1 | Introduction

1.1 Moving Boundary Problems

Heat transfer problems can be modeled as phase change problems or moving boundary problems. Moving boundary problems are defined as a set of partial differential equations that are to be solved for a domain whose boundaries are not known priori but it has to be determined as a part of solution. Even though the set of partial differential equations are linear, the above problems are highly nonlinear due to presence of moving interface condition. The position of the moving boundary is an important part in the required solution from theoretical and practical point of views. The moving boundary problems are naturally occur in physical and industrial processes like melting and freezing, solidification of alloys, chemical reaction, preservation of human blood, solar energy storage, casting and welding of metals and alloys, fluid flow in porous media with diffusion, aerodynamic ablation, energy storage, crystal growth and food processing and many others.

Moving boundary problems are often called Stefan problems or classical moving boundary problems. Generally the term classical is used to distinguish the classical formulation from weak formulation. The characteristic features of Stefan problem can be described as follows;

- the heat transfer governed by parabolic equations.

- both the phases are separated by a sharp interface.

- at interface, the known temperature and energy balance are prescribed.

- heat flux is discontinuous across the interface and the latent heat is absorbed and released at interface.

Solidification of an alloy is distinctly different in many respects from the phase change of pure substances. The basic physical phenomena for solidification of alloys was introduced by Flemings (1974); Kurz and Fisher (1989); Beckermann and Viskanta (1993); Beckermann and Wang (1995) and many others. In pure substances, the phase changes isothermally and the smooth interface exist between the phases, which is coincident with the isotherm corresponding to the phase change temperature T_f. Fig. 1.1(a) shows the solidification of pure substances. In this figure, the solid and liquid phases of pure substances are in equilibrium with each other at unique temperature, while Fig. 1.1(b) shows that the solid and liquid phases of an alloy may be in equilibrium with each other over a temperature range.
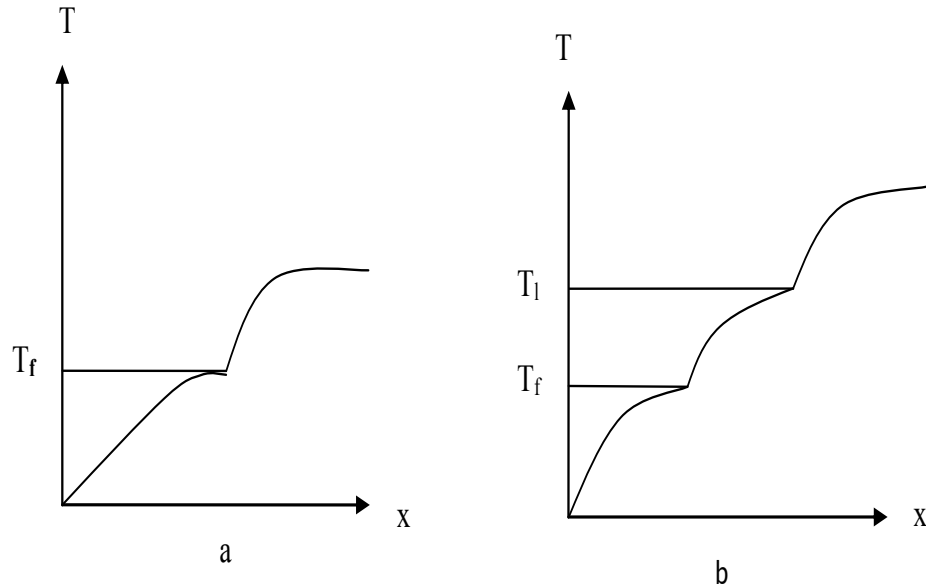
Figure 1.1: Solidification systems for (a) pure substance and (b) a binary substance.

An equilibrium phase diagram of binary eutectic system (A-B) is shown in Fig. (1.2). The phase diagram defines the temperature of regions and composition in which two or more phases may exists in equilibrium with each other. The temperature above the liquidus line, a single liquid phase exists as a solution of constituents A and B. The regions between liquidus and solidus lines, a solid-liquid mixture exists over a range of temperature up to a eutectic point. As the temperature of the solid-liquid interface is lowered, the composition of the solid and liquid at the

interface continuously change. At the eutectic point (lowest freezing/melting point than that of other alloy or mixture of the same ingredients), there is a three-phase of mixture of liquid and two solid phases exist. The two solid phases (α and β) of different composition form simultaneously and isothermally, such that the average composition is equal to the eutectic composition. Pure substances are represented along the left and right edges of the equilibrium phase diagram (i.e. $0\%B$ and $100\%B$) where the solidus and liquidus temperatures coincide. The temperature also coincide at eutectic composition f_e^B. However, for all other alloy compositions, freezing will occur over a temperature range defined by corresponding liquidus and solidus temperatures. Therefore, the solid-liquid region also known as mushy region exists and separates fully solidified and melted region during solidification.
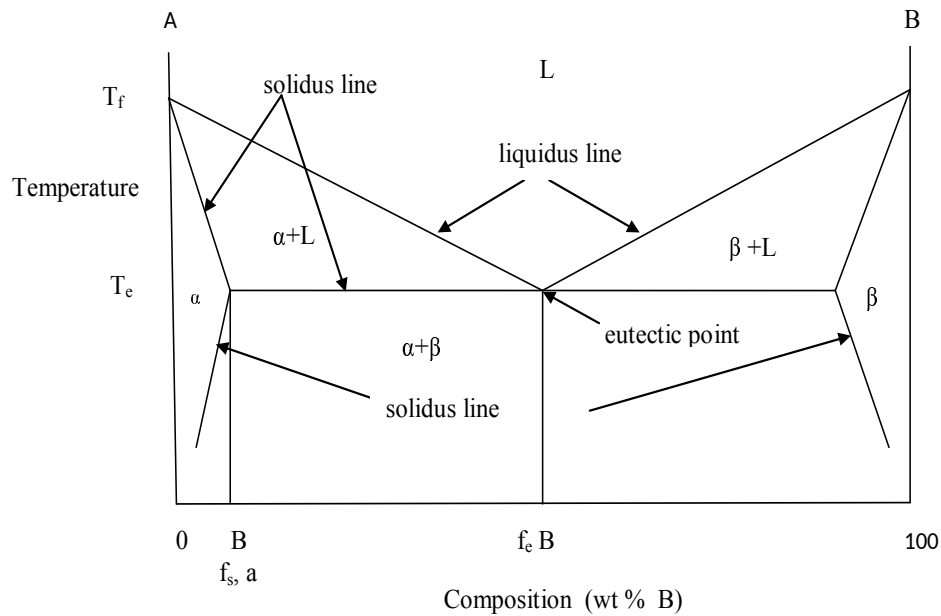

Figure 1.2: Equilibrium phase diagram of binary eutectic system (A-B).

The structure and extent of the mushy region, depends on several factors, such as the specific initial and boundary conditions. During solidification process, the latent heat is released at the interfaces which separates both the phases within the mushy region. The distribution of this energy depends on the specific structure of the multi-phase region. In solidification process, latent heat is transformed in the form of conduction in solid phase while in the liquid phase, it is transformed by the

combined effects of conduction and advection. The motion of fluid may be induced by external means and may be occur by thermal or solutal buoyancy forces, and it may be caused by expansion or contraction of the system due to the phase transformation. In mushy region, the flow can be estimated in two ways. The mushy region can be treated as a porous media where the solid is stationary and the liquid flows through the porous structure (Voller (1987b)). This behavior is convincing when solidification progresses in columnar mode. On the other hand, the mushy region can be considered as a mixture of solid and liquid. In this case the movement of both the solid and liquid is acceptable and this depiction is closer to the equiaxed mode of solidification. These two physical situations represent two edges. In many cases, however, solidification process takes place through columnar as well as equiaxed, i.e. in the beginning of solidification the columnar structure form and after that equiaxed structure form. In such cases, a morphological evolution from columnar to equiaxed takes place during the track of solidification. Therefore, an accurate depiction of mushy region can be through a combination of Darcy's law and variable viscosity formulation. Such depiction would also require a condition for columnar to equiaxed transition (CET) under transitory convection which is not willingly accessible. Moreover, at high solid fractions the equiaxed grains combined and solid phase can be treated as stationary with respect to mould. If the casting is moving with respect to inertial frame of reference, the solidified region, columnar structure of the mushy region, and combined equiaxed zone will move with a prescribed velocity (Us).

The driving force for the flow in mushy region and liquid region can be shrinkage and forced convection, thermal and solutal buoyancy. From the above discussion, it is noticed that during equiaxed solidification, solid grains in the mushy region can have independent velocity especially at low solid fraction and this requires the condition of an equation of motion for its resolution (Beckermann and Wang (1995)). An important results of the flow of solid and liquid in the mushy region is the large-scale transport of the solute components and as a result in addition to solute variations over the small scale representative volume element (REV) (microsegregation) the solute varies over the domain as a whole (macrosegregation).

1.2 Basic Definition of Thermodynamic Variables

In melting/solidification process, the phase change involves heat transfer, mass transfer, supercooling, absorption and release of latent heat, surface effects and change in thermo-physical properties (specific heat, thermal conductivity and densities) etc. This phase change process occur at macroscopic level. In case of transition from one phase to the other, the absorption or release of latent heat occurs at some temperature at which the stability of one phase breaks down in favour of other according to the available energy. The phase transition region where the solid and liquid coexist is called the interface and its thickness varies from few angstroms to few millimetres. The microstructure of interface thickness is much complex and depends on several factors such as rate of cooling, surface tension, temperature gradient in the liquid and material itself.

