Chapter 1

Introduction

1.1 Moving Boundary Problems

Moving boundary problems are the special type of the boundary value problems that involve partial differential equations in a domain in which a part of the boundary is not known in advance. This unknown part of the boundary is known as moving boundary (for example, interface between solid and liquid regions during melting or freezing process). The moving boundary is also a part of the solution to the problem. Therefore, researchers seek to determine the solution of the differential equations as well as the moving boundary. To solve partial differential equations, some boundary conditions on fixed boundary are prescribed in the formulation of the problem. But, to determine the moving boundary of the problem, an additional condition is imposed at the moving interface/ boundary besides the fixed boundary conditions. Moving boundary problem with phase change phenomenon is known as the Stefan problem which is associated with the eminent Austrian physicist Josef Stefan (1889). He is the most popular worker in this field because he presented first an extensive study of these problems.

In our daily life, we encounter many natural and industrial processes that include several examples of the moving boundary problems. One of the famous examples of these problems is melting of a solid material. When the left fixed boundary is subjected to a temperature T_0 greater than the melting temperature of the solid then the melting process starts and an interface between solid and liquid regions (moving boundary) is formed that propagates towards solid side. A schematic diagram of this process is given below:

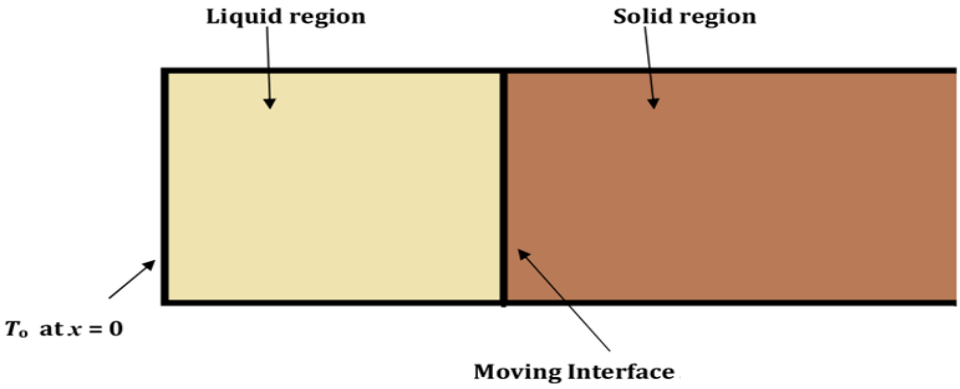

Fig. 1.1 Moving interface during melting process

Freezing process, oxygen diffusion process, tumor growth, evaporation of droplets, swelling of grains or polymers, sedimentation process near the shoreline, etc. are some other examples of moving boundary problems. All these processes contain either a moving interface or moving reaction front which is unknown initially. Moving boundary problems attract the researchers very much since nineteen century due to its various practical applications in the different domains of science, engineering and industry. The practical applications of these problems can be seen in the formation of ice, production of steel, vehicles design, preservation of foodstuffs, drug release processes, crystals growth, fluid flow in porous media, cryosurgery, geophysics, etc.

From the mathematical point of view, moving boundary problems are challenging problems because of the presence of moving interface and its inherent nonlinear nature. The solutions to these problems require a special treatment even in its simplest form. In literature, the exact solutions to these problems are available for some limit case only.

Therefore, many approximate methods like perturbation methods, variational approaches, Adomian decomposition method, homotopy perturbation methods, homotopy analysis method, etc. and numerical techniques like fixed grid method, variable space-step methods, variable time-step methods, etc. have been used by the researchers to get its solutions to study the phenomenon. In the field of moving boundary problem, mathematical formulation corresponding to the real problem, solution of the problem and qualitative results such as existence and uniqueness are the three important directions of research.

In this thesis, some mathematical models associated with the moving boundary problems are deliberated, and the approximate and analytical solutions of considered problems are presented. Moreover, existence and uniqueness of analytical solutions are also established in some cases. The approximate techniques implemented here are simple, efficient and sufficiently accurate, and these are mentioned in section 1.3 of this thesis.

