26-27 illustrate the effect of Rayleigh number on the solidified fraction and total solidification time for $Pr = 0.01$ and 10 , $T_c = -0.5$, $T_i = 0.5$, and $AR = 1$. Rayleigh numbers considered are 10^4 , 10^5 , and 10^6 . The times required for complete solidification are presented in Table 2 (Page 53). Figure 26 shows that for $Pr = 10$, the total solidification time is less at $Ra^* = 10^6$, than for $Ra^* = 10^4$ or 10^5 . Initially

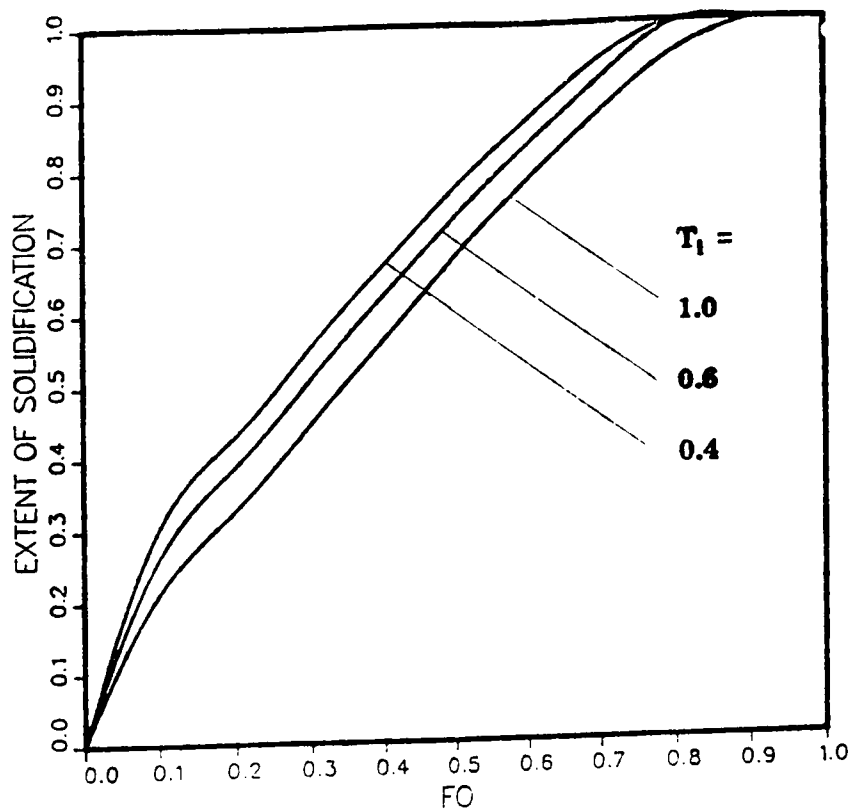


Figure 24 Effect of initial superheat on the volume fraction solidified.
 ($Pr=100, Ra^*=10^6, T_C = -1.0, Ar=1.0$) $T_i = 0.4, 0.6, 1.0$.

Table 2

Effect of various parameters on times for complete solidification for enclosures with
AR=1.0

Fo_{cs}	Pr	Ra^*	T_c	T_i
1.390	0.01	10^4	-0.5	0.5
1.350	0.01	10^5	-0.5	0.5
1.160	0.01	10^5	-0.6	2.0
0.485	0.01	10^5	-2.0	1.0
0.405	0.01	10^5	-2.0	0.1
0.7270	0.01	10^6	-1.0	1.0
0.7156	0.01	10^6	-1.0	0.6
0.8490	0.01	10^6	-0.8	0.6
1.2630	0.01	10^6	-0.5	0.6
1.2440	0.01	10^6	-0.5	0.5
1.430	10.0	10^4	-0.5	0.5
1.420	10.0	10^5	-0.5	0.5
0.329	10.0	10^5	-4.0	0.8
0.282	10.0	10^5	-4.0	0.3
0.350	10.0	10^5	-3.0	0.4
1.313	10.0	10^6	-0.5	0.5
1.430	100.0	10^4	-0.5	0.5
1.420	100.0	10^5	-0.5	0.5
1.374	100.0	10^6	-0.5	0.5
0.8150	100.0	10^6	-1.0	0.6
0.870	100.0	10^6	-1.0	1.0
0.772	100.0	10^6	-1.0	0.4
0.9669	100.0	10^6	-0.8	0.6
1.398	100.0	10^6	-0.5	0.6

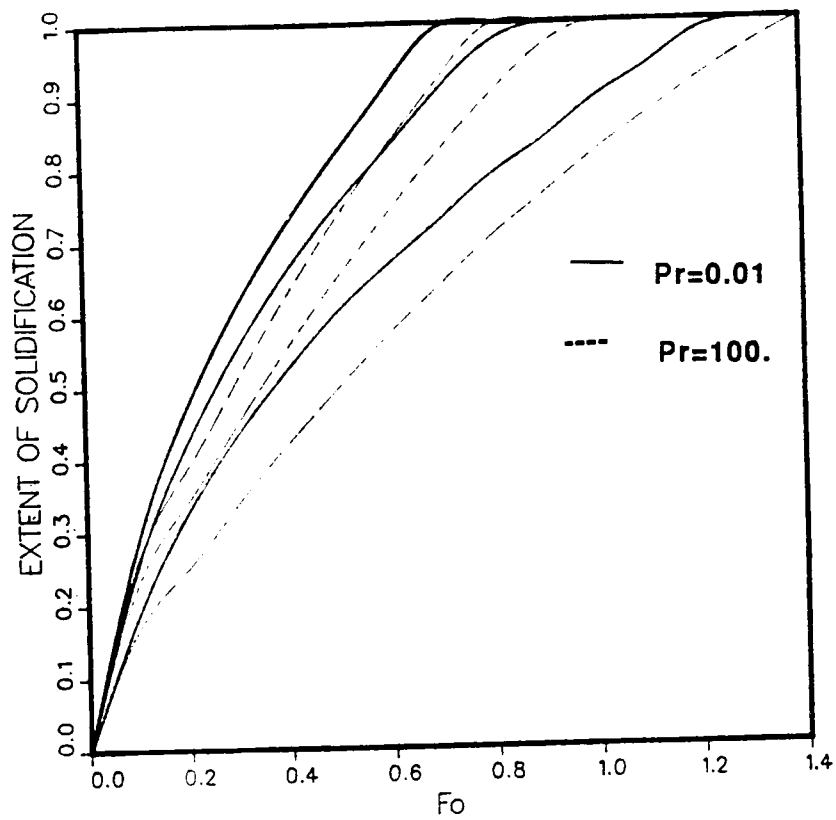


Figure25 Effect of cold wall temperature on the volume fraction solidified.
 ($Pr=.01$ and 100 , $Ra^*=10^6$, $T_i=0.6$, $AR=1.0$)
 $T_c = -0.5, -0.8, -1.0$.

