Chapter 1

Introduction

1.1 Moving Boundary Problems

In the literature, the moving boundary problem (MBP) is defined as a special type of boundary value problems that consists of the partial differential equation in some domain in which a part of boundaries is not known in advance. This unknown boundary of such domain is known as a moving boundary (for example, interface between solid and liquid regions during melting or freezing process). It is observed that the moving boundary is a part of the problem, and we have to determine it with the help of energy balance condition during the solution of the problem. The energy balance condition is defined at the moving boundary, and it is also known as the Stefan condition. This word "Stefan" is associated with an Austrian physicist Josef Stefan (1889) [1]. He was the first famous researcher in this field who studied a lot and presented an extensive work related to the melting and freezing process. Therefore, moving boundary problems are also known as Stefan problems.

Many examples of moving boundary problems (MBPs) can be found through various natural and industrial processes. Melting or freezing (a phase change problem) is one of the most popular examples which arises in our daily life. In a melting process, the left boundary of the melting material is subjected to an initial temperature higher than the melting temperature of the material. As time proceeds, the material begins to melt, and the transition interface (moving interface) is formed which propagates from left to right *i.e.*, the transition interface moves from higher temperature to lower temperature. In these problems, researchers investigate the temperature distribution in liquid and solid regions as well as locations of moving boundary. There are also some other processes that are governed by moving boundary problems for example, oxygen diffusion process in living bodies, treatment of tumors growth (cryosurgery and hyperthermia), sedimentation process near the seashore, preservation of foods, spreading and vanishing of the species, recrystallization of metals, thermal energy storage, plasma physics, etc.

Moving boundary problems are interesting because of their wide range of applications. From the mathematical point of view, these problems are difficult to find its solution because these problems involve unknown moving interface (a part of the boundary), and these are of nonlinear nature. Analytical solutions to these problems are not possible in most of the cases therefore, several numerical schemes like, fixed grid methods, variable space- step approaches, variable time- step approaches, etc. have been established by many researchers to handle these nonlinear problems. In this thesis, some mathematical models of moving boundary problems are presented, and the solutions of these models have been calculated with the help of appropriate numerical schemes. For some particular cases of the models, the exact solutions are also discussed. Based on the obtained solutions, the effects of various parameters on the considered processes and movement of moving boundary are also analyzed.

1.2 Historical Background

From the literature of the past decades, it is seen that the moving boundary problem related to phase change first came to light when Lame and Clapeyron [2] determined the thickness of the solid layer formed by the cooling of a liquid in positive half-space. In their study, it was determined that the movement of the crust is directly proportional to the $\sqrt{time}$, but they were unable to determine the proportionality constant. They used the concept of latent heat for their study. A two-phase problem similar to the Lame and Clapeyron's problem given by Hill [3] was solved in 1860 by the Franz Ernst Neumann, a German physicist, and mathematician in an unpublished article. In his honor, this solution was known as the Neumann solution. From the idea of Lame and Clapeyron, and Neumann solution, an Austrian physicist Joseph Stefan (1835-1893), one of the most popular researchers in the field of the moving boundary problem published the articles [1, 4] to elaborate the phase change processes systematically. Due to his methodical contribution, the MBPs are also known as the Stefan problems. Not much research has been done by researchers in the field of MBPs in the era from 1890 to 1930.

In 1929, Brillouin presented a method based on an integro-differential equation related to Stefan problem in his lecture at the institute Henri Poincare to procure the interest in the field of MBPs. Brillouin [5] proposed an article in 1931 related to the Stefan problem which reduced to the form of the system of the integro-differential equation after some strong limitations on initial and boundary conditions. An approximate method for the solution of the Stefan problem was given by Leibenzon [6], in which the true temperature within each phase is replaced by quasi-stationery solution. Apart from this, another method based on Appell transformation and Green's function was proposed by Huber [7] for the solution of one-dimensional MBPs. In the continuation of this area, Rubinstein [8] also proposed a method to solve the MBPs in which the moving boundary problem was transformed with the help of heat potential into the integral equation. In 1950, Laplace transformation method is used by Evans et al. [9] to obtain the solution of one phase one-dimensional MBP. In 1975, oxygen diffusion problem (a MBP) has been solved by Ockendon [10] with the help of the Laplace transformation method. Apart from this, Fourier transformation method is also used in semi-infinite and finite domains of the MBP by him to determine the solution. A MBP associated with Volterra integral equation has been formulated by Gliko and Efimov [11], and Laplace transformation method has been used to determine the solution including the moving phase front.

