Introduction

1.1 Moving boundary problems

Moving boundary problems involve heat/diffusion equation in a domain, a part of whose boundary is not known in advance. But, we have to determine this unknown boundary as a part of solution of the problem. The unknown part of boundary is called a moving boundary (e.g., the liquid-solid front during melting or freezing process). Moving boundary problem involving phase change process is also known as a Stefan problem. This name is associated with eminent Austrian physicist Josef Stefan (1889) who presented first an extensive study of these problems.

Several examples of moving boundary problem can be seen in the literature. One famous example of these problems is freezing process. During freezing process, solid and liquid phases are separated by an interface which propagates towards liquid side. This interface is the moving boundary. The other examples include melting of a solid, evaporation of droplets, oxygen diffusion problem, swelling of grains or polymers, tumor growth, basic shoreline problem, etc. All these processes involve either a moving interface or moving reaction front which is unknown. Moving boundary problems have many practical applications in industries, space vehicle design, preservation of foodstuffs, chemical process, diffusion process, growing crystal for semiconductors, cryosurgery, astrophysics, meteorology, geophysics, plasma physics, etc. The scientists and manufacturers are interested in controlling their processes so as to make moving boundary as smooth as possible.

Moving boundary problems are typical problems from point of view of mathematics because of its nonlinear nature and presence of moving interface.

Exact solutions of these problems are difficult to obtain except for a limited number of special cases (Wilson et al. (1975), Durack and Wendroff (1977)). In science and engineering, an extensive development in the field of moving boundary problems has been reported. Mathematically, this area is progressed in three main directions (Rubinstein (1971)), approximate analytical techniques, numerical methods and qualitative results such as existence and uniqueness.

The main aim of this thesis is to present some mathematical models related to moving boundary problems and its thorough study by approximate analytical techniques (given in section 1.3). Due to prevalence of these problems, there are a large number of methods exist in literature to solve these problems. The techniques adopted here are the recent and sufficient accurate ones which minimize the size and complexity of the calculations.

1.2 Literature Review

From the literature survey, it is found that Lame and Claperon (1831) were the first who studied a moving boundary problem in his paper. They discussed a problem to determine the thickness of the solid crust generated by the cooling of a liquid under a constant surface. They also discussed exact similarity solution of the problem and found that the thickness of the crust is proportional to the square root of the time but did not determine the coefficient of proportionality as mentioned by Rubinstein (1971). Similarity exact solutions of moving boundary problems are usually credited to Franz Newmann which is given in his unpublished lecture in 1860 (as pointed out by Weber (1919)). Then the most popular researcher in this area is an Austrian physicist Stefan (1889) who published altogether four papers in 1889. Stefan utilized Newmann's solutions and obtained exact analytical solutions of the problems (as given by Hill (1987)). His papers are based on

(a) Some problem in the theory of heat conduction.

(b) The theory of ice formation with reference to the Arctic sea.

(c) The diffusion of acid and alkaline solution through each other.

(d) Evaporation and condensation as diffusion processes.

From 1890 to 1930, no any profitable publication was observed in this field. In 1931, Brillouin (1931) published a paper in which he presented a method for reduction of Stefan problem to a system of non-linear integro-differential equations. But, this method is not feasible without taking extremely strong restrictions on the boundary data and initial data of the problem. In same year, Leibenzon (1931) proposed an effective approximation method for the solution of the Stefan problem. He used this technique to different type of the calculations for the time of solidification of the spherical earth from its original molten condition and this method was also used by Kovner for the solution of a problem of a thawed patch on a half-plane (as given by Rubinstein (1971)). After that, Huber (1939) presented a method based on Green's function to solve Stefan problem. This method was a generalization of the method of polygonal approximation of Cauchy-Lipschitz for the one-dimensional Stefan problem. But, this procedure was lengthy.

Another approach to the moving boundary problems was reported by Rubinstein (1947) who presented solution of a problem involving heat phenomenon. He reduced the problem into integral equations of Volterra type and also discussed the proof of existence and uniqueness of the solution. The next solution of the problem was presented by Evans et al. (1950). This solution was based on Laplace transform. Ockendon (1975) also used Laplace transform to find the solution of a moving boundary problem related to oxygen diffusion. Moreover, he has drawn an attention to the usefulness of Fourier transform in semi-infinite or finite domains.

In 1980, Gliko and Efimov (1980) utilized Laplace transformation to formulate Volterra linear integral equation corresponding to a moving boundary problem to investigate the motion of a phase interface.

Kolodner (1956) used Green's functions to formulated integral equations for a problem of freezing of a lake of finite depth. Rubinstein (1971) also used Green's functions to present an analysis of the existence, uniqueness and stability of the solution of moving boundary problems and this analysis was based on the formulation of integral equations. After that Rubinstein (1980) discussed the application of integral equation techniques to several moving boundary problems in his book. Some other researchers like Collatz (1978), Chuang and Szekely (1971), Chuang and Szekely (1972) and Hansen and Hougaard (1974) also used Green's functions to obtain the solutions of these problems. Carslaw and Jaeger (1987) presented the basic theory and solutions of some standard problems in terms of Green's functions.