In material there are three possibilities of heat transfer i.e. conduction, convection and radiation. In conduction, the kinetic energy transfer between the atoms by any number of ways, the movement of electrons from one atom to another atom or collision of neighbouring atoms. In this case, there is no flow or mass transfer of the material. In convection process, heat can also be transferred by the flow of particles in liquid form. In radiation, the heat transfer is in the form of electromagnetic wave. In conduction and convection medium is require but in radiation there is no requirement of medium. In phase change process heat and mass transfer by conduction, convection and radiation with gravitational, chemical, elastic and electromagnetic effects. If we take classical Stefan problem the heat transfer is isotropically by conduction only and assumes that interface structure is planner and sharp.

1.2.1 First Law of Thermodynamic

The internal energy of the system is the sum of all kinetic energy of motion and energy of interaction between the particles in the system. The internal energy can

be transformed to do work and produce heat

$$dU = dQ - dW, \tag{1.1}$$

where, dU is the change of internal energy of the system during the change of state p to another equilibrium state q. dQ is the heat flow into the system during the change of state. dW is the work done by the system changes its equilibrium state from p to q.

1.2.2 Fourier's Law

Fourier's law of heat conduction gives a linear relationship between the heat flow and temperature gradient and is given as

$$\vec{q} = -K\nabla T, \tag{1.2}$$

where, $\vec{q}$ is heat flux defined as the amount of heat crossing a unit area per unit time. The heat flux is a vector pointing in the direction of heat flow. In general it is a tensor with positive components varying with temperature. We shall assume isotropic conduction i.e. K is a scalar and $K > 0$. In one space dimension Fourier's law is expressed by

$$\vec{q} = -K\frac{\partial T}{\partial r}. \tag{1.3}$$

1.2.3 Single Phase Lagging Heat Conduction

Most of the available work in phase change literature assume that the heat transfer in solid and liquid region are described by classical Fourier law. In Fourier law, heat is propagate with infinite speed when ultra fast pulse heating on metal film. In this case, heat conduction appears with high heat flux and high unsteadiness. Cattaneo (1958) and Vernotte (1958, 1961) proposed a constitutive relation defined as

$$q(r, t + \tau_q) = -K\frac{\partial T(r, t)}{\partial r}. \tag{1.4}$$

It is commonly known as CV constitutive relation or single-phase-lagging (SPL) heat conduction model. Here $\tau_q > 0$ is called the relaxation time. According to

which the temperature gradient established at a point r at a time t gives rise to a heat flux at r at later time $t + \tau_q$. The CV model gives rise to a wave type of heat conduction equation called the hyperbolic heat conduction equation. The first order Taylor's expansion of $q(r, t + \tau_q)$ in Eq. (1.4) is defined as

$$q(r,t) + \tau_q \frac{\partial q(r,t)}{\partial t} = -K \nabla T(r,t). \tag{1.5}$$

The one-dimensional energy conservation equation for such problem is given as

$$\rho c \frac{\partial T}{\partial t} = -\frac{\partial q}{\partial r}. \tag{1.6}$$

Elimination of q between Eq. (1.5) and Eq. (1.6) leads to a hyperbolic heat conduction equation

$$\rho c \tau_q \frac{\partial^2 T}{\partial t^2} + \rho c \frac{\partial T}{\partial t} = -K \frac{\partial^2 T}{\partial r^2}. \tag{1.7}$$

1.2.4   Thermal Conductivity

Thermal conductivity is the property of materials to conduct heat. It is evaluated primarily in terms of Fourier's law of heat conduction. Thermal conductivity can be defined as the quantity of heat transmitted through a unit thickness of material in a direction normal to a surface of unit area due to a unit temperature gradient under steady state condition. It is measured in watts per meter kelvin (W/mK).

1.2.5   Thermal Diffusivity

Thermal diffusivity of material indicates the rate of cooling and heating of a material under transient condition. When thermal conductivity considered constant, then the thermal diffusivity is defined as

$$a = \frac{K}{\rho c}. \tag{1.8}$$

The general heat equation can be written in form

$$T_t = a \nabla^2 T + F. \tag{1.9}$$

Which is now a linear parabolic equation. In one-dimension when no internal sources are present, the Fourier law, general heat conduction equation, and heat equation

takes the forms

$$q = -K\frac{\partial T}{\partial r}, \tag{1.10}$$

$$\rho c\frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial r^2}, \tag{1.11}$$

$$\frac{\partial T}{\partial t} = a\frac{\partial^2 T}{\partial r^2}. \tag{1.12}$$

1.2.6 Latent Heat

When a solid metal piece is heated, then temperature rises and reaches an equilibrium temperature T_m. When more heat is supplied, the heat is first absorbed without changing the temperature of metal piece. The heat absorbed is called latent heat of melting. It is expressed as the ratio of the heat absorbed per unit mass of the substances under going the phase change.

This heat is absorbed because in solid metals, the free atoms are packed closely. The atomic arrangement is disordered in liquids as compare to that in solids. So the latent heat of fusion is the energy required to pull the atoms apart to the more openly packed structure of the liquid.

In general, when solid convert into liquid or liquid convert into vapour or solid convert into vapour, the system absorbs heat. In phase change transformations, the absorb heat is called the latent heat of fusion or latent heat of vaporization or latent heat of sublimation respectively. If a liquid solidifies latent heat is released. Latent heat released per unit mass is taken as positive and denoted by L.

1.2.7 Specific Heat Capacity or Specific Heat

If no phase change take place in a process, then the heat capacity c at any temperature is defined by the equation

$$dQ = cdT. \tag{1.13}$$

dQ is the quantity of heat added to the system which changes its temperature by dT. The process may be reversible or irreversible. If there is no change in volume the system does not change in the process, then c is denoted by c_V and is called

heat capacity at constant volume $dV = 0$. From the first law of thermodynamic

$$dQ = dU + PdV = \left(\frac{\partial U}{\partial T}\right)_V dT + \left[\left(\frac{\partial U}{\partial V}\right)_T + P\right] dV = \left(\frac{\partial U}{\partial T}\right)_V dT, \quad (1.14)$$

where the work is done by the pressure P in changing the volume. From Eq. (1.14) we get,

$$c_V = \left(\frac{\partial U}{\partial T}\right)_V. \quad (1.15)$$

It may be assumed that Q is not a function of temperature. Therefore, c is not derivative of Q with respect to T but it is the ratio of dQ and dT or the ratio of very small amount of heat supplied and the change in temperature. The specific heat may be defined as the amount of heat per unit mass required to raise the temperature by $1\,°C$ and denoted by c.

1.2.8   Interface Condition

Consider a region Ω occupied by the phase change material. If melting starts, the region Ω will be subdivided into two region i.e. liquid and solid, separated by a sharp interface $\sum$ of zero thickness. According to the conservation of energy in each region demands that a heat conduction Eq. (1.12) must be satisfied there. The specific heat and thermal conductivity are assumed in the solid region c_1 and K_1 and in the liquid region, c_2 and K_2 respectively. The interface comprises part of the boundary of both the liquid and solid regions. Hence, we need a boundary condition from each side in order to complete the initial boundary value problem in each phase. At $T = T_m$, the temperature must be continuous, and interface is an isotherm. Therefore, we have taken

$$\lim_{\substack{r \to interface \\ r \in liquid}} T(r,t) = T_m \text{ and } \lim_{\substack{r \to interface \\ r \in solid}} T(r,t) = T_m. \quad (1.16)$$

If the interface location were known we would have enough conditions to determine the temperature inside the liquid and the solid region. Since the location is unknown therefore, we need an additional condition to determine it and obtained from energy conservation across the interface. Now, for one-dimensional case, the Stefan condition derives directly from global energy balance. Consider a slab of

material $0 < r < l$, of constant cross sectional area A. Heat is input and output at the faces $r = 0$ and $r = l$ by some means, the liquid region $0 < r < s(t)$ and the solid region $s(t) < r < l$ are separated by a sharp interface at $r = s(t)$, at each time $t > 0$. We assumed that the density in each phase are constant. The total enthalpy in the slab at time $t > 0$, referred to the melt temperature T_m is

$$E(t) = A \left[\int_0^{s(t)} \{\rho c_2(T(r,t) - T_m) + \rho L\} dr + \int_{s(t)}^l \{\rho c_1(T(r,t) - T_m)\} dr \right], \quad (1.17)$$

Global heat balance demands,

$$\frac{dE}{dt} = \text{net heat flow into the slab} = Aq(0,t) - q(l,t), \quad (1.18)$$

Where $q(0,t)$ and $-q(l,t)$ are the heat fluxes into the slab through the faces $r = 0$ and $r = l$ respectively. Leibnitz's rule enables us to compute

$$\frac{1}{A} \frac{dE}{dt} = \rho c_2 \{(T(s(t),t) - T_m)\} s'(t) + \int_0^{s(t)} \rho c_2 (T_t(r,t)) dr + \rho L s'(t)$$

$$-\rho c_1 \{(T(s(t),t) - T_m)\} s'(t) + \int_{s(t)}^l \rho c_1 (T_t(r,t)) dr. \quad (1.19)$$

Using $T(s(t),t) = T_m$ and substituting the heat Eq. (1.11) for each phases, we obtain

$$\frac{1}{A} \frac{dE}{dt} = K_2 T_r(s(t)^-,t) - K_2 T_r(0,t) + \rho L s'(t) + K_1 T_r(l,t) - K_1 T_r(s(t)^+,t). \quad (1.20)$$

Where $T_r(s(t)^\mp,t)$ denotes the values of $T_r(r,t)$ as $r \to s(t)^\mp$, i.e. from the left or right and $-K_2 T_r(0,t)$ and $+K_1 T_r(l,t)$ are precisely the fluxes $q(0,t)$ and $-q(l,t)$. Therefore, Eq. (1.18) yields the Stefan condition (Interface condition)

$$\rho L s'(t) = K_1 T_r(s(t)^+,t) - K_2 T_r(s(t)^-,t). \quad (1.21)$$

Expressing energy conservation across the interface $r = s(t)$ in the one-dimensional case as follow

$$(q_2 - q_1)_{s(t)} = K_1 T_r(s(t)^+,t) - K_2 T_r(s(t)^-,t), \quad (1.22)$$

Where, q_1, q_2 are heat flux in solid and liquid region respectively. Stefan condition says that the rate of change in latent heat $\rho L s'(t)$ equals the amount by which the heat flux jumps across the interface.