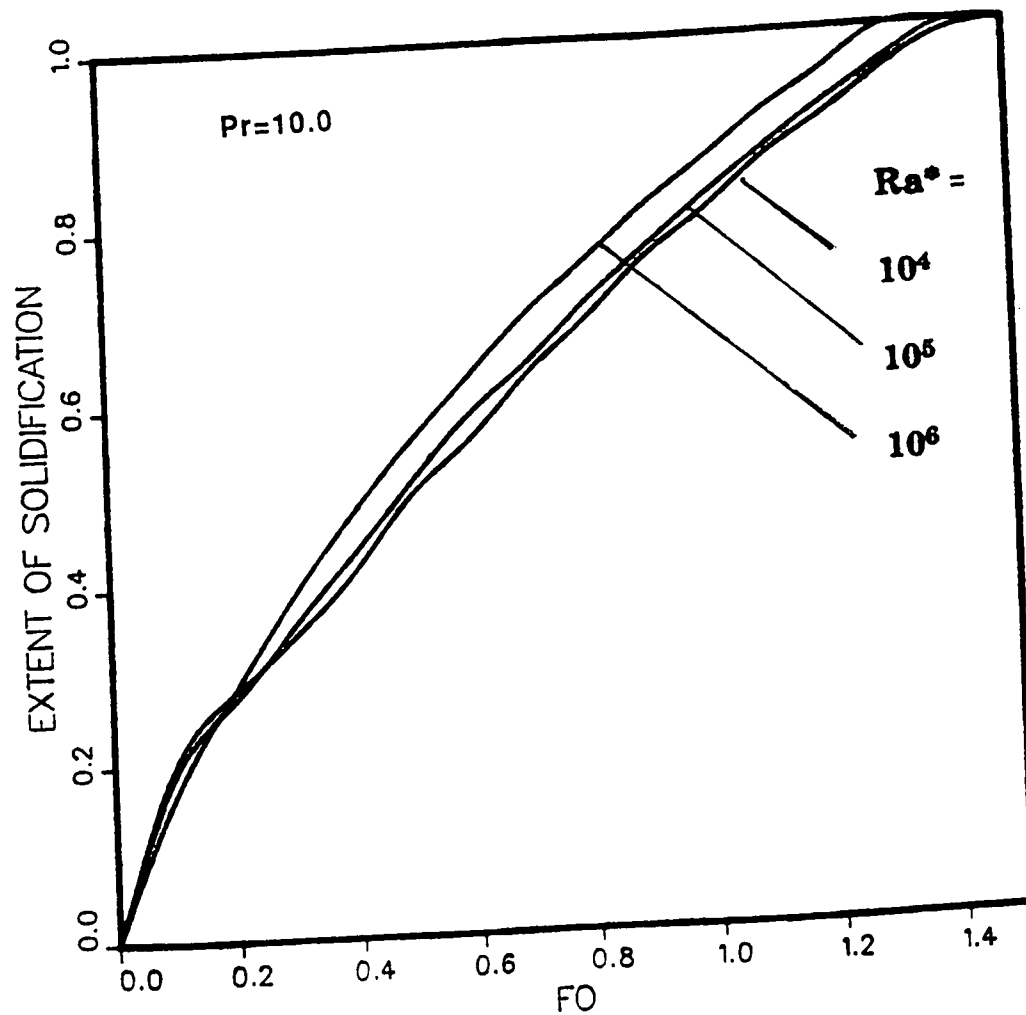


Figure 26. Effect of Rayleigh number on the solidified fraction.
 ($Pr=10$, $T_c = -0.5$, $T_i = 0.5$, $AR=1.0$) $Ra^* = 10^4, 10^5, 10^6$

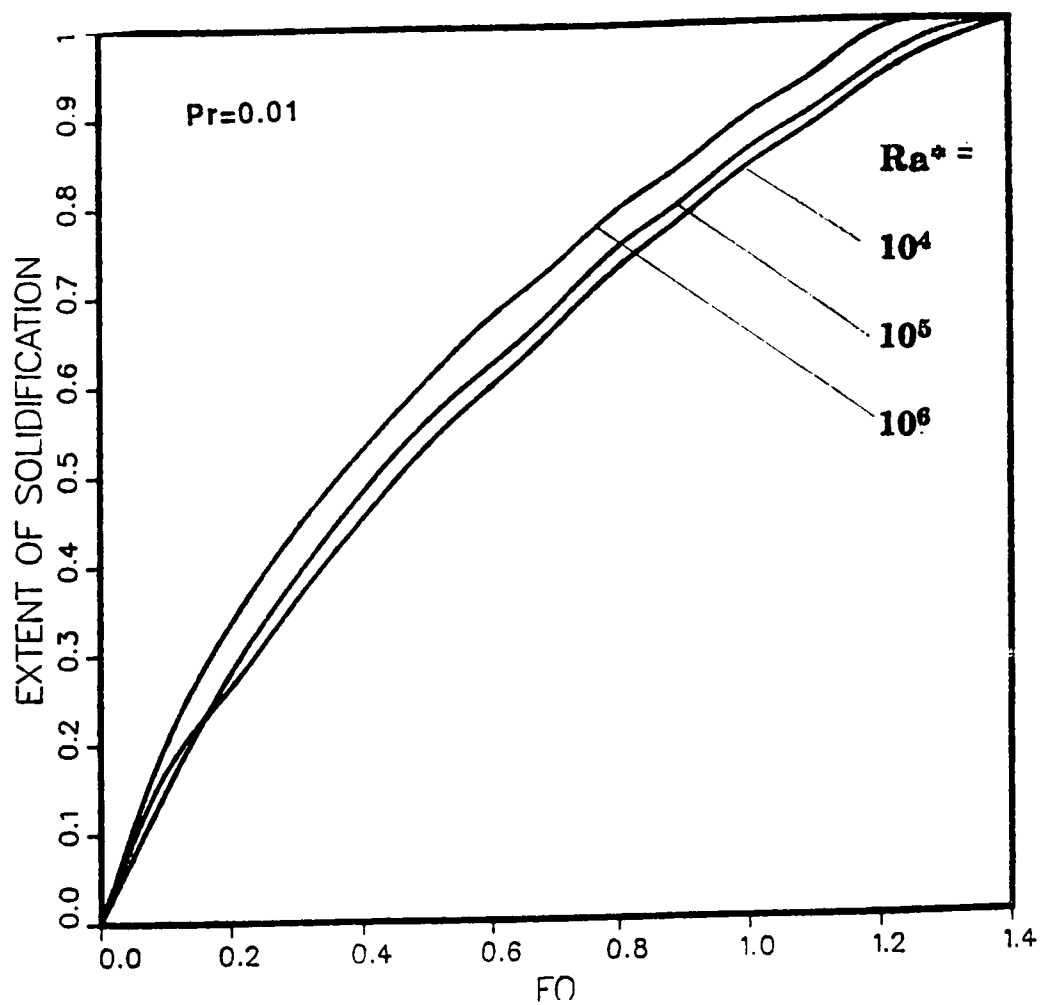


Figure27 Effect of Rayleigh number on the solidified fraction.
 ($Pr=0.01$, $T_c = -0.5$, $T_i = 0.5$, $AR=1.0$) $Ra^* = 10^4, 10^5, 10^6$