As the year passed, the new techniques and its applications have been derived by the researchers to determine the solution of MBP. A moving boundary problem associated with the freezing of a lake whose formulation was based on the integral equation has been solved by Kolodner [12] with the application of Green's function. After that, the application of Green's function in the integral equation has been derived by Rubinstein [13], and he presented the stability, existence and uniqueness along with the solution of the MBPs. In 1987, Green's function and its application have been used by one of the great mathematician Hill [3] to obtain the solution of the MBP. The application of Greens' function has also been used by many researchers to obtain the solution of the MBPs, some of the researchers are Carslaw and Jaeger [14], Chuang and Szekely [15] and Hansen and Hougaard [16]. Their solutions of the problems were coming out through the integral equation with the aid of applications of Green's function.

A great mathematician of those days, Goodman [17] developed a new integral method known as Heat Balance Integral Method (HBIM), and applied this method to obtain the approximate solutions of phase change problems. In 1960, the approximate solution of the two-phase MBP in an infinite domain has also been presented by Goodman and Shea [18] with the help of HBIM. After that, many researchers showed their interest to apply this method to determine the approximate solutions to the MBPs, and some of them are Lardnern and Pohle [19], Poots [20], Goodman [21], Boley and Entenssoro [22], Yuen [23], etc. Rectification and modification of HBIM have also been done by many researchers to make the application of this method wider and wider. Wood [24] and, Mosally and Wood [25] have used the energy balance equation and developed a new look to solve the phase change problems by HBIM. Mitchell and Myres [26], Mitchell and Myres [27], Mitchell and Myres [28] have shown a wide application of HBIM for determining the solution of MBPs related to phase change processes with improved accuracy. In the last decade, Hristov [29, 30, 31, 32] presented a lot of work with HBIM to solve the different kinds of phase change problems (MBPs) including integers and fractional differential operators. Kumar and Rajeev [33] have also discussed a time-fractional Stefan problem with Robin boundary condition and temperature-dependent thermal conductivity.

The next approach to solve MBPs (phase change problems) was embedding method which was developed by Boley [34, 35] in 1961. After sometime, Boley and Yagoda [36] modified this method to solve a three-dimensional MBPs. Wilson [37] and Gupta [38] have also used this method to present the solution of a phase change problem including moving boundary. In 1970, Chernousko [39] discussed the solution of a MBP with nonlinear diffusion by using the isotherm migration method. After that Crank and Phahle [40], Crank and Gupta [41], Crank and Crowley [42] also applied this method to obtain the solution of MBPs.

In literature, so many other approximate methods have been discussed to obtain the solution of the MBPs. Some important schemes are perturbation method (Kreith and Romie [43], Weinbaum and Jiji [44], Dragomirescu et al. [45], Font [46]); variational method (Biot [47], [48], Elliott and Ockendobn [49]); nodal integral method (Rizwan-Uddin [50], Caldwell and Savovic [51]); Adomian decomposition method (Grzymkowski and Slota [52], Das and Rajeev [53], Rajeev et al. [54]); Homotopy perturbation method (Li et al. [55], Das et al. [56], Singh et al. [57], Rajeev and Kushwaha [58]); Spectral method (Hussaini and Zang [59], Doha et al.[60], Kumar et al. [61]). Besides these methods, many numerical techniques have also been discussed by many researchers to establish the solution of a different kind of MBPs. In those numerical techniques, finite difference method is very popular among researchers as its solution is much more accurate, and easy to apply to the complicated MBPs. Some of the finite difference schemes are discussed by Gupta and Kumar [62], Voller [63], Zerroukat and Chatwin [64], Rizwan-Uddin [65], Savovic and Caldwell [66], Mitchell and Vynnycky [67], Jain et al. [68], Kumar and Rajeev [69], Kumar and Rajeev [70], and many more. There are also some other numerical methods used by many researchers to handle the complex problems related to moving boundary. Finite element method (Comini et al. [71], Kawahara and Umetsu [72]) and boundary element method (Brebbia et al. [73], Wendland [74]) are also very famous numerical tools to obtain the solution of MBPs in complex geometry.