1.3 Classification of Moving Boundary Problems

In melting and solidification process, the moving boundary problems can be classified in three types (one phase; two phase and multiphase). The classification of melting and freezing depends on the properties of the phase change material and the initial condition. The melting/solidification of single components occurs at a single temperature. For example pure water melts at a uniform temperature of $0°C$ while pure n- octadecane ($C_{18}H_{38}$) melts at $28°C$. For the solidification (meting) process, if the initial temperature T_i equal to the freezing temperature T_f, the temperature in the liquid (solid) phase remains uniformly equal to the freezing point throughout the process. In this case, the temperature in solid (liquid) phase needs to be determined. Thus, the temperature only in one phase is unknown and the problem is called one phase problem. In solidification process the surface temperature T_0 is below the freezing temperature T_f and in melting process the surface temperature T_0 is greater than the melting temperature T_m.

If the initial temperature T_i is above (below) the freezing temperature T_f (melting temperature T_m), the temperature distribution in both solid and liquid region must be determined and the problem is called two phase solidification (melting) problem.

For multi-component phase change material, the phase change occurs over a range of temperature (T_{f_1}, T_{f_2}) instead of a single temperature. The phase change material is liquid if its temperature is above T_{f_2} and solid when its temperature is below T_{f_1}. Between the solid and liquid phases there is a mushy zone where the temperature falls within the phase change temperature range (T_{f_1}, T_{f_2}). The temperature distribution in solid region, mushy region and liquid region must be determined therefore, the problem is referred to as multi phase solidification problem. The mathematical model for one phase; two-phase and multi-phase are described as follows:

1.3.1 One Phase Moving Boundary Problem

Consider a semi infinite medium consisting of melt is initially kept at freezing temperature T_f. At time $t > 0$, the surface $r = 0$ is cooled at a temperature T_0 below than the freezing temperature. Therefore, the freezing process starts at the surface $r = 0$ and liquid-solid interface moves in the positive r- direction. The temperature in the solid phase is unknown and the liquid phase being at a constant temperature. Hence, the problem is one phase problem. The mathematical formulation of classical Stefan problem can be described by following differential equation:

$$\rho c \frac{\partial T}{\partial t} = K \frac{\partial^2 T}{\partial r^2}, \ 0 < r < s(t), \ t > 0, \tag{1.23}$$

and associated initial and boundary conditions are

$$T(r, 0) = T_f, \tag{1.24}$$

$$T(r, t) = T_0, \ r = 0, \tag{1.25}$$

$$T(r, t) = 0, \ r = s(t), \tag{1.26}$$

where ρ is density, c is specific heat, K is thermal conductivity and are assumed to be constant.

The energy balance equation at the interface is

$$-K \frac{\partial T}{\partial r} = \rho L \frac{ds}{dt}, \ r = s(t), \tag{1.27}$$

$$s(0) = 0, \tag{1.28}$$

where L is latent heat.

1.3.2 Two Phase Moving Boundary Problem

Consider a semi infinite medium consisting of a melt initially kept at temperature T_i which is greater than the freezing temperature T_f. At time $t > 0$, the surface $r = 0$ is cooled at a temperature T_0 which is below the freezing temperature. The freezing starts and solid-liquid interface moves in positive r-direction. The region is divided into two regions; $0 < r < s(t)$ is solid region and $s(t) < r < \infty$ is liquid region

which are shown in Fig. (1.3). The heat occurs in both solid and liquid region. Let $T_1(r,t)$ and $T_2(r,t)$ are the temperature of solid and liquid region respectively.
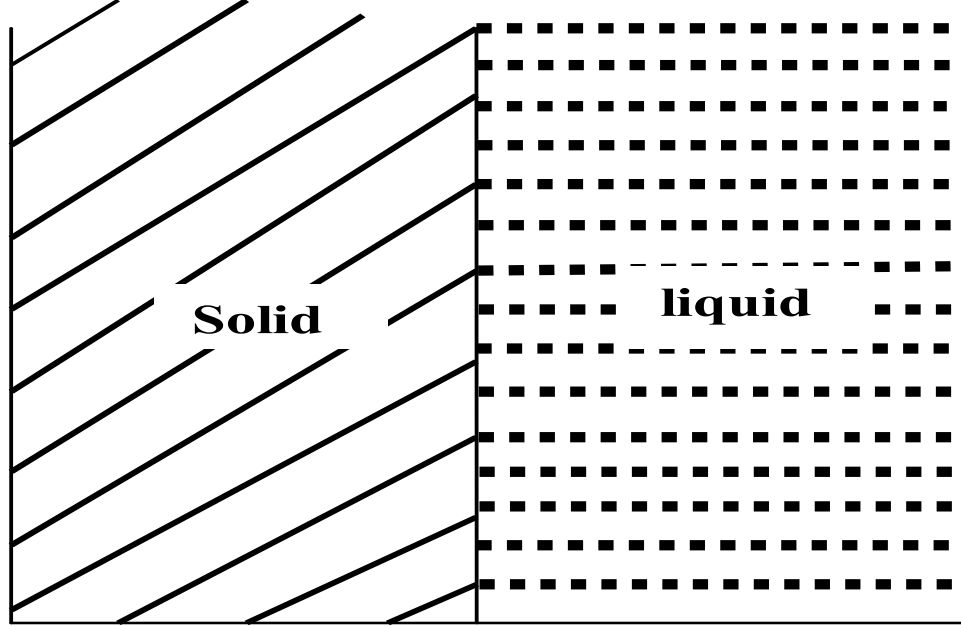

Figure 1.3: Two phase diagram

The dynamics of freezing can be described by the following equations:

In solid region

$$\rho_1 c_1 \frac{\partial T_1}{\partial t} = K_1 \frac{\partial^2 T_1}{\partial r^2}, \ 0 < r < s(t), \ t > 0. \tag{1.29}$$

In liquid region

$$\rho_2 c_2 \frac{\partial T_2}{\partial t} = K_2 \frac{\partial^2 T_2}{\partial r^2}, \ s(t) < r < \infty. \tag{1.30}$$

The initial and boundary conditions are

$$T_1(r,0) = T_i, \tag{1.31}$$

$$T_1(r,t) = T_0, \ r = 0, \tag{1.32}$$

on moving interface the temperature continuity and energy balance equations are defined as

$$T_1(r,t) = T_2(r,t) = T_f, \tag{1.33}$$

$$K_1 \frac{\partial T_1}{\partial r} - K_2 \frac{\partial T_2}{\partial r} = \rho L \frac{ds(t)}{dt}, \ r = s(t), \tag{1.34}$$

as $r \to \infty$, the temperature of material is equal to the initial temperature T_i.

$$T_2(r, t) = T_i, \ r \to \infty, \tag{1.35}$$

where ρ_1, ρ_2 are densities, c_1, c_2 are heat capacities and K_1 and K_2 are thermal conductivities of solid and liquid respectively. There is no volume change due to densities on freezing hence, assumed constant i.e. $\rho_1 = \rho_2 = \rho$.

1.3.3 Multi Phase Moving Boundary Problem

When a binary alloy is cooled and solidified, an interface formed and separating the solid and liquid region. The crucial point for solidification is that the heat is continuously remove from the interface, first to cool the liquid to its freezing temperature T_f, then to enable the solidification to proceed. The solidification interface deform with the local velocity of propagation which depends on the local temperature gradients on both sides of the interface. In the case of solidification of binary alloy, the composition of forming solid is different from the composition of the liquid ahead of the interface. Hence, at the interface boundary, one component must be rejected from the system and then removed away from the interface. This removal is enhanced near protrusions of solid into the liquid and solid is growing faster. Therefore, the solidification interface is morphologically unstable and highly complicated.