the extent of solidification is more for $Ra^* = 10^4$ or 10^5 . The results show that for $Pr=10$ and $Ra^* = 10^4$ and 10^5 , conduction aids solidification at earlier times more than convection inhibits it. However for $Ra^*=10^6$ and $Pr=10$ heat transfer is predominantly convective. Figure 27 shows that at $Pr=.01$ and $Ra^*=10^4$, the extent of solidification is initially larger when compared to $Pr=.01$ and $Ra^* = 10^5$. However, these values never go above the volume fraction for $Pr=.01$ and $Ra^* = 10^6$. It can be concluded that at $Pr=.01$ and $Ra^*=10^5$ and 10^6 convection inhibits solidification initially and aids it at later times while at $Pr=.01$ and $Ra^*=10^4$ there is less convection and therefore it inhibits solidification less at earlier times and does not help solidification at later times as compared to $Ra^* = 10^5$ and 10^6 .

A simple correlation for complete solidification time is computed using a SAS package. The correlation is found to be

$$Fo_{cs} = 0.9935 (Pr)^{.0094} (Ra^*)^{-0.0167} (|T_c|)^{-.7647} (T_i)^{.0334}$$

valid for the following range of parameters:

$$0.01 \leq Pr \leq 100$$

$$10^4 \leq Ra^* \leq 10^6$$

$$-4.0 \leq T_c \leq -0.5$$

$$0.1 \leq T_i \leq 2.0$$

$$10^2 \leq Gr^* \leq 10^8$$

$$AR = 1.0$$

The average absolute error was found to be 2.7 percent and the correlation coefficient was 0.997. It can be seen from this correlation that complete solidification time depends weakly on Pr and Ra^* .

For $Pr=.01$ and $Ra^*=10^5$, additional computations were performed to investigate the influence of aspect ratio on the extent of solidification and the nature of the

phase-front. For $T_i = 0.5$, $T_c = -0.5$, and $Fo = 0.2$, for the aspect ratios within the range of 0.1 to 10.0 the extent of solidification was found to be within 0.27 to 0.30 indicating that the aspect ratio is also a weak parameter. For aspect ratios of 0.1 and 0.2, as shown in Figure 28, the phase front is vertical at about $X = 0.3$. In general for aspect ratios less than 0.5, the phase front was found to be vertical and the isotherms indicate that the heat transfer in the liquid is conduction dominated. It was observed that the nondimensional velocities are on an average higher for higher aspect ratios than for lower ones. Figures 29-30 show that as the aspect ratio increases from 1 to 5, the front propagation at the bottom of the enclosure is essentially unaffected where as at the top of the enclosure it is progressively retarded indicating that the influence of convection becomes increasingly important.

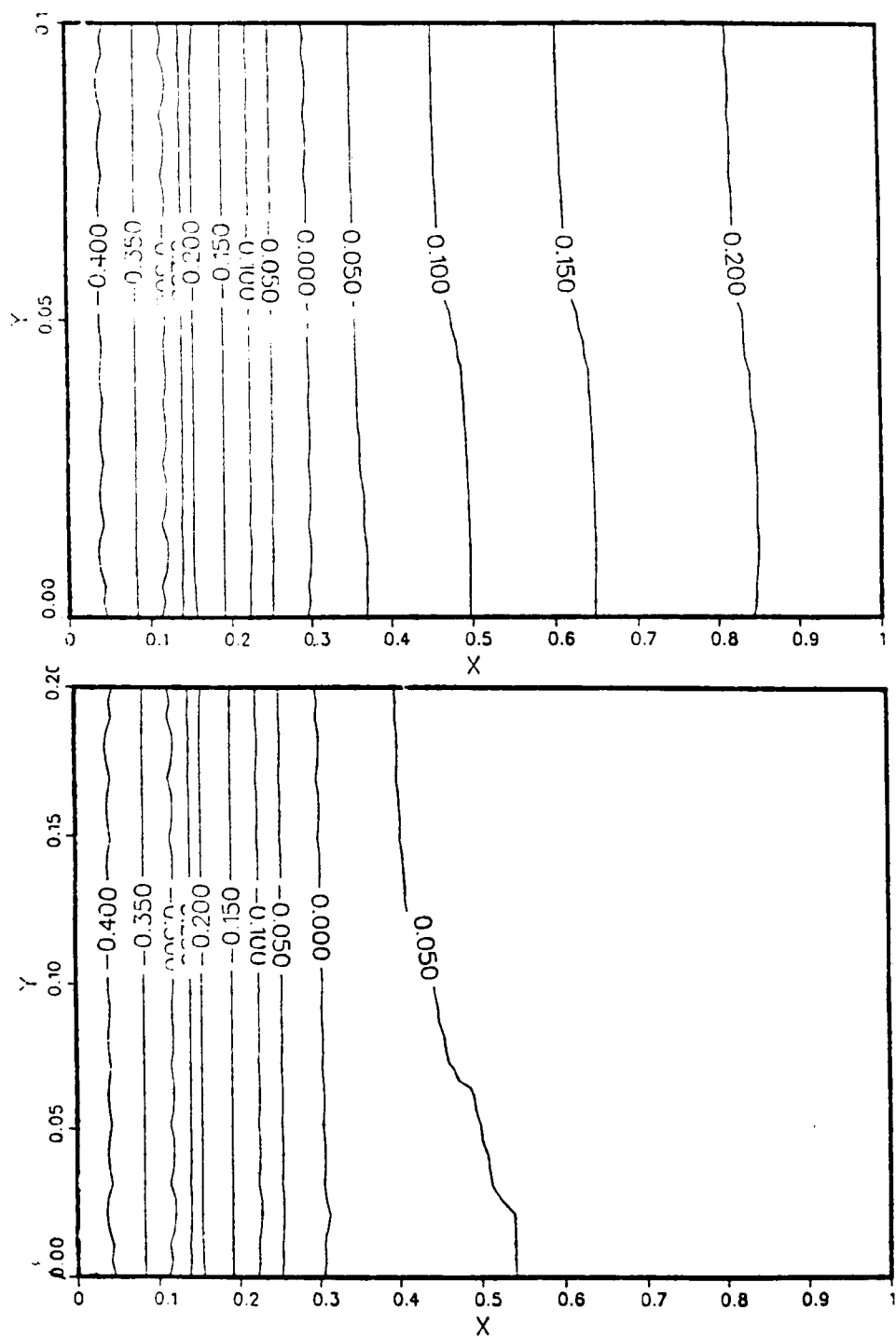


Figure 28 Effect of aspect ratio on the nature of the front and the isotherms
 ($Pr=0.01$, $Ra^*=10^5$, $T_c = -0.5$, $T_i = 0.5$, $AR=0.1$ and $.2$)