Apart from the above approximate solutions, the impacts of the analytic solution to the MBPs are always a bigger and ore interesting part of the solution. Due to the non-linearity nature of the problem, it becomes much more difficult to obtain the analytic solution to the complex MBPs, and sometimes it needs a special care for getting analytic solution. In the literature, the analytic solutions of the MBPs for some particular cases have been discussed by many researchers and some of solutions are reported by Cho and Sunderland [75], Oliver and Sunderland [76], Ramos et al. [77], Voller et al. [78], Briozzo et al. [79], Briozzo et al. [80], Voller and Falcini [81], Zhou et al. [82], Zhou and Xia [83], Ceretani et al. [84], Singh et al. [85, 86], Kumar et al. [87, 88], etc.

1.3 Fractional calculus

Differential calculus and its applications are very important and well-known topics of research. We also understand the notion of n^{th} order derivative which means that the differential operator has to apply n-times on the differentiable function in succession, where n is a positive integer. In 1965, G. de L'Hospital and G. W. Leibniz thought about the possibility of n to be other than an integer, and that was the day when fractional calculus came to light. After that day, many researchers have made this question as a topic of their research and contributed in the field of fractional calculus. Some of them are L. Euler, P. Laplace, J-L. Lagrange, S. F. Lacroix, J. Fourier, N.H. Abel, J. Liouville and many more. Apart from these, fractional calculus has also been contributed by B. Riemann, H. Weyl, G. Leibniz, A. K. Grunwald, and A.V. Letnikov. From the 17^{th} to 18^{th} century, the literature of arbitrary order derivative is missing from the field of mathematics. In this period, the derivative of an arbitrary order was only mentioned by L. Euler and J. Fourier but they did not use in their further work. After that, in the 19^{th} century, the derivative of arbitrary order of a function x^m is defined with the help of the Gamma function by S. F. Lacroix, which is given as

$$D_x^{\alpha} x^m = \frac{\Gamma(m)}{\Gamma(m-\alpha)} x^{m-\alpha}. \tag{1.1}$$

In 1823, the evolution of the fractional derivative in the field of fractional calculus has been given by Ross [89] in his book. In this book, it is also mentioned that the fractional derivative was used by N. H. Able to solve the Tautochrone problem. J. Liouville got the motivation from this work, and presented a logical definition in 1832 for the derivative of fractional order for any arbitrary function by expanding the function in the series of exponential. After that, the definition of fractional order derivative faced many controversies between the years 1835 to 1850. But, in 1853, G. F. Bernhard Riemann gave a different definition of the fractional order derivative which involves the definite integral. After that, Sonin [90] started to define the differentiation of arbitrary order by using Cauchy's integral formula. Later in 1884, Riemann-Liouville fractional order derivative has been developed by Laurent [91] by using an open circuit instead of a closed circuit. In 1967, the most significant contribution to the field of fractional calculus was given by M. Caputo which deals with the major drawback of Riemann-Liouville's definition of fractional derivative. As time passes, a large number of researchers showed their interest in fractional calculus and a large number of books have also been written by many authors. Some of those are Nishimoto [92], Miller and Ross [93], Kiryakova [94], Rubin [95], Podlubny [96], Hilfer [97], Kilbas et al. [98], etc. The next sub-section will consist of the definition of Caputo derivative and it's properties used in this thesis.