Consider a line heat sink of strength Q, is kept at $r = 0$ in a large body of liquid which is initially at uniform temperature T_i higher than the liquidus temperature T_l. The heat sink is activated at time $t = 0$ and absorbs heat continuously for time $t > 0$. The solidification process start and propagate in positive r-direction. Since, we have considered a binary system in which the two phase region consisting of solid and liquid mixture exist between purely solid and purely liquid region shown in Fig. (1.4). All the thermo-physical properties are constant and different from different phases. When solid is continuously formed with in two phase region, the heat released during solidification is treated as a volumetric heat generation term and expressed as

$$A = \rho L \frac{df_s}{dt}, \tag{1.36}$$

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where f_s is solid fraction present in mushy region. Thus, the rate of change of solid fraction with respect to the time with in mushy region provides a heat generation effect.
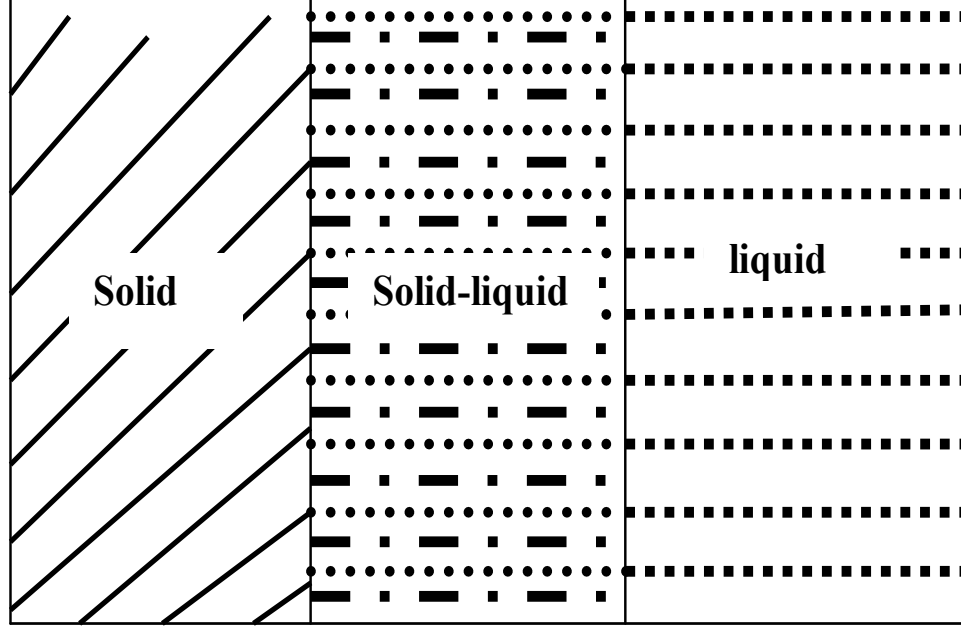

Figure 1.4: Multi phase diagram

The solid fraction depends on various physical parameters such temperature dependent and distance dependent. The solid fraction temperature relationship was given by Tien and Geiger (1968). Özisik and Uzzell (1979) considered two models for determining the solid fraction in mushy region.

Model I: In this model, a linear relationship is assumed between the solid fraction and temperature in mushy region and defined as

$$f_s = f_{su}\left(1 - \frac{T_2 - T_l}{T_2 - T_f}\right). \qquad (1.37)$$

Model II: In this model, the solid fraction present in mushy region has a linear relationship with distance and defined as

$$f_s = f_{su}(1 - R), \quad R = \left(\frac{r - s_1(t)}{s_2(t) - s_1(t)}\right). \qquad (1.38)$$

The differential equations of heat conduction for the solid, mushy and liquid regions are given as

In solid region,

$$\rho_1 c_1 \frac{\partial T_1}{\partial t} = K_1 \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_1}{\partial r} \right), \ 0 < r < s_1(t). \tag{1.39}$$

In mushy region,

$$\rho_2 c_2 \frac{\partial T_2}{\partial t} = K_2 \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_2}{\partial r} \right) + A, \ s_1(t) < r < s_2(t). \tag{1.40}$$

In liquid region,

$$\rho_3 c_3 \frac{\partial T_3}{\partial t} = K_3 \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_3}{\partial r} \right), \ s_2(t) < r < \infty. \tag{1.41}$$

The heat sink at origin should satisfy the energy balance equation

$$\lim_{r \to \infty} \left(2\pi r K_1 \frac{\partial T_1}{\partial r} \right) = Q. \tag{1.42}$$

The boundary conditions at the solidus front are

$$T_1(r, t) = T_2(r, t) = T_f, \ \ r = s_1(t). \tag{1.43}$$

The energy equation at solid-mushy boundary

$$K_1 \frac{\partial T_1}{\partial r} - K_2 \frac{\partial T_2}{\partial r} = \rho L (1 - f_{su}) \frac{ds_1(t)}{dt}, \ \ r = s_1(t). \tag{1.44}$$

$$T_2(r, t) = T_3(r, t) = T_l, \ \ r = s_2(t). \tag{1.45}$$

The energy equation at mushy-liquid boundary

$$K_2 \frac{\partial T_2}{\partial r} = K_3 \frac{\partial T_3}{\partial r}, \ \ r = s_2(t). \tag{1.46}$$

As $r \to \infty$, the liquidus temperature is equal to initial temperature i.e.

$$T_3(r, t) = T_i, \ \text{as} \ r \to \infty. \tag{1.47}$$

1.3.4 Two Dimensional Moving Boundary Problem

The two-dimensional moving boundary problem is described by following differential equation:

$$\rho c \frac{\partial T}{\partial t} = K \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right), \ 0 < r < s(t), \ t > 0. \tag{1.48}$$

The energy balance equation defined for one dimensional case is now generalized for multidimensional case. For the two-dimensional problem involving the (x, z, t)

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variables, if the position of the solid-liquid interface is specified by the relation $F(x, z, t) = z - s(x, t) = 0$, then the interface condition is described by

$$\left(1 + \left(\frac{\partial s}{\partial x}\right)^2\right)\left(K_1\frac{\partial T_1}{\partial z} - K_2\frac{\partial T_2}{\partial z}\right) = \rho L\frac{\partial s}{\partial t}, \quad z = s(x, t). \qquad (1.49)$$

The initial and boundary conditions are defined in Eqs.(1.24-1.26).

1.3.5 Three Dimensional Moving Boundary Problem

The three dimensional moving boundary problem is defined as

$$\rho c\frac{\partial T}{\partial t} = K\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right), \quad 0 < r < s(t), \ t > 0. \qquad (1.50)$$

In case of three dimensional region, the solid-liquid phases are separated by a sharp interface defined by the equation

$$F(x, y, z, t) = 0. \qquad (1.51)$$

The temperature continuity at the interface becomes

$$T_1(x, y, z, t) = T_2(x, y, z, t) = T_f, \quad at \ F(x, y, z, t) = 0. \qquad (1.52)$$

The interface energy-balance equation is written as

$$K_1\frac{\partial T_1}{\partial n} - K_2\frac{\partial T_2}{\partial n} = \rho L v_n, \qquad (1.53)$$

where $\frac{\partial}{\partial n}$ denotes the derivative at the interface along the normal direction vector n at any location p on the interface and pointing towards the liquid region and v_n is the velocity of this interface at the location p in the direction of n. Here we assumed that the densities of the solid and liquid phases are the same. The interface energy-balance Eq. (1.53) is not in a suitable form for analytical or numerical solutions of phase changes problems. Hence an alternative form of this equation is given by

$$\left[1 + \left(\frac{\partial s}{\partial x}\right)^2 + \left(\frac{\partial s}{\partial y}\right)^2\right]\left[K_1\frac{\partial T_1}{\partial n} - K_2\frac{\partial T_2}{\partial n}\right] = \rho L\frac{\partial s}{\partial t} \quad at \ z = s(x, y, t). \quad (1.54)$$

This form is more suitable form for analytical or numerical solution of problems.

1.3.6 Melting Problem

The problems defined in Eqs. (1.23 - 1.35) is a solidification problem as the phase change from liquid to solid. The melting problem can be formulated for minor changes in Eq. (1.23 - 1.35). In solidification process latent heat is released but during melting latent heat is absorbed. The mathematical formulation for both solidification and melting are analogous. Consider a solid in a semi infinite region having a phase change temperature T_m. Initially, the solid is at uniform temperature T_i that is lower than the phase change temperature T_m. At time $t = 0$, the temperature at the surface $x = 0$ is suddenly raised to a temperature T_0, which is higher than the melting temperature T_m and maintained at that temperature for times $t > 0$. The solid-liquid interface moves in the positive x- direction. The region is divided into two regions, the region $0 < r < s(t)$ is liquid region and $s(t) < r < \infty$ is solid. Assuming that the thermo-physical properties for each phases are constant. The governing differential equations for two phase problem are given by

In liquid region

$$\rho_1 c_1 \frac{\partial T_1}{\partial t} = K_1 \frac{\partial^2 T_1}{\partial r^2}, \ 0 < r < s(t), \ t > 0. \tag{1.55}$$

In solid region

$$\rho_2 c_2 \frac{\partial T_2}{\partial t} = K_2 \frac{\partial^2 T_2}{\partial r^2}, \ s(t) < r < \infty. \tag{1.56}$$

The initial and boundary conditions are

$$T_1(r, 0) = T_i, \tag{1.57}$$

$$T_1(r, t) = T_0, \ r = 0. \tag{1.58}$$

On moving interface the temperature continuity and energy balance equations are defined as

$$T_1(r, t) = T_2(r, t) = T_m, \tag{1.59}$$

$$K_1 \frac{\partial T_1}{\partial r} - K_2 \frac{\partial T_2}{\partial r} = \rho L \frac{ds(t)}{dt}, \ r = s(t), \tag{1.60}$$

as $r \to \infty$ the temperature of material is equal to the initial temperature T_i i.e.

$$T_2(r, t) = T_i, \ r \to \infty. \tag{1.61}$$

The basic concepts on modelling and analysis for classical stefan problems has been described by Carslaw and Jaegar (1959); Alexiades and Solomon (1993); Gupta (2003).