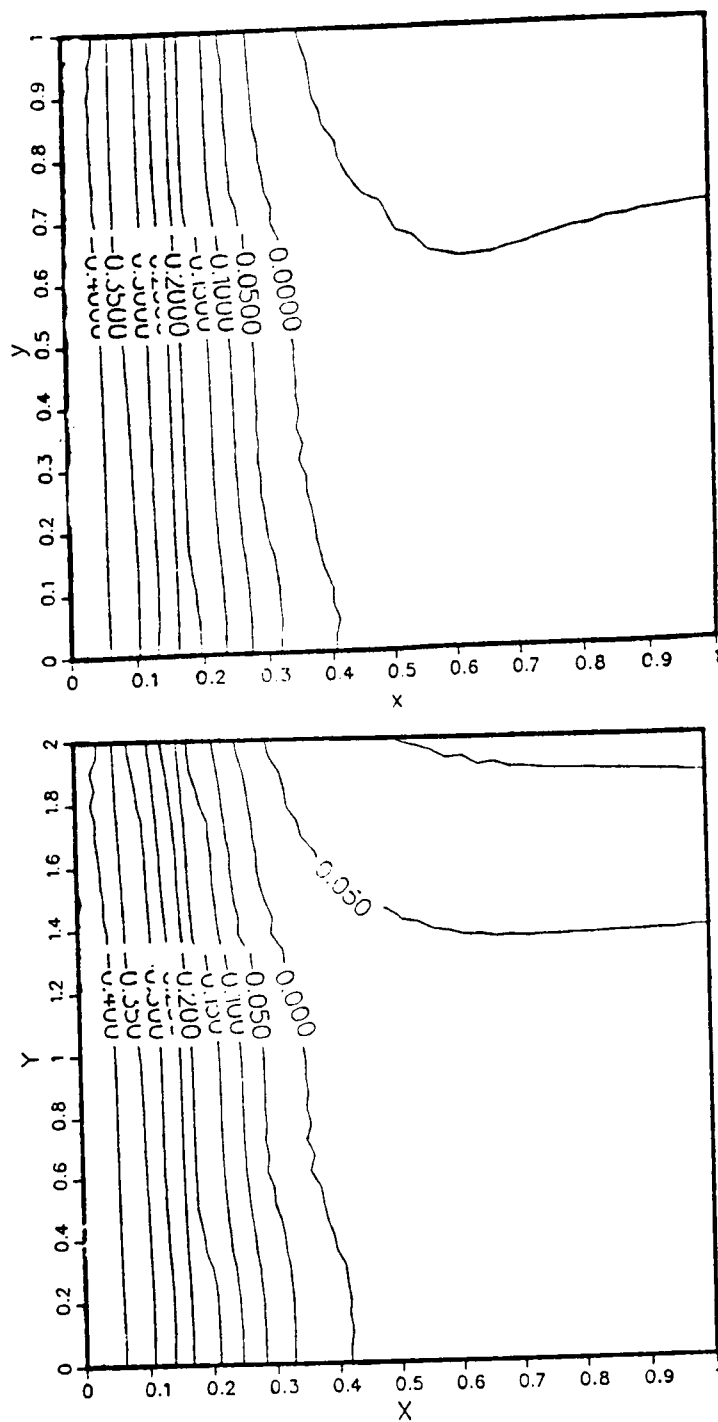


Figure29 Effect of aspect ratio on the nature of the front and the isotherms
 ($Pr=0.01$, $Ra^*=10^5$, $T_c = -0.5$, $T_i = 0.5$, $AR=1$ and 2)

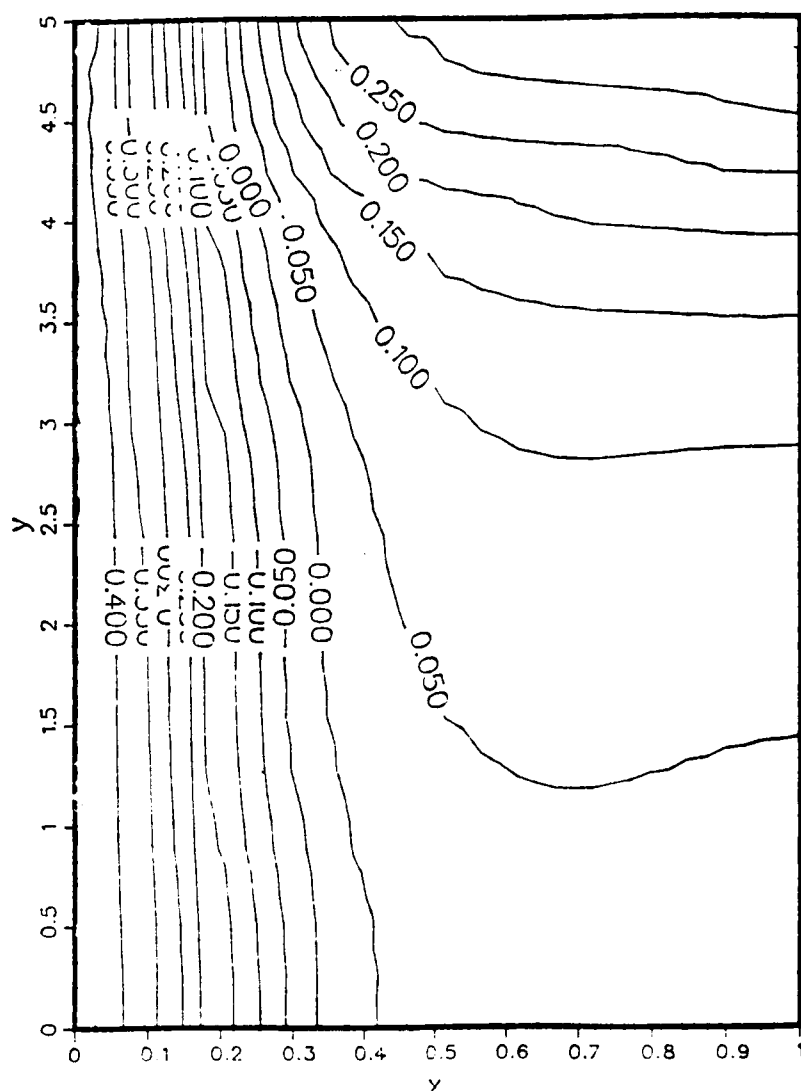


Figure 30 Effect of aspect ratio on the nature of the front and the isotherms
 ($Pr=0.01$, $Ra^*=10^5$, $T_c = -0.5$, $T_i = 0.5$, $AR=5.0$)