1.2 Historical Background

From the literature, it is found that the first work of interest in the field of moving boundary problem related to phase change was reported by Lame and Clapeyron (1831) for the determination of the thickness of solid crust formed by the cooling of liquid in positive half space. They found that the thickness of the crust is directly prepositional to the square root of the time but they could not find out the proportionality constant. This study was based on the concept of latent heat. In the 18^{th} century, the Scottish medical doctor Joseph Black as mentioned by Eddy and Daniel (2014, 2015) was the first who introduced the concept of latent heat to understand the physical mechanism of phase change. In an unpublished lecture in 1860, Franz Ernst Neumann, a German physicist and mathematician, presented the solution of a two phase problem as given by Hill (1987) in detailed similar to the problem of Lame and Clapeyron. This solution is known as Neumann solution in the honour of the German scientist. Latter on, the most popular researcher in the field of moving boundary problems is an Austrian physicist J. Stefan (1835-1893) who published all together four papers (Stefan, 1889a, 1889b, 1889c, 1889d) in 1889 to describe the phase change processes systematically by utilizing the idea of Lame and Clapeyron, and Neumann solution.

From 1890 to 1930, no any profitable work was received in field of moving boundary problems (Hill, 1987). In 1931, a paper related to the reduction of a Stefan problem to system of integro-differential equation was reported by Brillouin (1931). But, this procedure was feasible only for extremely strong limitations on initial and boundary conditions of the problems. Actually, Brillouin presented this method in his lecture in 1929 at the institute Henri Poincare to improve the interest in the field of moving boundary problems. Leibenzon (1931) presented an effective approximate technique for the solution of phase change problem which was based on the replacement of true temperature within each phase by a quasi-stationary solution. After that, Huber (1939) proposed a lengthy method for one dimensional moving boundary problems with the aid of the invariance of the diffusion equation under an Appell transformation and Green’s function.

The next method to solve the moving boundary problems was received by Rubinstein (1947). His approach was based on the reduction of the moving boundary problem to integral equation with the help of heat potential. Evans et al. (1950) utilized Laplace transform for the solution of one phase moving boundary problems. Ockendon (1975) also utilized Laplace transform to find the solution of oxygen diffusion problem.

Further, he has drawn an attention towards the applicability of Fourier transform for the solution of moving boundary problems in semi-infinite or finite domains. Gliko and Efimov (1980) formulated Volterra linear integral equation associated to a moving boundary problem and the solution was presented with the aid of Laplace transform to investigate movement of moving interface.

Another step towards the solution of moving boundary problems was the application of Green's functions (Hill, 1987). Kolodner (1956) presented the solution of a freezing problem of a lake of finite depth which was based on formulation of integral equation with the help of Green's function. After that Rubinstein (1971) reported the application of the integral equation technique with the aid of Green's function to the phase change problems. He had also presented an analysis of stability, existence and uniqueness of the solutions. Some researchers like Chuang and Szekely (1972), Hansen and Hougaard (1974), Collatz (1978) also used Green's function to obtain the solution of moving boundary problems. Carslaw and Jaeger (1987) also utilized some appropriate Green's functions to present the basic theory and solution of few standard phase change problems.

Heat balance integral method was the other approximate technique to find the solution of the phase change problems. Goodman (1958) applied this technique to the moving boundary problems involving phase change processes. Goodman and Shea (1960) also reported the solution of a two phase melting problem in an infinite domain by using heat balance integral method. After that, this technique was applied by many researchers to solve different types of moving boundary problems, and few of them are Lardnern and Pohle (1961), Poots (1962), Goodman (1964), Boley and Entenssoro (1977), Yuen (1980).

The next method was reported by Boley (1961, 1968) who used embedding technique to solve melting and solidification problems. After that, modified form of this embedding method was presented to solve a three dimensional moving boundary problem by Boley and Yagoda (1971). Ferriss and Hill (1974) discussed an embedding solution of a moving boundary problem associated to oxygen diffusion process. Boley (1975) summarized the uniqueness of the various solutions of moving boundary problems obtained by embedding technique. Further, the study in this direction is reported by Wilson (1978) and Gupta (1986).

In 1970, isotherm migration method was applied on moving boundary problem with nonlinear diffusion by Chernousko (1970). After that this method was applied by Crank and Phale (1973), Crank and Gupta (1975), Crank and Crowley (1978). In the literature, several other approximate methods have been used to solve different moving boundary problems, and some of them are variational method (Biot, 1957, 1959; Biot and Daughaday, 1962; Vujanovic and Baclic, 1976; Elliott and Ockendobn, 1982); non integral method (Annamalai et al., 1986); perturbation method (Kreith and Romie, 1955; Pedroso and Demoto, 1973; Weinbaun and Jiji, 1977; Dragomirescu et al., 2016; Font, 2018); nodal integral method (Rizwan-Uddin, 1999; Savovic and Caldwell; 2003); Adomian decomposition method (Grzymkowski and slota, 2006; Das and Rajeev, 2010; Rajeev et al., 2013); Homotopy perturbation method (Li et al., 2009; Das et al., 2011; Singh et al., 2011a; Rajeev and Kushwaha, 2013).