1.4 Methods of Solution

The exact solution of moving boundary problems was given by first Neumann (1912) and by Stefan (1889). They considered a semi infinite material with simple initial and boundary conditions. The exact solution of moving boundary problem is established in terms of the similarity variables $r/t^{1/2}$ and position of the interface boundary is found to be proportional to $t^{1/2}$. This means that the problem is solved by a similarity transformation, i.e. the partial differential equations of the problem are reduced into the ordinary differential equations. The reduction of partial differential equation into ordinary differential equation is possible only when the domain is semi infinite and initial and boundary conditions are defined in some special forms.

1.4.1 Approximate Analytical Solution

1.4.1.1 Heat Balance Integral Method

Since the exact solutions are exist only for semi infinite problems with constant parameters at each phase with simple initial and boundary condition. The exact solutions are not applicable for constant heat flux. So approximate analytical solutions have been developed. One of the approximate solution is introduced by Goodman (1958) known as heat balance integral method and based on Karmann Pohlhuasen's method of momentum integral in the boundary layer theory. In this method Goodmann developed the integral equation which describes the overall heat balance of system by integrating the one-dimensional heat conduction equation with respect to spatial variable r and using the boundary conditions. The heat balance integral method is defined as

- assume that the temperature distribution depends on the spatial variable in

the particular form which is consistent with the boundary conditions, for example a polynomial relationship;

- integrate the heat conduction equation with respect to the spatial variable over the appropriate interval and substitute the assumed form of the temperature distribution to attain the heat balance integral;

- solve the integral equation to obtain the time dependence of the temperature distribution and of moving boundaries.

1.4.1.2 Method of Weighted Residual (MWR)

Method of weighted residual is an approximate method to find the solution of differential equations. Let us consider a linear differential operator $\mathcal{L}$ acting on a function u to produce a function p i.e.

$$\mathcal{L}(u(r)) = p(r). \tag{1.62}$$

We wish to approximate u by a function U_N, which is a linear combination of basis functions chosen from a linearly independent set. That is,

$$u \cong U_N = \sum_{i=1}^{n} c_i \phi_i, \tag{1.63}$$

where c_i are unknown constants and ϕ_i are called the trial functions. The trial functions should be linearly independent. Now, when substituted the approximate function U_N into the differential operator $\mathcal{L}$, the result of the operations is not, in general, $p(r)$. Hence a error or residual will exist:

$$R(x) = \mathcal{L}(U_N(r)) - p(r) \neq 0. \tag{1.64}$$

The parameters c_i are determined by setting the weighted average of the residual over the computational domain to zero i.e.,

$$\int_{\Omega} R(r) W_i dr = 0, \quad i = 1, 2, 3, \cdots\cdots, n. \tag{1.65}$$

The functions W_i are called weight functions. The number of weight functions W_i is an exactly equal to the number of unknown constants c_i present in an approximate

function U_N. The result is a set of n algebraic equations for the unknown constants c_i. There are several sub-methods for choices of weight function W_i.

- **Galerkin Method**

  In Galerkin method, the weight function is chosen from the same family of functions as the trial functions in Eq. (1.65) i.e. $W_i = \phi_i, \;\; i = 1, 2, \cdots, n$.

- **Petrov-Galerkin Method**

  In Petrov-Galerkin method, the weight function is represented by $W_i = \phi_i^1 \neq \phi_i, \;\; i = 1, 2, \cdots, n$. The more details of Petrov-Galerkin method are given in book of Reddy (2002).

- **Collocation Method**

  In this method, the weight functions are taken from the family of Dirac δ functions in the domain i.e. $W_i = \delta(r - r_i), \;\; i = 1, 2, \cdots, n$. The dirac δ function is defined by

  $$\delta(r - r_i) = \begin{cases} 1, & r = r_i \\ 0, & \text{otherwise.} \end{cases} \tag{1.66}$$

  Hence, the integration of the weighted residual statement results in the forcing of the residual to zero at specific points in the domain. That is, integration of Eq. (1.65) with weight function $W_i = \delta(r - r_i), \;\; i = 1, 2, \cdots, n$ is $R(r_i) = 0$.

1.4.2   Legendre Polynomial

The Legendre polynomials, $P_n(r), n = 0, 1, 2, \cdots$ are eigen solutions to the Sturm-Liouville problem

$$\frac{d}{dr}\left[(1 - r^2)\frac{dP_n(r)}{dr}\right] + n(n + 1)P_n(r) = 0, \tag{1.67}$$

where $p(r) = 1 - r^2, q(r) = 0$ and $w(r) = 1$ with eigen values $\lambda_n = n(n + 1)$. $P_n(r)$ is even if n is even and odd if n is odd. If $P_n(r)$ is normalized so that $P_n(1) = 1$, then for any n

$$P_n(r) = \frac{1}{2n}\sum_{k=0}^{[n/2]}(-1)^k\binom{n}{k}\binom{2n - 2k}{n}r^{n-2k}, \tag{1.68}$$

where $[n/2]$ denotes the integral part of $n/2$.

The Legendre polynomials can be expressed by Rodrigues formula

$$P_n(r) = \frac{(-1)^n}{2^n n!} \frac{d^n}{dr^n}[(1 - r^2)^n]. \tag{1.69}$$

The three term recurrence relation for Legendre polynomials

$$(n + 1)P_{n+1}(r) = (2n + 1)rP_n - nP_{n-1}(r), \tag{1.70}$$

yields a direct way to evaluate the Legendre polynomials of arbitrary order.

The generating function of a Legendre polynomial is

$$\frac{1}{\sqrt{1 - 2rt + t^2}} = \sum_{n=0}^{\infty} P_n(r)t^n. \tag{1.71}$$

Legendre polynomials $P_n(r)$, $n = 0, 1, 2, \cdots$ form a complete orthogonal set on the interval $-1 \le r \le 1$. It can be shown that

$$\int_{-1}^{1} P_m(r)P_n(r)dr = \begin{cases} 0, & m \ne n \\ \frac{2}{2n+1}, & m = n. \end{cases} \tag{1.72}$$

1.4.3   Spectral Galerkin Method

The spectral method employs global polynomials as the trial functions for the discretization of partial differential equations. It provides very accurate approximations with a relatively small number of unknowns. Consequently it has gained increasing popularity in the last two decades, especially in the field of computational fluid dynamics (Canuto (1987), Gottlieb (1977)). This method is distinguished not only by the fundamental type of the method (Galerkin, Collocation, Galerkin with numerical integration or tau) but also by the particular choice of trial functions. The most frequently used trial functions are trigonometric polynomials, Chebyshev polynomials and Legendre polynomials. In this section we shall discussed the basic principles of spectral Galerkin method. Consider a differential equation

$$\frac{\partial u}{\partial t} = \mathcal{L}(u), \tag{1.73}$$

where $u(r,t)$ is the solution and $\mathcal{L}$ is a differential operator (linear or nonlinear) that contains all the spatial derivatives of u. An approximate solution is given as

$$U_N = \sum_{i=1}^{n} c_i(t)\phi_i(r). \tag{1.74}$$

The ϕ_i are the trial functions, whereas the c_i are the unknown coefficients. In general, U_N will not satisfy Eq. (1.73), i.e. the residual

$$\frac{\partial U_N}{\partial t} - \mathcal{L}(U_N), \tag{1.75}$$

will not vanish. For minimizing the residual, we take residual orthogonal to trial functions. i.e.

$$\int_{\Omega} \left[\frac{\partial U_N}{\partial t} - \mathcal{L}(U_N) \right] \phi_i(r) dr = 0, i = 1, 2, 3 \cdots, n. \tag{1.76}$$

Eq. (1.76) represents the system of ordinary differential equations of the form

$$\frac{d\bar{C}}{dt} = \bar{f}(t, \bar{C}), \tag{1.77}$$

where, $\bar{f}$ and $\bar{C}$ are column matrix and defined as $\bar{f} = [f_1, f_2, f_3......, f_n]^T$, $\bar{C} = [c_1, c_2, c_3, ..., c_n]^T$ respectively. The solution of Eq. (1.77) provides the unknown C. Substituting C in Eq. (1.74), we get required solution.

1.4.4 Spectral Petrov-Galerkin Method

Consider a differential equation defined in Eq. (1.73). Let U_N is an approximate solution of Eq. (1.73) defined as

$$U_N = \sum_{i=1}^{n} c_i(t)\phi_i(r). \tag{1.78}$$

For minimizing the residual, we take residual is orthogonal to test function which is different from the trial function ($\phi_i^1 \neq \phi_i$), i.e.

$$\int_{\Omega} \left[\frac{\partial U_N}{\partial t} - \mathcal{L}(U_N) \right] \phi_i^1(r) dr = 0, i = 1, 2, 3 \cdots, n. \tag{1.79}$$

Eq. (1.79) gives the system of differential equation in unknown $\bar{C}$.

1.4.5   Numerical Solutions

1.4.5.1   Fixed Grid Method

In this method, the heat flow equation is to be solved by using finite difference replacements for derivatives in order to compute values of temperature T_{ij}, at discrete points $(i\delta r, j\delta t)$ on a fixed grid in the (r, t) plane. At any time $j\delta t$, the moving boundary will be located between two neighbouring grid points, say $i\delta r$ and $(i+1)\delta r$. As seen, the numerical solution of the method is carried out on a space grid that remains fixed throughout the calculation.