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

An enthalpy formulation, isolating latent heat effects in the "source term", is used for the convection/diffusion phase-change process. The numerical solution is compared with the experimental data for the solidification of 98% pure Caprillic acid and the melting of 99.99% pure tin. The numerical predictions and experimental results are in good agreement for the phase-front locations and in reasonable agreement for temperature-time history. This gives confidence in the numerical scheme. Caprillic acid with its less than ambient melting point and low volume reduction upon solidification seems to be a good candidate for solidification experiments.

Parametric study illustrates that modified Rayleigh number, Prandtl number, and modified Grashoff number play a significant role in the nature of the front, the extent of solidification, and time for complete solidification. It was observed that for $Ra^* \geq 10^3$, Gr^* determines whether convection is a predominant mode of heat transfer. For $Gr^* \geq 10^4$ convection plays an important role in the solidification process. For $Ra^* < 10^3$ solidification process is conduction dominated irrespective of Gr^* or Pr . A correlation is presented for complete solidification time for enclosures with $AR = 1.0$. It is shown that aspect ratio has less influence on the solidified fraction, and the phase-front is more slanted for higher aspect ratios than for the lower ones. For aspect ratios less than 0.5, the phase-front is flat indicating a diffusion dominated solidification process. For aspect ratios larger than 1, convection plays a significant role.

Flow visualization was attempted using Methyl blue dye in Caprillic acid. The dye is useful for short-time visualization but was found to diffuse and not very useful for

large times. Aluminum powder was found to be heavier than Caprillic acid. The author feels that flow visualization is an area open for further investigation to resolve the flow structure especially near the corners of the enclosure. Glycol with traces of Aluminum powder can be one of the candidates for flow visualization experiments. Much work is also needed in convection/diffusion solidification of alloys.

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APPENDICES

APPENDIX A

SOLUTION METHODOLOGY

The conservation equations governing the convection/diffusion phase change are the continuity momentum and energy equations. Throughout this work the properties will be assumed constant, i.e. $k_S = k_l$; $c_S = c_l$; $\rho_S = \rho_l$. The governing equations take the following form, :

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (A - 1)$$

$$\rho \left[\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right] = - \frac{\partial P}{\partial x} + \mu \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right] \quad (A - 2)$$

$$\rho \left[\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right] = - \frac{\partial P}{\partial y} + \mu \left[\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right] + g\beta (T - T_m) \quad (A - 3)$$

$$\rho \left[\frac{\partial H}{\partial t} + u \frac{\partial H}{\partial x} + v \frac{\partial H}{\partial y} \right] = \frac{DP}{Dt} + \text{Div}(k \nabla T) + \Phi \quad (A - 4)$$

$$\Phi = \mu \left[2 \left(\frac{\partial u}{\partial x} \right)^2 + 2 \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 \right] + \lambda \left[\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)^2 \right] \quad (A - 5)$$

where u, v are the velocities in the X and Y directions respectively. H is specific enthalpy which consists of the sensible heat $h = c(T - T_m)$ and the latent heat. Using the following non-dimensional parameters

$$x^* = \frac{x}{L}; y^* = \frac{y}{L}; u^* = \frac{u}{(\alpha / L)}; v^* = \frac{v}{(\alpha / L)};$$

$$P^* = \frac{P}{\rho \left(\frac{\alpha}{L} \right)^2}; Fo = \frac{\alpha t}{L^2}; T^* = \frac{T - T_m}{\lambda / c}; H^* = \frac{H}{\lambda} \quad (A - 6)$$

and dropping the superscript $*$ the governing equations reduce to

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (A - 7)$$

$$\frac{Du}{DFo} = \text{Pr}[\nabla^2 u] - \frac{\partial P}{\partial x} \quad (A - 8)$$

$$\frac{Dv}{DFo} = \text{Pr}[\nabla^2 v] - \frac{\partial P}{\partial y} + \text{Ra}^* T \quad (A - 9)$$

where Pr is the Prandtl number $c_p \mu / k$ and Ra^* is the modified Rayleigh number, $\text{Ra}^* = [\beta g L^3 \lambda_p^2 / \mu k] \text{Pr}$. The energy equation reduces to

$$\frac{DH}{DFo} = \frac{(\alpha / L)^2}{\lambda} \frac{DP}{DFo} + \nabla^2 h + \frac{\mu(\alpha / L)^2}{\alpha \rho \lambda} \Phi \quad (A - 10)$$

The coefficients of the first and of the last term on the right hand side are dependent on the Mach number and are very small when the velocities involved are much less than sonic velocity and therefore, can be neglected. The energy (enthalpy equation) therefore reduces to

$$\frac{DH}{DFo} = \nabla^2 h \quad (A - 11)$$

where h is the normalized sensible enthalpy (= dimensionless T) and H is the normalized total enthalpy (sensible plus latent). Introducing the liquid fraction $f(T)$ as in (5), page 16, H is expressed as

$$H = h + f(T) = \begin{cases} T + 1 & \text{if } T > 0 \\ f(T) & \text{if } T = 0 \\ T & \text{if } T < 0 \end{cases} \quad (A - 12)$$

Substituting $H = h + f(T)$ into equation (A-11) and noting that at the interface the velocity is zero, the dimensionless energy equation becomes

$$\frac{\partial h}{\partial Fo} + \left[u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} \right] - \nabla^2 h + \frac{\partial f(T)}{\partial Fo} = 0 \quad (A - 13)$$

The value of $f(T)$ determines the phase in the problem as follows,

$$f(T) = \begin{cases} 1, & T > 0 & \text{liquid} \\ 0 < f(T) < 1, & T = 0 & \text{two-phase control volume} \\ 0, & T < 0 & \text{solid} \end{cases} \quad (A - 14)$$

Boundary conditions for equations (A-7),(A-8), (A-9), (A-13), are as follows:

Left Wall (x=0)

$$u=v=0$$

$$T = T_c$$

Top and Bottom Walls (Y=1 and Y=0)

$$u=v=0$$

$$dT/dy=0$$

Right Wall (X=1)

$$u=v=0$$

$$dT/dx=0$$

Initial Condition

$$T = T_i \text{ at } t=0$$

Control Volume Discretization of a General Conservation Law in Two

Dimensions

Major portion of the following formulation is taken from Reference 62.