1.3.1 Definition of Caputo fractional derivative and its properties

Definition 1.1. Let us consider, γ:$\mathbf{R} \to \mathbf{R}$, x $\to \gamma(x)$, then the Caputo fractional derivative of order α is defined as

$$
{}_0^C D_x^\alpha \gamma(x) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \int_0^x (x-y)^{m-\alpha-1} \gamma^{(m)}(y) dy, & m-1 < \alpha < m, \\ \gamma^{(m)}(x), & \alpha = m, \end{cases}
$$

where $m \in N$ and N is the set of natural number.

Property 1. Let $\gamma(x) = C$, where C is a constant, then

$$ {}_0^C D_x^\alpha \gamma(x) = 0. \tag{1.2} $$

Property 2. Let $\gamma(x) = Cx^n$, where $n \geqslant 1$ and C is a positive real constant then

$$ {}_0^C D_x^\alpha \gamma(x) = C \frac{\Gamma(1+n)}{\Gamma(1+n-\alpha)} x^{n-\alpha}. \tag{1.3} $$

Property 3. Let $x = kz(k > 0)$ and ${}_0^C D_x^\alpha \gamma(x)$ $(p - 1 < \alpha \leq p)$ exists, then the following result is true:

$$ {}_0^C D_x^\alpha \gamma(x) = k^{-\alpha} {}_0^C D_z^\alpha \gamma(kz). \tag{1.4} $$

1.4 Some Methods for treatment of moving boundary problems

1.4.1 Finite Difference Method (FDM)

The finite difference is one of the most popular and accurate methods for solving differential equations. In the past few decades, the presence of computers, and software makes it easy to determine numerical solutions to a wide variety of scientific and engineering problems. Recently, the interest of many researchers in the field of FEM has increased in comparison to other numerical schemes, like finite volume method or finite element methods because it is easier to apply to the complex differential equations than other numerical schemes.

In this section, the fundamentals of the FDM along with the front fixing method (Landau-type transformation) are discussed. In the front fixing method, the time dependent domain of the MBPs is converted into a fixed domain [0,1] by using an appropriate transformation (Landau-type transformation). After that, the domain is discretized into the finite number of mesh points, and appropriate approximations of space derivative and time derivative by using Taylor's series expansion are considered for the solution of the problem. This generates a system of algebraic equations and solution of the problem can be found by solving this algebraic system.

In this thesis, an explicit FDM is used. Therefore, the approximations of the time derivative and space derivative of the dependent variable ($U(\xi, t)$) are based on the forward difference and central difference, respectively at the mesh points (ξ_i, t^n) which are given as

$$\frac{\partial U(\xi_i, t^n)}{\partial t} \approx \frac{U_i^{n+1} - U_i^n}{k}, \qquad \frac{ds(t^n)}{dt} \approx \frac{s^{n+1} - s^n}{k} \tag{1.5}$$

$$\frac{\partial U(\xi_i, t^n)}{\partial \xi} \approx \frac{U_{i+1}^n - U_{i-1}^n}{2h}, \qquad \frac{\partial^2 U(\xi_i, t^n)}{\partial \xi^2} \approx \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{h^2} \tag{1.6}$$

In this work, the error between the exact and approximate solutions have been discussed by replacing the differential operator with a difference operator which is known as truncation error. The stability and convergence of this method have also been presented. In the chapter 3, the finite difference method for the case of fractional derivative is also discussed.

1.4.2 Heat Balance Integral Method

Goodman [17] developed a popular approximate method to determine the solution of the moving boundary problem (phase change problem) which is known as the Heat Balance Integral Method (HBIM). The classical HBIM is used to solve the heat conduction problem by converting the governing partial differential equation into an ordinary differential equation. The PDE can be converted into ODE by the following procedures:

(i) We assume a suitable approximation for the temperature profile that satisfies the available boundary condition.