1.4.5.2   Variable Grid Method

The fixed grid method sometimes breakdown as boundary moves a distance larger than space increment in a time step. The problem associated with the fixed grid method can be avoided by using the variable grid method. In the variable grid method, the number of spatial intervals are kept constants and the spatial intervals are adjusted in such manner so that the moving boundary lies on a particular grid points. Thus, in this method the spatial intervals are a function of time. The substantial temperature derivative of each grid point is

$$\left(\frac{dT}{dt}\right)_i = \left(\frac{\partial T}{\partial r}\right)_t \left(\frac{dr}{dt}\right)_i + \left(\frac{\partial T}{\partial t}\right)_r, \tag{1.80}$$

where the moving rate of each grid point is related to the moving boundary by

$$\left(\frac{dr}{dt}\right)_i = \frac{r}{s(t)}\frac{ds}{dt}. \tag{1.81}$$

Substitute Eq. (1.81) and Eq. (1.23) in Eq. (1.80). The one-dimensional heat equation becomes

$$\left(\frac{dT}{dt}\right)_i = \frac{r}{s(t)}\frac{ds}{dt}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2}, \tag{1.82}$$

and $s(t)$ is updated at each time step by using, for example, a suitable finite-difference form of the boundary condition $ds/dt = -\partial T/\partial r$ on $r = s(t)$.

1.4.5.3 Enthalpy Method

The essential feature of the basic enthalpy method is that the evaluation of latent heat is accounted for by the enthalpy as well as the relationship between enthalpy and temperature. The method can be illustrated by considering a one-dimensional heat conduction controlled phase problem. An appropriate equation for such a case can be expressed by

$$\rho\frac{\partial h}{\partial t} = \frac{\partial}{\partial r}\left(K\frac{\partial T}{\partial r}\right).$$

(1.83)

The relationship between the enthalpy and temperature can be defined in terms of the latent heat release characteristic of the phase change material. This relationship assumed to be a step function for isothermal phase change problem and a linear function for non-isotherm phase change cases defined in Fig. (1.5). The enthalpy as a function of temperature for both cases is given by

for isotherm phase change

$$h = \begin{cases} c_s T, & T \leq T_m \ \text{solid phase} \\ c_l T + H_f, & T \geq T_m \ \text{liquid phase} \end{cases}$$

(1.84)

for non-isotherm phase change

$$h = \begin{cases} c_s T, & T \leq T_s \ \text{solid phase} \\ c_{in}T + \frac{H_f(T-T_s)}{(T_l-T_s)}, & T_s \leq T \leq T_l \ \text{solid/liquid phase} \\ c_l T + H_f + c_{in}(T_l - T_s), & T \geq T_l \ \text{liquid phase} \end{cases}$$
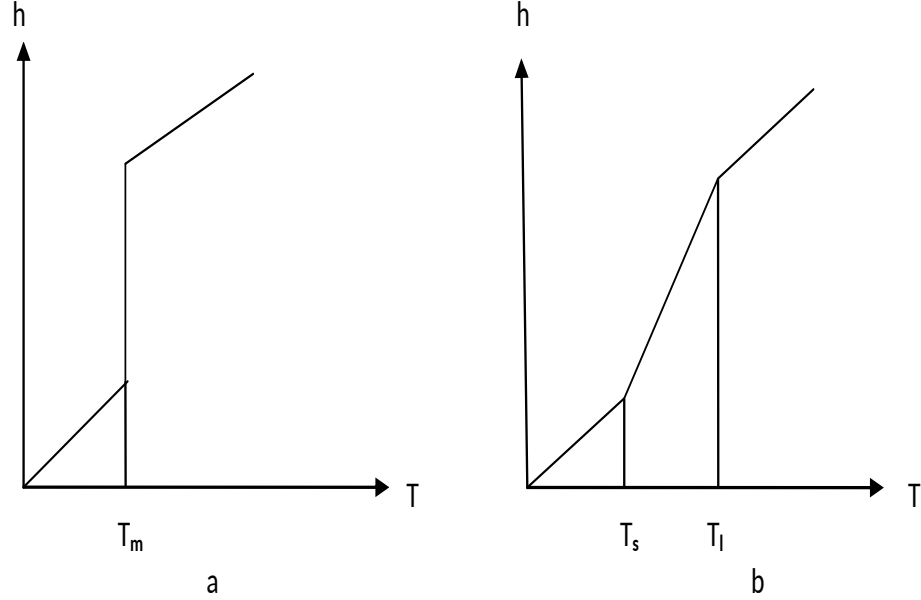
(1.85)

Figure 1.5: Enthalpy as a function of temperature for (a) isothermal phase change (b) non-isothermal phase change.

1.5 Wavelets

In this section, we described some preliminary concepts of wavelets, Legendre wavelets, basis function and their properties, operational matrix of integration and differentiation.

Wavelets constitute a family of functions constructed from dilation and translation of a single function called the mother wavelets. When the dilation parameters a and the translation parameters b vary continuously, we have the following family of wavelets as

$$\psi_{a,b}(t) = |a|^{-1/2}\psi\left(\frac{t-b}{a}\right), \quad a, b \in R, \ a \neq 0. \tag{1.86}$$

1.5.1 Legendre Wavelets

The Legendre wavelets $\psi_{nm}(t) = (k, \hat{n}, m, t)$ have four arguments, where $k = 1, 2, 3......$, $\hat{n} = 2n - 1$, $n = 1, 2, .., 2^{k-1}$, m is the order of Legendre polynomial and t is normalized time and all are defined by Razzaghi and Yousefi (2000) on the

interval $[0,1]$ as follows:

$$\psi_{nm}(t) = \begin{cases} \sqrt{(m+1/2)}2^{k/2}P_m(2^k t - \hat{n}) & , \quad \frac{\hat{n}-1}{2^k} \le t \le \frac{\hat{n}+1}{2^k} \\ 0 & , \quad \text{otherwise,} \end{cases} \tag{1.87}$$

where $m = 1, 2, .., M-1$, $P_m(t)$ is denoted by Legendre polynomial of order m which are orthogonal with respect to the weight function $w(t) = 1$, $t \in [-1, 1]$ and satisfying the following formula

$$P_0(t) = 1, \ P_1(t) = t, \ P_{m+1}(t) = \left(\tfrac{2m+1}{m+1}\right) t P_m(t) - \tfrac{m}{m+1} P_{m-1}(t), \quad m = 1, 2, 3..... \ .$$

1.5.2 Function Approximation

A function $f(t)$ defined in domain $[0,1]$, may be expressed by Legendre wavelets series as

$$f(t) = \sum_{n=1}^{\infty} \sum_{m=0}^{\infty} c_{nm}\psi_{nm}(t), \tag{1.88}$$

where c_{nm} is Fourier coefficient. The infinite series in Eq. (1.88) is truncated and can be written as

$$f(t) \simeq \sum_{n=1}^{2^{k-1}} \sum_{m=0}^{M-1} c_{nm}\psi_{nm}(t) = C^T\psi(t), \tag{1.89}$$

where C and ψ are matrices of order $2^{k-1} M \times 1$ and given by

$$C = \quad [c_{10}, c_{11}, ..., c_{1M-1}, c_{20}, c_{21}, ..., c_{2M-1}...., c_{2^{k-1}0}, ..., c_{2^{k-1}M-1}]^T, \tag{1.90}$$

$$\psi(t) = \quad [\psi_{10}(t), \psi_{11}(t), ...\psi_{1M-1}(t), \psi_{20}(t), \psi_{21}(t)...\psi_{2M-1}(t), ...(t), ...,$$

$$\psi_{2^{k-1}0}, \psi_{2^{k-1}1}...., \psi_{2^{k-1}M-1}(t)]^T. \tag{1.91}$$

1.5.3 Operational Matrix of Integration

The operational matrix of integration is defined by Razzaghi and Yousefi (2001) as follow

$$\int_0^t \psi(s)ds = P\psi(t), \ t \in [0, 1], \tag{1.92}$$

where P is operational matrix of integration of order $2^{k-1}M \times 2^{k-1}M$.

$$P = \frac{1}{2^k} \begin{pmatrix} L & O & O & \cdots & O \\ 0 & L & O & \cdots & O \\ 0 & 0 & L & \cdots & O \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & O \\ 0 & 0 & 0 & \cdots & O \end{pmatrix} \qquad (1.93)$$

where O and L are $M \times M$ matrices given by

$$O = \begin{pmatrix} 2 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

and

$$L = \begin{pmatrix} 1 & \frac{1}{\sqrt{3}} & 0 & 0 & \cdots & 0 & 0 & 0 \\ \frac{-1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{15}} & 0 & \cdots & 0 & 0 & 0 \\ 0 & \frac{-1}{\sqrt{15}} & 0 & \frac{1}{\sqrt{35}} & \cdots & 0 & 0 & 0 \\ 0 & 0 & \frac{-1}{\sqrt{35}} & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{1}{\sqrt{(2M-3)(2M-1)}} & 0 & \frac{1}{\sqrt{(2M-3)(2M-5)}} \\ 0 & 0 & 0 & 0 & \cdots & 0 & \frac{-1}{\sqrt{(2M-1)(2M-3)}} & 0 \end{pmatrix}$$

respectively.

1.5.4 Property of Legendre Wavelets

The Legendre wavelets satisfying the following property

$$\int_0^1 \psi(t)\psi^T(t) = I. \qquad (1.94)$$

1.5.5 Property of Product of Two Legendre Wavelets

If E is a given wavelets vector then we have a property

$$E^T \psi(t)\psi^T(t) = \psi^T(t)\hat{E}, \qquad (1.95)$$

where $\hat{E}$ is $2^{k-1}M \times 2^{k-1}M$ matrices depend on the wavelet vector E.