The conservation laws (A-7,A-8,A-9, A-13) in the model are P.D.E.s of the general form

$$\frac{\partial [\rho \phi]}{\partial t} + \frac{\partial [\rho u_j \phi]}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\Gamma \frac{\partial \phi}{\partial x_j} \right] + S, \quad (A - 15)$$

where ϕ stands for any of the quantities u, v , or h . Equation (A-15) can be written as

$$\frac{\partial[\rho\phi]}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = S, \text{ where}$$

$$J_x = \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \quad (A - 16)$$

$$J_y = \rho v \phi - \Gamma \frac{\partial \phi}{\partial y}$$

Integrating the equation over a control volume and over a time step we find

$$\begin{aligned} & \int_w^e \int_s^n \int_t^{t+\Delta t} \frac{\partial[\rho\phi]}{\partial t} dx dy dt + \int_t^{t+\Delta t} \int_w^e \int_s^n \frac{\partial J_x}{\partial x} dy dx dt + \int_t^{t+\Delta t} \int_s^n \int_w^e \frac{\partial J_y}{\partial y} dx dy dt \\ &= \int_t^{t+\Delta t} \int_w^e \int_s^n S dx dy dt \end{aligned} \quad (A - 17)$$

For the transient term, assume ρ_p and ϕ_p to prevail over the entire control volume, so that

$$\begin{aligned} & \int_w^e \int_s^n \int_t^{t+\Delta t} \frac{\partial[\rho\phi]}{\partial t} dt dx dy = \Delta x \Delta y \int_t^{t+\Delta t} \frac{\partial[\rho\phi]}{\partial t} dt \\ &= (\rho_p \phi_p - \rho_p^o \phi_p^o) \Delta x \Delta y \end{aligned} \quad (A - 18)$$

()^o = Old values

The flux terms can be written as

$$\int_t^{t+\Delta t} \int_w^e \int_s^n \frac{\partial J_x}{\partial x} dy dx dt = (J_e - J_w) \Delta t, \quad (A - 19)$$

and similarly,

$$\int_t^{t+\Delta t} \int_s^n \int_w^e \frac{\partial J_y}{\partial y} dx dy dt = (J_n - J_s) \Delta t, \quad (A - 20)$$

where $J_{e,w} = J_x \Delta y$, and $J_{s,n} = J_y \Delta x$.

Linearizing the source term as follows[62],

$$\int_t^{t+\Delta t} \int_w^e \int_s^n S dx dy dt = [S_c + S_p \phi_p] \Delta x \Delta y \Delta t$$

we obtain the discretized form of (A-17):

$$[\rho_p \phi_p - \rho_p^o \phi_p^o] \Delta x \Delta y / \Delta t + J_e - J_w + J_n - J_s = [S_c + S_p \phi_p] \Delta x \Delta y \quad (A - 21)$$

Integrating the Continuity equation in the same manner

$$\frac{\partial \rho}{\partial t} + \frac{\partial [\rho u]}{\partial x} + \frac{\partial [\rho v]}{\partial y} = 0 \quad (A - 22)$$

$$\int_w^e \int_s^n \int_t^{t+\Delta t} \frac{\partial \rho}{\partial t} dt dy dx + \int_t^{t+\Delta t} \int_w^e \int_s^n \frac{\partial [\rho u]}{\partial x} dy dx dt + \int_t^{t+\Delta t} \int_s^n \int_w^e \frac{\partial [\rho v]}{\partial y} dx dy dt = 0$$

the following discretized form of the continuity equation is obtained

$$\frac{[\rho_p - \rho_p^o]}{\Delta t} \Delta x \Delta y + [F_e - F_w] + [F_n - F_s] = 0 \quad (A - 23)$$

$$\text{where, } F_e = (\rho u)_e \Delta y; F_w = (\rho u)_w \Delta y; F_s = (\rho v)_s \Delta x; F_n = (\rho v)_n \Delta x$$

Multiplying equation (A-23) by ϕ_p and subtracting the result from equation (A-21) we obtain

$$\frac{(\phi_p - \phi_p^o)}{\Delta t} \rho_p^o \Delta x \Delta y + [J_e - F_e \phi_p] - [J_w - F_w \phi_p]$$

$$+ [J_n - F_n \phi_p] - [J_s - F_s \phi_p] = (S_c + S_p \phi_p) \Delta x \Delta y \quad (A - 24)$$

Assuming J's are uniform over the control volume faces and that J prevails over the entire face of the control volume, 1-d practice [Patankar, 62] can be employed giving

$$J_e - F_e \phi_p = a_E (\phi_p - \phi_E)$$

$$J_w - F_w \phi_p = a_W (\phi_W - \phi_p) \quad (A-25)$$

$$J_n - F_n \phi_p = a_N (\phi_N - \phi_p)$$

$$J_s - F_s \phi_p = a_S (\phi_p - \phi_S) \text{ where,}$$

$$a_E = D_e A(|P_e|) + \text{Max}(-F_e, 0)$$

$$a_W = D_w A(|P_w|) + \text{Max}(F_w, 0) \quad (A - 26)$$

$$a_N = D_n A(|P_n|) + \text{Max}(-F_n, 0)$$

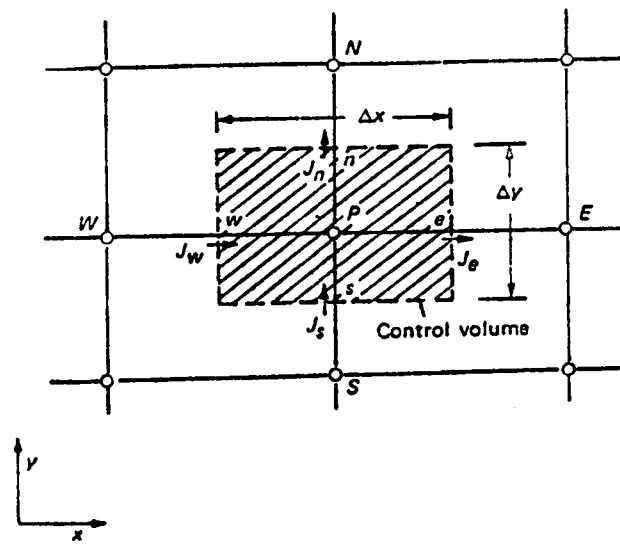
$$a_S = D_s A(|P_s|) + \text{Max}(F_s, 0)$$