In the literature, various numerical methods have been also frequently used by many researchers for the solution of moving boundary problems. Finite difference method is the most popular choice of researchers for the numerical solution of these problems. Fixed grid methods, variable space state methods and variable time step methods are the main three finite difference methods for solving moving boundary problems. Applications of finite difference methods to these problems are reported by Gupta and Kumar (1980), Voller (1990), Zerroukat and Chatwin (1994), Asaithambi (1997), Rizaudin-Uddin (1999), Caldwell and Savovic (2002), Savovic and Caldwell (2003), Mitchell and Vynnycky (2009) and many more. Due to the ability to handle these problems in complex geometry, finite element method (Finn and Voroglu, 1979; Kawahara and Umetsu, 1986) and boundary element method (Brebbia et al., 1984; Wendland, 1985) have been also utilized for the solution of different types of moving boundary problems.

Besides above mentioned techniques, the establishment of the exact solutions to the moving boundary problems are always an interesting direction of research since the beginning of this area because of the complexity associated with these problems. These problems are nonlinear and need a special treatment for getting exact/analytical solution. In the literature, many researchers presented exact solutions of these problems for some particular cases and some of them are reported by Cho and Sunderland (1974), Oliver and Sunderland (1987), Ramos et al. (1992), Tritscher and Broadbridge (1994), Tarzia (2004), Voller et al. (2004), Briozzo et al. (2007), Voller (2010), Briozzo et al. (2010), Voller and Falcini (2013), Zhou et al. (2014), Zhou and Xia (2015), Ceretani et al. (2018), Kumar et al. (2018a, 2018b), Singh et al. (2018a, 2018b). The matter in this section is presented with the help of Rubinstein (1971), Crank (1984), Hill (1987) and Kushwaha (2015). Motivated by all above works, some mathematical models associated with moving boundary problems and its solutions are presented in this thesis.

1.3 Some Methods

In this thesis, the following three methods are used:

1.3.1 The shifted Chebyshev polynomials

As we know that the Chebyshev polynomials $\{T_i(t); i = 0,1,...\}$ are defined on the interval $(-1, 1)$. In order to use these polynomials on the interval $x \in (0, L)$, we introduce a new variable $t = \frac{2x}{L} - 1$ in $T_i(t)$ which is called as shifted Chebyshev polynomials (Doha et al.,2011b; Ghoreishi and Yazdani, 2011).

Let the shifted Chebyshev polynomials $T_i\left(\frac{2x}{L} - 1\right)$ be denoted by $T_{L,i}(x)$, satisfying the following recurrence formula:

$$T_{L,i+1}(x) = 2\left(\frac{2x}{L} - 1\right)T_{L,i}(x) - T_{L,i-1}(x), \quad i = 1, 2, ..., \tag{1.1}$$

where $T_{L,0}(x) = 1$ and $T_{L,1}(x) = \frac{2x}{L} - 1.$

The following properties of first kind shifted Chebyshev polynomials given in Doha et al. (2011b), Ghoreishi and Yazdani (2011) are used:

(a) A square integrable function $u(x)$ in $(0, L)$ can be expressed in terms of the shifted Chebyshev polynomials as:

$$u(x) = \sum_{j=0}^{\infty} c_j T_{L,j}(x), \tag{1.2}$$

where the coefficients c_j are given by

$$c_j = \frac{1}{h_j}\int_0^L u(x) T_{L,j}(x) w_L(x) dx, \quad j = 0, 1, 2, \ldots. \tag{1.3}$$

For practice purpose, only the first $(N+1)$-terms shifted Chebyshev polynomials can be considered for the approximation of the function $u(x)$. Hence, we can write

$$u_N(x) \approx \sum_{j=0}^{N} c_j T_{L,j}(x) = C^T \phi(x), \tag{1.4}$$

where C^T is the transpose of shifted Chebyshev coefficient vector and $\phi(x)$ is the shifted Chebyshev vector which are given by

$$C^T = [c_0, c_1, \ldots, c_N] \text{ and } \phi(x) = [T_{L,0}(x), T_{L,1}(x), \ldots, T_{L,N}(x)]^T . \tag{1.5}$$