1.5.6 Two-Dimensional Legendre Wavelets

The two-dimensional Legendre wavelets which is defined on the interval $[0, 1] \times [0, 1]$ by Parsian (2005) as follows:

$$\psi_{nmn'm'}(x, y) = \begin{cases} \sqrt{(m+1/2)(m'+1/2)}2^{(k+k')/2}P_m(2^k x - \hat{n})P'_m(2^k y - \hat{n}'), \\ \qquad \frac{\hat{n}-1}{2^k} \le x \le \frac{\hat{n}+1}{2^k}, \quad \frac{\hat{n}'-1}{2^{k'}} \le y \le \frac{\hat{n}'+1}{2^{k'}} \qquad (1.96) \\ 0, \qquad \text{otherwise} \end{cases}$$

where $m = 0, 1, 2, ..., M-1$, $m' = 0, 1, 2, ...,M'-1$, $\hat{n} = 2n-1$, $\hat{n}' = 2n'-1$, $n = 1, 2...., 2^{k-1}$ and $n' = 1, 2...., 2^{k'-1}$. $P_m(x)$ and $P_{m'}(y)$ are Legendre polynomials of order m and m' and orthogonal to weight function $w(x) = w(y) = 1$ defined over the interval $[-1, 1]$. The recursive formula for $P_m(x)$ and $P_{m'}(y)$ are

$$P_0(x) = 1, \quad P_1(x) = x, \quad (m+1)P_{m+1}(x) = (2m+1)P_m(x) - mP_{m-1}(x), \quad (1.97)$$

and

$$P_0(y) = 1, \quad P_1(y) = y, \quad (m'+1)P_{m'+1}(y) = (2m'+1)P'_m(y) - m'P_{m'-1}(y), \quad (1.98)$$

respectively.

1.5.7 Function Approximation

A function $f(x, y)$ is defined in domain $[0, 1] \times [0, 1]$ may be expressed as

$$f(x, y) = \sum_{n=1}^{\infty}\sum_{n'=1}^{\infty}\sum_{m=0}^{\infty}\sum_{m'=0}^{\infty} c_{nmn'm'}\psi_{nmn'm'}(x, y), \qquad (1.99)$$

where $c_{nmn'm'}$ is Fourier coefficient. The infinite series in Eq. (1.99) is truncated and can be written as

$$f(x, y) \simeq \sum_{n=1}^{2^{k-1}}\sum_{n'=1}^{2^{k'-1}}\sum_{m=0}^{M-1}\sum_{m'=0}^{M'-1} c_{nmn'm'}\psi_{nmn'm'}(x, y) = C^T\psi(x, y), \qquad (1.100)$$

where C and $\psi(x,y)$ are the column vector of order $2^{k-1}2^{k'-1}MM' \times 1$ which is given by

$$
\begin{aligned}
C = \quad & \big[c_{1010}, \cdots, c_{101M'-1}, c_{1020} \cdots c_{102M'-1}, c_{102^{k'-1}0} \cdots c_{102^{k'-1}M'-1}, \cdots, \cdots, \\
& c_{1M-110}, \cdots, c_{1M-11M'-1}, c_{1M-120}, \cdots, c_{1M-12M'-1}, \cdots, c_{1M-12^{k'-1}0}, \cdots, \\
& c_{1M-12^{k'-1}M-1}, c_{2010}, c_{201M'-1}, c_{2020}, \cdots c_{202M'-1}, \cdots, c_{202^{k'-1}0}, \cdots, \cdots, \\
& c_{202^{k'-1}M'-1}, c_{2M-110}, \cdots, c_{2M-11M'-1}, c_{2M-120}, \cdots, c_{2M-12M'-1}, \cdots, \cdots, \\
& c_{2M-12^{k'-1}0}, \cdots, c_{2M-12^{k'-1}M'-1}, \cdots, c_{2^{k-1}010}, \cdots, c_{2^{k-1}01M'-1}, c_{2^{k-1}020}, \cdots, \\
& c_{2^{k-1}02M'-1}, \cdots, c_{2^{k-1}02^{k'-1}0}, \cdots, c_{2^{k-1}M-12^{k'-1}M'-1}\big]^T
\end{aligned}
\tag{1.101}
$$

and

$$
\begin{aligned}
\psi = \quad & \big[\psi_{1010}, \cdots, \psi_{101M'-1}, \psi_{1020} \cdots \psi_{102M'-1}, \psi_{102^{k'-1}0} \cdots \psi_{102^{k'-1}M'-1}, \cdots, \cdots, \\
& \psi_{1M-110}, \cdots, \psi_{1M-11M'-1}, \psi_{1M-120}, \cdots, \psi_{1M-12M'-1}, \cdots, \psi_{1M-12^{k'-1}0}, \cdots, \\
& \psi_{1M-12^{k'-1}M-1}, \psi_{2010}, \psi_{201M'-1}, \psi_{2020}, \cdots \psi_{202M'-1}, \cdots, \psi_{202^{k'-1}0}, \cdots, \cdots, \\
& \psi_{202^{k'-1}M'-1}, \psi_{2M-110}, \cdots, \psi_{2M-11M'-1}, \psi_{2M-120}, \cdots, \psi_{2M-12M'-1}, \cdots, \cdots, \\
& \psi_{2M-12^{k'-1}0}, \cdots, \psi_{2M-12^{k'-1}M'-1}, \cdots, \psi_{2^{k-1}010}, \cdots, \psi_{2^{k-1}01M'-1}, \cdots, \cdots, \\
& \psi_{2^{k-1}020}, \cdots, \psi_{2^{k-1}02M'-1}, \cdots, \psi_{2^{k-1}02^{k'-1}0}, \cdots, \psi_{2^{k-1}M-12^{k'-1}M'-1}\big]^T.
\end{aligned}
\tag{1.102}
$$

1.5.8 Operational Matrix of Integration for x Variable

Theorem 1.1 *Let $\psi(x,y)$ be the two-dimensional Legendre wavelets vector defined in Eq. (1.99) then*

$$
\int_0^x \psi(s,y)ds = P_x\psi(x,y),
\tag{1.103}
$$

where, P_x is $2^{k-1}2^{k'-1}MM' \times 2^{k-1}2^{k'-1}MM'$ operational matrix of integration defined as

$$P_x = \frac{1}{M'2^{k'+k-1}} \begin{pmatrix} L & F & F & \cdots & F \\ O & L & F & \cdots & F \\ O & O & L & \cdots & F \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O & O & O & \cdots & F \\ O & O & O & \cdots & L \end{pmatrix},$$ (1.104)

and; F, L and O matrices of order $2^{k-1}MM' \times 2^{k-1}MM'$ are given as

$$F = \begin{pmatrix} 2D & O' & O' & \cdots & O' \\ O' & O' & O' & \cdots & O' \\ O' & O' & O' & \cdots & O' \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O' & O' & O' & \cdots & O' \\ O' & O' & O' & \cdots & O' \end{pmatrix},$$

$$L = \begin{pmatrix} D & \frac{1}{\sqrt{3}}D & O' & \cdots & O' \\ -\frac{1}{\sqrt{3}}D & O' & \frac{1}{\sqrt{15}}D & \cdots & O' \\ O' & -\frac{1}{\sqrt{15}}D & O' & \cdots & O' \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O' & O' & O' & \cdots & O' \\ O' & O' & O' & \cdots & O' \end{pmatrix},$$

and

$$O = \begin{pmatrix} O' & O' & O' & \cdots & O' \\ O' & O' & O' & \cdots & O' \\ O' & O' & O' & \cdots & O' \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O' & O' & O' & \cdots & O' \\ O' & O' & O' & \cdots & O' \end{pmatrix},$$

where D is the matrix of order $2^{k'-1}M' \times 2^{k'-1}M'$ which is given as

$$D = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix},$$

O' is zero matrix of order $2^{k'-1}M' \times 2^{k'-1}M'$.

1.5.9 Operational Matrix of Integration for y Variable

Theorem 1.2 *Let $\psi(x,y)$ be the two-dimensional Legendre wavelets vector defined in Eq. (1.99) then*

$$\int_0^y \psi(x,s')ds' = P_y\psi(x,y), \tag{1.105}$$

where, P_y is operational matrix of integration of order $2^{k-1}2^{k'-1}MM' \times 2^{k-1}2^{k'-1}MM'$, is given as

$$P_y = \frac{1}{M2^{k-1}} \begin{pmatrix} P & P & P & \cdots & P \\ P & P & P & \cdots & P \\ P & P & P & \cdots & P \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ P & P & P & \cdots & P \end{pmatrix},$$

in which P is

$$P = \frac{1}{2^{k'}} \begin{pmatrix} L & F & F & \cdots & F \\ O & L & F & \cdots & F \\ O & O & L & \cdots & F \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O & O & O & \cdots & L \end{pmatrix},$$

where, O, L and F are $M \times M'$ matrices. O is the zero matrix and L, F are given as

$$L = \begin{pmatrix} D & \frac{1}{\sqrt{3}} & 0 & \cdots & 0 \\ -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{15}} & \cdots & 0 \\ 0 & -\frac{1}{\sqrt{15}} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

and

$$F = \begin{pmatrix} 2 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

1.6 Literature Survey on Moving Boundary Problems

The analysis of heat transfer problems in melting/solidification process, called moving boundary problems. Moving boundary problems have been studied first by Lamé and Clapeyron (1831), concerning ice formation. However the mathematical model of this phenomenon is traditionally named after the Austrian physicist Stefan (1889), who published four papers as follows:

- On some problem in the theory of heat conduction.