Function $A(|P|)$ for the power law scheme recommended by Patankar [62] is $A(|P|) = (1 - 0.1|P|^5)$. For upwinding scheme $A(|P|) = 1$. In this work powerlaw scheme of Patankar is used. Two-dimensional discrete equation can be written as

$$a_p \phi_p = a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S + b, \text{ where}$$

$$b = S_c \Delta x \Delta y + a_p^o \phi_p^o, a_p^o = \frac{\rho_p^o}{\Delta t} \Delta x \Delta y$$

$$a_p = a_E + a_W + a_S + a_N + a_p^o - S_p \Delta x \Delta y$$



A Regular Two-dimensional Control Volume.

$$D_e = \frac{\Gamma_e}{\Delta x} \Delta y ; D_w = \frac{\Gamma_w}{\Delta x} \Delta y ; D_n = \frac{\Gamma_n}{\Delta y} \Delta x ; D_s = \frac{\Gamma_s}{\Delta y} \Delta x$$

$$P_e = \frac{F_e}{D_e} ; P_w = \frac{F_w}{D_w} ; P_n = \frac{F_n}{D_n} ; P_s = \frac{F_s}{D_s} \quad (A - 27)$$

$$F_e = (\rho u)_e \Delta y ; F_w = (\rho u)_w \Delta y ; F_n = (\rho v)_n \Delta x ; F_s = (\rho v)_s \Delta x$$

Calculation of Flow Field and the SIMPLE/SIMPLER Algorithm

The method described so far can solve the general differential equation (A-15) for the variable ϕ in the presence of a given flow field. The real difficulty in the calculation of the flow(velocity) field lies in the unknown pressure field. Pressure appears as a source term in the momentum equations. The pressure field is indirectly specified by the continuity equation. i.e. the velocity solution resulting from a correct pressure field will satisfy the continuity equation.

To avoid situations in which a zigzag pressure field will appear as uniform one and a nonrealistic velocity field may satisfy the continuity equation, a **staggered grid** is employed for the velocities[62].

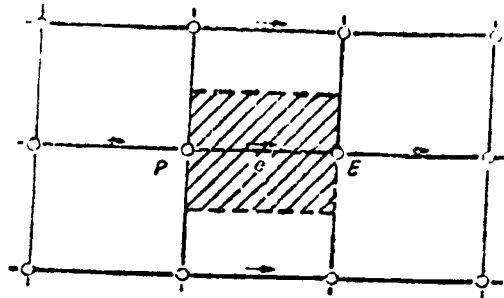
The discretized X-momentum equation can be written as

$$a_e u_e = \sum a_{nb} u_{nb} + b + (P_P - P_E) A_e, \quad (A-28a)$$

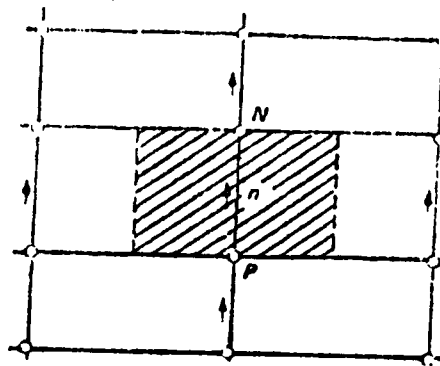
with a's and b are as defined before (equation A-26), but the pressure force term is not included in the source term. Similarly Y-momentum equation can be written as

$$a_n v_n = \sum a_{nb} v_{nb} + b + (P_P - P_N) A_n. \quad (A-28b)$$

Where $A_e = \Delta Y$ and $A_n = \Delta X$. Equations (A-28a), (A-28b) can be solved only when the pressure distribution is known. Let P^* denote the latest value of pressure and u^* , v^* represent the corresponding values of the velocity components. Equation (A-28) therefore can be



A Control Volume Staggered in X -direction.



A Control Volume Staggered in Y-direction.

written as

$$a_e u_e^* = \sum a_{nb} u_{nb}^* + b + (P_p^* - P_E^*) A_e \quad (A-29a)$$

$$a_n v_n^* = \sum a_{nb} v_{nb}^* + b + (P_p^* - P_N^*) A_n \quad (A-29b)$$

A procedure is needed to adjust the estimated pressure , P^* , such that u^*, v^* approach the correct velocity field (i.e. the field which satisfies the continuity equation). Let

$$P = P^* + P'$$

$$u = u^* + u'$$

$$v = v^* + v'$$

where ' denotes corrections in respective quantities.

Subtract (A-29a) from (A-28 a) and (A-29 b) from (A-28b). This results in velocity correction equations,

$$a_e u_e' = \sum a_{nb} u_{nb}' + (P_p' - P_E') A_e \text{ and}$$

$$a_n v_n' = \sum a_{nb} v_{nb}' + (P_p' - P_N') A_n$$

For now drop the first term on the right hand side (see reference 62 for further discussion of this step) Therefore, the expression for velocity corrections becomes

$$u_e' = (P_p' - P_E') d_e, \quad d_e = (A_e / a_e) \quad (A-30a)$$

$$v_n' = (P_p' - P_N') d_n, \quad d_n = (A_n / a_n) \quad (A-30b)$$

and

$$u_e = u_e^* + u_e' \quad (A-31a)$$

$$v_n = v_n^* + v_n' \quad (\text{A-31b})$$

Pressure Correction Equation

$P_P', P_N', \dots$ etc. are still to be determined. Assume ρ not to be a function of pressure. Assume p_p prevails over the entire control volume and so does u_p, v_n etc. The discrete conservation of mass equation is (A-23), namely,

$$\frac{(\rho_p - \rho_p^o)}{\Delta t} \Delta x \Delta y + [(\rho u)_e - (\rho u)_w] \Delta y + [(\rho v)_n - (\rho v)_s] \Delta x = 0$$

Substitute equations (A-31a), (A-31b) into the above equation and rearrange, to obtain the pressure correction equation:

$$a_P P_P' = a_E P_E' + a_W P_W' + a_N P_N' + a_S P_S' + b, \quad (\text{A-32})$$

where

$$a_E = \rho_e d_e \Delta y, a_W = \rho_w d_w \Delta y, a_N = \rho_n d_n \Delta x, a_S = \rho_s d_s \Delta x \quad (\text{A-33a})$$

$$a_P = a_E + a_S + a_N + a_W \quad (\text{A-33b})$$

$$b = \left\{ \frac{\rho_p^o}{\Delta t} \Delta x \Delta y + [(\rho u)_w^* - (\rho u)_e^*] \Delta y + [(\rho v)_s^* - (\rho v)_n^*] \Delta x \right\} \quad (\text{A-33c})$$