(b) The derivative of the vector $\phi(x)$ is given by

$$\frac{d\phi(x)}{dx} = D^{(1)}\phi(x), \tag{1.6}$$

where $D^{(1)}$ is the $(N+1)\times(N+1)$ operational matrix of derivative given by

$$D^{(1)} = (d_{ij}) = \begin{cases} \dfrac{4i}{\varepsilon_j L}, & j = 0, 1, \ldots, i = j + k, \begin{cases} k = 1, 3, 5, \ldots, N, & \text{if } N \text{ is odd}, \\ k = 1, 3, 5, \ldots, N-1, & \text{if } N \text{ is even}. \end{cases} \\ 0, & \text{otherwise}. \end{cases}$$

and $\varepsilon_0 = 2, \varepsilon_k = 1, k \geq 1$.

(c) The n^{th} order derivative of the vector $\phi(x)$ is given by

$$\frac{d^n\phi(x)}{dx^n} = (D^{(1)})^n \phi(x), \tag{1.7}$$

where $n \in N$ and $(D^{(1)})^n$ denotes n$^{\text{th}}$ powers of $D^{(1)}$ i.e.,

$$D^{(n)} = (D^{(1)})^n, \qquad n = 1, 2, \dots. \tag{1.8}$$

1.3.2 Some properties of shifted Legendre polynomials

To use classical Legendre polynomials $\{L_i(x);\ i = 0,1,\dots\}$ on the interval $[a,b]$, the shifted Legendre polynomials $L_i^*(x)$ are defined as

$$L_i^*(x) = L_i\left(\frac{2x - a - b}{b - a}\right), \qquad i = 0,1,2,\dots, \tag{1.9}$$

which satisfy the following recurrence formula:

$$(i+1)\, L_{i+1}^*(x) = (2i+1)\left(\frac{2x - a - b}{b - a}\right) L_i^*(x) - i\, L_{i-1}^*(x), \qquad i = 0,1,2,\dots, \tag{1.10}$$

where $L_0^*(x) = 1$ and $L_1^*(x) = \dfrac{2x - a - b}{b - a}$.

In this method, we will use the following properties of the shifted Legendre polynomials (Abd-Elhameed et al., 2015):

(a) First, we define a space

$$L_0^2[a,b] = \left\{\phi(x) \in L^2[a,b] : \phi(a) = \phi(b) = 0\right\}, \tag{1.11}$$

and select the basis functions in the Hilbert space $L_0^2[a,b]$ as

$$\phi_j(x) = (x-a)(x-b) L_j^*(x), \qquad j = 0,1,2,\dots. \tag{1.12}$$

Now, a function $u(x) \in L_0^2[a,b]$ can be written in terms of the shifted Legendre polynomials as:

$$u(x)=\sum_{j=0}^{\infty} c_j \phi_j(x), \tag{1.13}$$

where the coefficients c_j are given by

$$c_j=\frac{2j+1}{b-a}\int_a^b u(x)\phi_j(x)\,w(x)dx, \quad j=0,1,2,..., \tag{1.14}$$

and the weight function $w(x)=\dfrac{1}{(x-a)^2(x-b)^2}$.

For numerical computation purpose, the series given in Eq. (1.13) for the function $u(x)$ can be approximated as

$$u(x)\approx u_N(x)=\sum_{j=0}^{N} c_j\,\phi_j(x)=\boldsymbol{C}^T\boldsymbol{\Phi}(x), \tag{1.15}$$

where $\boldsymbol{C}^T$ is the transpose of shifted Legendre coefficient vector and $\boldsymbol{\Phi}(x)$ is the shifted Legendre vector which are given by

$$\mathbf{C}^T=\left[c_0,\, c_1,...,c_N\right] \text{ and } \boldsymbol{\Phi}(x)=\left[\phi_0(x),\,\phi_1(x),...,\phi_N(x)\right]^T. \tag{1.16}$$

(b) First derivative of the shifted Legendre vector $\boldsymbol{\Phi}(x)$ can be approximated as:

$$\frac{d\boldsymbol{\Phi}(x)}{dx}=D\boldsymbol{\Phi}(x)+\boldsymbol{\delta}, \tag{1.17}$$

where $D=\left(d_{ij}\right)_{0\le i,j\le N}$, is a square operational matrix of derivative of order $(N+1)$ and its elements are given by

$$D=(d_{ij})=\begin{cases}\dfrac{2}{b-a}(2j+1)(1+2H_i-2H_j), & i>j,(i+j)\,\text{odd},\\ 0, & otherwise,\end{cases} \tag{1.18}$$

and

$$\boldsymbol{\delta} = [\delta_0(x), \delta_1(x), \delta_2(x), ..., \delta_N(x)]^T, \tag{1.19}$$

$$\delta_i(x) = \begin{cases} a+b-2x, & \text{when } i \text{ is even,} \\ a-b, & \text{when } i \text{ is odd.} \end{cases} \tag{1.20}$$