(ii) In the second step, we integrate the heat equation with respect to the space variable over a suitable interval to create a heat balance integral.

(iii) Finally, ODE resulting from step (ii) is solved.

It is assumed that the temperature profile in different forms [26] of polynomials for example quadratic temperature profile, cubic temperature profile, exponential temperature profile, etc. For phase change problems some profiles for temperature distribution ($T(x,t)$) are given below:

1.4.2.1 Quadratic temperature profile

$$T(x,t) \approx a\Big(1 - \frac{x}{s(t)}\Big) + b\Big(1 - \frac{x}{s(t)}\Big)^2, \tag{1.7}$$

where $a \geqslant 0$ and $b \geqslant 0$ are constants and $s(t)$ is the moving phase front.

1.4.2.2 Cubic temperature profile

$$T(x,t) \approx a\Big(1 - \frac{x}{s(t)}\Big) + b\Big(1 - \frac{x}{s(t)}\Big)^2 + c\Big(1 - \frac{x}{s(t)}\Big)^3, \tag{1.8}$$

where $a \geqslant 0$, $b \geqslant 0$ and $c \geqslant 0$ are constants.

1.4.2.3 Exponential temperature profile

$$U(x,t) = a + \frac{bx}{s(t)} e^{-cx^2/s(t)^2}. \tag{1.9}$$

where $a \geqslant 0$, $b \geqslant 0$ are constants and $s(t)$ is the moving phase front.

1.4.3 Genocchi Operational Matrix Method

In this approach, first, the residual corresponding to the given differential equation is constructed by taking the approximations of the dependent variable and it's derivatives. In this thesis, the derivatives of the dependent variable are approximated with the help of the operational matrices based on the transformed Genocchi polynomials. In the next step, the constructed residual is set to zero at various collocation points of the given domain. This process produces a system of algebraic equations, and its solution gives an approximate solution of the problem. The detail of this approach is mentioned in the fifth chapter of the thesis.

1.5 Research Gap, Objective and Novelty of the Thesis

In the literature, the mathematical models related to the parabolic PDEs including moving interfaces (moving boundary problems) are discussed under some assumptions. Therefore, there is still scope to modify the models related to these problems which is more near to the real physical processes. Moreover, there are many important physical processes associated to moving boundary problems which have not been adequately studied and are not understood till now. To have a deeper understanding of such complex physical mechanics of these important problems, a detailed studies need to be performed to present more realistic mathematical model of moving boundary problems and its solution.

From the mathematical point, moving boundary problems are challenging problems because these problems are nonlinear in nature and its moving interface is not known in advances. Due to these inherent difficulties, the solutions of 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 numerical techniques like fixed grid method, variable space-step methods, variable time-step methods, etc. have been developed by the researcher to get its solutions to study the phenomenon. But, it is still required to develop more simple, efficient and accurate techniques for the moving boundary problems involving complex phenomenon to present a systematized study of the problem.

In view of above facts, the objectives of the thesis are

(a) Identification of some complicated moving boundary problems having physical relevance and importance in real world.

(b) Modifications in the mathematical models of the considered problems if it is needed.

(c) First, we will try to find exact solutions/analytical solutions to the identified problems. If there is difficulty to get the analytical solution to a problem then we will try to establish numerical solution of the problem.

(d) Based on obtained solution, we will see the dependence of considered process on different parameters involved in the mathematical model. We will also see how the parameters affect the moving interface and how to control it.

In this thesis, four different modified non-classical models are presented in which three are related to the phase change problems and one problem is associated with diffusion logistic population model governing the processes of spreading and vanishing of the species. To solve these problems, finite difference method, heat balance integral techniques, and operational matrix method based on Genocchi polynomials are applied with a special care. The accuracy of each used technique is discussed chapter wise of this thesis. The analytical solutions to these problems for some particular cases are also established. The dependence of the phase change processes, and spreading/vanishing of the species on various parameters of the considered models are also analyzed.

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