"b" serves as a mass generation term which is to be driven to zero by the iterative process. The SIMPLE algorithm for the calculation procedure is as follows,

SIMPLE Algorithm

- 1) Guess a value for P^*
- 2) Solve the Momentum equations for u^* and v^* from (A-29)
- 3) Solve the P' equation, (A-32)

- 4) Compute $P^* + P'$
- 5) Compute u, v , using equations (A-31)
- 6) Solve discretized energy equation
- 7) Let the corrected pressure serve as P^* & return to step (2)

The approximation of omitting the term $\sum a_{nb} u_{nb}'$ in the P' equation leads to exaggerated pressure corrections, and therefore underrelaxation of pressure correction becomes essential to avoid divergence. To overcome these difficulties Patankar[62] developed a revised algorithm SIMPLER. The momentum equation is written as

$$u_e = \frac{\sum a_{nb} + b}{a_e} + d_e(P_P - P_E), \quad (A - 34)$$

$$d_e = \frac{A_e}{a_e}. \quad (A - 35)$$

Defining a pseudo-velocity u_e by

$$\hat{u}_e = \frac{\sum a_{nb} + b}{a_e}, \text{ we have } u_e = \hat{u}_e + d_e(P_P - P_E), \quad (A - 36a)$$

and similarly

$$v_n = \hat{v}_n + d_n(P_P - P_E). \quad (A - 36b)$$

The resulting pressure equation can be written as

$$a_P P_P = a_E P_E + a_W P_W + a_N P_N + a_S P_S + b, \quad (A - 37)$$

where the a 's are given by equation (A-33a) and (A-33b) and b is given by

$$b = \frac{(\rho_p^o - \rho_p)\Delta x \Delta y}{\Delta t} + [(\rho \hat{u})_w - (\rho \hat{u})_e]\Delta y + [(\rho \hat{v})_s - (\rho \hat{v})_n]\Delta x \quad (A - 38)$$

Although the pressure equation and the pressure correction equation are almost identical, there is one major difference. No guess is made in deriving the pressure equation. Thus if a correct velocity field were used to compute pseudo-velocities, the pressure equation would generate a correct pressure solution. The SIMPLER algorithm is as follows

- 1) Start with a guessed velocity field
- 2) Calculate the coefficients for the momentum equation and hence calculate u and v
- 3) Calculate the coefficients of pressure equation (A-37) and solve it to obtain the pressure field.
- 4) Treating this pressure field as P^* , solve the momentum equations (A-29) to obtain u^*, v^* .
- 5) Calculate the mass source b and equation (A-32) for P' .
- 6) Correct the velocity field, but do not correct the pressure.
- 7) Solve the discretized energy equation.
- 8) Return to step 2 and repeat until convergence (mass source within the tolerance limit).

In the above described SIMPLER algorithm the energy equation is solved last in the iteration process. For solidification processes, this works fine at early times because there is a strong driving potential for natural convection flow. As time progresses the convective flow decays and the algorithm stops iterating on velocities. In order to avoid difficulties arising from decaying convection and melting at early times, the SIMPLER algorithm is modified by solving the energy equation (step 7) after step 2 in the iteration process. The rest of the algorithm is same as SIMPLER.

Since the latent heat effects are isolated in the source term of the energy equation, to apply the control volume discretization of the general conservation law and the SIMPLER algorithm described earlier two major problems need to be addressed,

- 1) How to treat the latent heat source term
- 2) How to insure that the velocities are zero in the solid during the solution iterations.

The source term in the discretized nondimensional energy equation is,

$$b = \alpha_p \left[h_p^\circ + (f(T)_p^\circ - f(T)_p) \right] . \quad (A - 39)$$

To slowly make the velocities in the control volumes changing phase approach zero, Voller [61] has proposed to add a large term (taken to be 50000 in this work) in the leading coefficient of the momentum equations. This term will depend on the value of the latent heat in the control volume.

$$S_p = \text{Large term} \cdot (1 - f(T)), \quad (A-40)$$

is added to a_p .

The method for dealing with $f(T)$ during the solution iterations is as follows. On commencement of the SIMPLE algorithm over one time step, initial estimates for $f(T)$ are the values at the previous time values,

$$(f(T)_p)_0 = f(T)_p^0 \quad (A-41)$$

After solving for the nodal enthalpies at the i^{th} iteration, it is temporarily assumed that all control volumes are changing phase. Under this assumption the predicted enthalpies $(h_p)_i$ should be zero and any deviation should be taken up in the source term,

$$(f(T)_p)_{i+1} = (f(T)_p)_i + (h_p)_i . \quad (A-42)$$

Since the assumption that all control volumes are changing phase is wrong, corrections have to be made for $f(T)_p$. Knowing that if $(h_p)_i > 0$ and $(f(T)_p)_i = 1$ the phase is liquid

and if $(h_P)_i < 0$ and $(f(T)_P)_i = 0$ the phase is solid, the corrections are

$$\text{If } (f(T)_P)_{i+1} > 1 \text{ set } (f(T)_P)_{i+1} = 1 \quad (\text{A-43})$$

$$\text{If } (f(T)_P)_{i+1} < 0 \text{ set } (f(T)_P)_{i+1} = 0. \quad (\text{A-44})$$

After these corrections, the $(i+1)^{\text{th}}$ sweep in SIMPLER can continue. On convergence, any phase changing control volume will have $h=0$ and $f(T)$ between 0 and 1.

VITA

Satish Prabhakar Ketkar was born in Poona, India, on November 25, 1960. He attended elementary and secondary school at Nutan Marathi Vidyalaya, Poona, through tenth standard and received his secondary school certificate in 1975. He received his higher secondary school certificate in 1977. He represented his school in interschool Cricket.

In 1977, he enrolled in The College of Engineering, Poona, India. He played for his college in intercollegiate Cricket tournaments. In August 1981 he received a Bachelor of Engineering degree with a major in Mechanical Engineering. In Fall of 1982 the author enrolled in the Masters program in Mechanical Engineering at The University of Tennessee, Knoxville, U.S.A. He earned the degree in March 1985. He continued for a Doctoral at The University of Tennessee, Knoxville. This degree was awarded in August 1989. The author has co-authored a few technical research papers which have been published in archive journals. The field of his expertise is Thermal Sciences. The author wishes to pursue a teaching and research career in the general area of Thermal Engineering. The author is a Associate Member of The American Society of Mechanical Engineers.