In Eq. (1.18), H_i and H_j are harmonic numbers which are defined as

$$H_n = \sum_{k=1}^{n} \frac{1}{k} \quad \text{with} \quad H_0 = 0. \tag{1.21}$$

(c) We can take the following approximation for the second derivative of the shifted Legendre vector $\boldsymbol{\Phi}(x)$:

$$\frac{d^2\boldsymbol{\Phi}(x)}{dx^2} = D^2\boldsymbol{\Phi}(x) + D\boldsymbol{\delta} + \boldsymbol{\delta}', \tag{1.22}$$

where

$$\boldsymbol{\delta}' = [\delta_0'(x), \delta_1'(x), \delta_2'(x), ..., \delta_N'(x)]^T \text{ and } \delta_i'(x) = \begin{cases} -2, & \text{when } i \text{ is even,} \\ 0, & \text{when } i \text{ is odd.} \end{cases} \tag{1.23}$$

1.3.3 Homotopy Analysis Method

To understand the homotopy analysis method (Liao, 2009; Abbasbandy, 2006), we assume the following differential equation

$$N[u(\tau)] = 0, \quad \tau \in \Omega, \tag{1.24}$$

where N is the non-linear operator and u represents the unknown function with τ as the independent variable.

By means of generalizing the traditional homotopy method, Liao (2003) builds the, so called, zero-order deformation equation as

$$(1-q)\,L[\phi(\tau;q)-u_0(\tau)] = q\mu\,H(\tau)N[\phi(\tau;q)], \tag{1.25}$$

where $q\in[0,1]$ denotes the embedding parameter, L is the auxiliary linear operator, $u_0(\tau)$ represents the initial guess, $\mu\neq 0$ is the auxiliary parameter, $H(\tau)\neq 0$ is the auxiliary function. If we substitute $q=0$ and $q=1$ in Eq. (1.25) then we simply obtain $\phi(\tau;0)=u_0(\tau)$ and $\phi(\tau;1)=u(\tau)$, respectively.

This indicates that when q tends 1 from 0, the initial estimate $u_0(\tau)$ shifts towards $u(\tau)$ which satisfies the proposed problem.

Now, the expansion of the function $\phi(\tau;q)$ in Taylor series with respect to q is given by

$$\phi(\tau;q)=\phi(\tau;0)+\sum_{m=1}^{\infty}u_m(\tau)q^m\,, \tag{1.26}$$

where

$$u_m(\tau)=\frac{1}{m!}\frac{\partial^m\phi(\tau;q)}{\partial q^m}\bigg|_{q=0,}\qquad m=1,2,3,..., \tag{1.27}$$

For $q=1$, the required solution of the problem is given by

$$u(\tau)=\sum_{m=0}^{\infty}u_m(\tau)\,, \tag{1.28}$$

provided that the series is convergent.

For the convergence of the series, the auxiliary linear operator, the initial solution, the auxiliary parameter and function have to be properly chosen.

To evaluation the function u_m, we differentiate Eq. (1.25) *m*-times with respect to q and divide the result by $m!$. By setting $q = 0$, we find the *m*-th order deformation equation ($m > 0$):

$$L[u_m(\tau) - \chi_m u_{m-1}(\tau)] = \mu\, H(\tau) R_m(\bar{u}_{m-1}, \tau), \tag{1.29}$$

where $\bar{u}_{m-1} = \{u_0(\tau), u_1(\tau), ..., u_{m-1}(\tau)\}$,

$$\chi_m = \begin{cases} 0, & m < 2, \\ 1, & m \geq 2 \end{cases} \tag{1.30}$$

and

$$R_m(\bar{u}_{m-1}, \tau) = \frac{1}{(m-1)!} \left(\frac{\partial^{m-1}}{\partial q^{m-1}} N\left(\sum_{i=0}^{\infty} u_i(\tau) q^i \right) \right) \Bigg|_{q=0}. \tag{1.31}$$

For practical applications, we use the approximate solution of the considered equation in the following form of partial sum of the series (1.28):

$$u_n(\tau) = \sum_{m=0}^{n} u_m(\tau). \tag{1.32}$$

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