- On the diffusion of acid and alkaline solution through each other.

- On the theory of ice formation with reference to the Arctic sea.

- On evaporation and condensation as diffusion processes.

The first paper deals with the freezing of ground and in this paper he considered two problems: one problem is semi infinite $(0, \infty)$ region and second problem is infinite region $(-\infty, \infty)$. In the same work, Stefan gave an analogous description

of processes of neutralization for diffusion transport of material in a reaction zone. In his hard work, he examined the problem of melting of a layer of ice with initial temperature equal to zero, subject to the influence of the temperature $f(t)$ at the boundary $r = 0$. This problem had been solved in closed analytic form only for f is constant. Finally, Stefan published his fourth work related to evaporation and condensation. Since, the nonlinear form of energy balance at moving interface is present. Therefore, an exact solution of moving boundary problems are possible in limited cases. The simplest one-phase problem first solved analytically by Stefan (1889). The Laplace transform technique is used to solve one phase moving boundary problem by Evans *et al.* (1950). Ockenden and Hodgkins (1975) has shown the integral formulation of the oxygen diffusion problem described by the use of Laplace transform and has drawn attention to the usefulness of Fourier transform in semi infinite or finite domain.

Neumann (1912) extended the Stefan's solution to the two-phase problem. The one dimensional two-phase Stefan problem was formulated by Rubinstein (1947a) in terms of a system of integral equations and proved existence and uniqueness of a solution in a small time interval. Further integral formulations of the one-dimensional Stefan problem were then studied. Several techniques were used to prove well-posedness, results of approximation, regularity, asymptotic behaviour and some other properties.

In melting and freezing of binary alloy, Ruddle states in his monograph on solidification. A very serious disadvantage of all mathematical methods is that they are only applicable to materials which freeze at constant temperatures and are not capable when alloys solidifying over a extended range of temperature. The melting and freezing temperatures of a binary alloy are not constant values and they vary with the composition of the alloy. The solidification of the binary alloy for a given composition actually occurs at a temperature below the liquidus line. Hence, the solidification problem of a binary alloy is definitely more elaborate and complex than the classical Stefan problem for a pure metal. A known exact solution of the problem exists. This solution is, of course for a binary alloy in a semi infinite region with constant initial and boundary conditions. Boley has also examined the problem

by his embedding technique and obtained a short time solution. In his study the solidus and liquidus line are assumed to be straight line; the solution is therefore limited to dilute binary alloys. In addition there are some other studies for various aspects of solidification of binary alloy in which straight solidus and liquidus lines are also assumed. Mushy regions were first investigated for the one-dimensional Stefan problem by Atthey (1974), Lacey and Tayler (1983), Fasano and Primicerio (1985), Meirmanov (1981, 1983), Primicerio (1983) and many others. After the introduction of weak solutions, these regions were also studied in several space dimensions by Andreucci (1993), Bertsch *et al.* (1986), Bertsch and Klaver (1989), Götz and Zaltzman (1991a,b), Lacey and Herraiz (2000, 2002).

To find the solution of moving boundary problems many different mathematical techniques and approximate method have been described. An approximate analytical methods were developed by London and Seban (1943) and analysed the process of ice formation for different boundary conditions and geometries like cylinder, sphere, and flat plate. Goodman and Shea (1960) developed the heat balance integral method and used to solve the one-phase melting-ice problem with various boundary conditions. Further, Goodman and Shea (1960) applied the heat balance method to the two phase problem of melting of finite slab, which is initially at a uniform temperature below the melting point. Poots (1962) used the heat balance integral method to single phase melting problem using a two parameters quadratic profile. Noble (1975) proposed a spatial subdivision scheme in which quadratic profiles are used in each subregion. After that Bell (1978) modified Noble's scheme to solve a single-phase melting problem. Crank and Gupta (1972) have been solved a moving boundary problems in heat flow using cubic splines or polynomials. This technique was also used by Yuen (1980) in melting problems with initial subcooling. Landau (1950) proposed a transformation of coordinates such that in the new coordinate system the moving interface can be immobilized and the solution can be realized in the fixed domain.

Douglas and Gallie (1955) proposed to determine a variable time step, as part of the solution, such that the moving boundary coincides with a grid line in space. Murray (1959) proposed two methods for numerical solutions of phase-change prob-

lems using finite difference approach. The numerical methods for the solution of phase-change problems can be subdivided into two main groups: fixed grid methods based on the enthalpy concept and moving grid methods utilizing the interface immobilization technique. The moving grid method is equivalent to the Landau transforms, where the grid points move following the interface. From the numerical point of view a fixed grid in the Landau transformed plane is equivalent to a moving grid in the physical domain. This method was applied by Heitz and Westwater (1970) to solve a one-dimensional problem of solidification with the liquid initially at saturated temperature. They incorporated the volume change and a higher value of liquid thermal conductivity to simulate the effect of fluid flow. The complications due to the non-uniform grid size around the moving boundary were avoided by the methods of Crank and Gupta (1972), in which the entire uniform grid system moves with the velocity of the moving boundary. They presented two schemes of obtaining the interpolated values of temperatures at the new grid points, to be used for the next step, in terms of cubic spline or polynomials. The two methods (fixed grid method and variable grid method) are compared by Furzerland (1980) for the solution of a specific test problem of one dimension pure conduction heat transfer. Gupta and Kumar (1980) formulated the same set of finite difference equation as Douglas and Gallie but they used the Stefan condition to update the time step. The instability, that develops as the depth of the moving boundary increases, was avoided with Gupta and Kumar's method. Goodling and Khader (1974) gave another variable time step method in which the finite difference form of the Stefan condition was incorporated into the system of the equations to be solved. The system is solved for an arbitrary value of the temperature of the node adjacent to the moving boundary, which is then updated from the Stefan condition. However, Gupta and Kumar (1981), in a study of a convective boundary condition at the fixed end, found that Goodling and Khader's method does not converge as the computation progresses in time. They showed a satisfactory agreement between their results and those obtained by using other variable time step methods and the Goodman (1958) integral method.

Several other more general ways of formulating moving boundary problem in terms of integral equations and their solution have been found useful. One advantage of introducing integral equation in linear heat flow problems generally is that only the value of the unknown on the boundaries of the domain either into the formulation. The use of Green's function for the solution of heat flow problems subjected to conditions prescribed on fixed boundaries is well known. Carslaw and Jaegar (1959) give the basic theory and solutions to a selection of standard problems in terms of appropriate Green's functions. Chuang and Szekely (1972) employed Green's functions to solve in integral equation form, the problem of a solid slab, symmetrically placed in its own melt. Later papers by Chuang and Szekely (1972) and Chuang and Ehrich (1974) deal with corresponding cylindrical and spherical problems. For most geometries and boundary conditions encountered in practice, simple exact solution can not always be obtained in terms of standard analytic functions.

In 1946, The enthalpy approach was proposed by Eyres *et al.* (1946) to avoid nonlinearity in a heat conduction problem. The earliest application of an enthalpy formulation to a finite difference scheme appears to be Rose (1960). Shamsunder and Sparrow (1975) employed the enthalpy method with a fully-implicit finite difference scheme for solidification in a square geometry with convective boundary conditions. They verified their results by the results from an enthalpy formulation used with the Crank-Nicholson scheme. The enthalpy method have been used by Esen and Kutluay (2004); Caldwell and Chan (2000). perturbation solution was used by Yagit (2007); Singh *et al.* (2011a). A finite difference methods have been employed by Furzeland (1977), and Rai and Singh (1998).

Recent, several others numerical methods have been used by Kutluay (2005), Jana *et al.* (2007), Yagit (2008), Rajeev *et al.* (2009a,b). The use of numerical methods (fixed grid, variable grid, front fixing, adaptive grid generation, and enthalpy methods) for obtaining solution of moving boundary problems was reported by Ozisik (1994). On the other hand, the variety of approximate analytical methods such as the energy integral method, perturbation methods, and similarity solutions can be found in the available literature.

1.7 Dimensionless Variables

The dimensionless variables have wide acceptance in tracing the problem of heat and mass transfer phenomena. It is not only reduce the number of parameters but it also generalized the results and creates a firm scientific phenomena. The various dimensionless variable and similarity criteria which have been used in the problem are listed as:

1.7.1 Fourier Number

The Fourier number is defined by

$$Fo = \frac{at}{l^2}. \tag{1.106}$$

It is a measure of the rate of heat conduction in comparison with the heat storage in the given volume element. Larger the Fourier number, deeper is the penetration of heat into a solid over a given period of time.

1.7.2 Stefan Number

The Stefan number Ste, is strictly positive and signifies the importance of sensible heat relative to the latent heat. Thus

$$Ste = \frac{C\Delta T}{L}, \tag{1.107}$$

$\Delta T = T_f - T_0$.

1.7.3 Predvoditelev Number

The Predvoditelev number is defined as

$$Pd = \frac{bl^2}{a\Delta T}, \tag{1.108}$$

The Predvoditelev number Pd describes the rate of change of temperature in medium. Where, b is constant rate.

1.7.4 Kirpichev Number

Kirpichev number is ratio of external heat transfer intensity to the internal heat transfer intensity and defined as

$$Ki = \frac{ql}{K\Delta T}.$$ (1.109)

1.7.5 Biot Number

The Biot number is the ratio of the internal thermal resistence to the external thermal resistence and defined as

$$Bi = \frac{\alpha l}{K}.$$ (1.110)

It may vary in the range from 0 to ∞ and the temperature increases as increase the Biot number increases.