The next step toward the solution of these problems was reported by Goodman (1958) who applied the heat balance integral method to a phase change problem. Goodman and Shea (1960) also used this method to solve a two-phase problem of melting of finite slab. Poots (1962) considered quadratic profile and used the heat balance integral method to solve a single phase melting problem. Lardner and Pohle (1961), Goodman ((1961), (1964)), Boley and Entenssoro (1977) and Yuen (1980) also applied this technique to solve various types of moving boundary problems.

Another technique for the solutions of moving boundary problems was embedding method. Boley (1961, 1968) applied this technique to solve moving boundary problems which was valid for short times. Later on, Boley and Yagoda (1971) extended their embedding technique to obtain three dimensional starting solutions for a melting slab. Applications of embedding method for moving boundary problems were also observed by Boley (1971, 1975), Ferriss and Hill (1974) and Wilson (1978). Further study in this direction was done by Gupta (1986) who used this technique and presented a short time analytical solution for the axisymmetric melting of a long cylinder due to an infinite flux.

Beside above approximate analytical methods, other approximate analytical methods such as variational method (Biot (1957, 1959), Biot and Daughaday (1962), Kumar (1971), Vujanovic and Baclic (1976), Elliott and Ockendobn (1982)), non integral method (Rai and Rai (1982), Annamalai et al. (1986), Lau and Kondepudi (1986)), regular perturbation method (Kreith and Romie (1955), Theofanous and Lim (1971), Nayfeh (1973), Pedroso and Demoto (1973), Riley et al. (1974), Weinbaum and Jiji (1977)), strained coordinate method (Pedroso and Demoto (1973), Parang et al. (1990)), semi-analytical technique known as the nodal integral method (Savovic and Caldwell (2003)), etc. are also available in the literature for solving moving boundary problems.

Several numerical techniques are also available in the literature for the solution of moving boundary problems. Numerical treatments of moving boundary problems have been mostly based on finite-difference and finite-element methods. A variety of numerical methods for moving boundary problems was reported by Masters et al. (1971), Furzeland (1977), Finn and Vorog´lu (1979), Gupta and Kumar (1980), Dalhuijsen and Segal (1986), Kawahara and Umetsu (1986), Voller (1990), Usmani et al. (1992), Asaithambi (1997), Savovic and Caldwell (2003) and by many other authors. Some other numerical approaches like the enthalpy method (Caldwell and Chan (2000), Esen and Kutluay (2004), Voller et al. (2006)), isotherm migration method (Chernousko (1970), Crank and Phahle (1973), Turland and Wilson (1977), Durak and Wendroff (1977), Crank and Crowley (1978, 1979)), solution using automatic differentiation (Sweilam et al. (2007)), etc. have also been reported in the literature.

Most of the above methods have been applied to moving boundary problems with integer ordered derivatives (standard problem). In recent years, mathematical models of these problems with fractional derivatives are of great interest. The main aim for considering these types of mathematical models is to describe phenomena of anomalous (non-Fickian) diffusion through complex and/or disordered systems. First mathematical model with fractional derivatives related to moving boundary problem is presented by Liu and Xu (2004). After that Li et. al (2007), Liu et al. (2009), Das and Rajeev (2010), Voller (2010), etc. also discussed these types of models. The moving boundary problems with fractional derivatives are a special problem which is difficult to get the exact solution. Hence, many approximate techniques have been used to solve these problems by Li et al. (2009), Yin and Xu (2009), Das and Rajeev (2010), Singh et al.(2011), Rajeev and Kushwaha (2013), etc.

1.3 Some methods

In this thesis, the following three methods are used:

(I) Homotopy perturbation method

Consider a differential equation

$$L(u)+N(u)=f(x), \qquad x\in\Omega, \tag{1.3.1}$$

with boundary conditions

$$B(u,\frac{\partial u}{\partial t})=0, \qquad x\in\Gamma, \tag{1.3.2}$$

where L is a linear operator, N is nonlinear operator, B is boundary operator, Γ is the boundary of the domain Ω and $f(x)$ is known analytic function.

As given by He (2003, 2004, 2005), constructing a homotopy for (1.3.1) as:

$$v(x,p):\Omega\times[0,1]\rightarrow R \ ,$$

which satisfy

$$H(v,p)=(1-p)[L(v)-L(u_0)]+p[L(v)+N(v)-f(x)]=0\,, \qquad (1.3.3)$$

or

$$H(v,p)=L(v)-L(u_0)+p\,L(u_0)+p[N(v)-f(x)]=0\,, \qquad (1.3.4)$$

where $x\in\Omega$ and $p\in[0,1]$ is an imbedding parameter and u_0 is an initial approximation which satisfy the given boundary conditions.

when $p=0$, then (1.3.1) gives

$$L(v)-L(u_0)=0\,, \qquad (1.3.5)$$

and if $p=1$, then (1.3.1) becomes

$$L(v)+N(v)=f(x)\,. \qquad (1.3.6)$$

Clearly, as embedding parameter p changes from zero to unity, $v(x,p)$ varies from $u_0(x)$ to $u(x)$.

The basic assumption is that the solution of equation (1.3.3) or (1.3.4) can be expressed as a power series

$$v=v_0+p\,v_1+p^2v_2+\cdots. \qquad (1.3.7)$$

The approximate solution of (1.3.1) can be obtained as:

$$u=\lim_{p\rightarrow 1}v=v_0+v_1+v_2+\cdots\,. \qquad (1.3.8)$$

(II) Adomian decomposition method

In Adomian decomposition method (Adomian (1988, 1994, 1998), Wazwaz (2007)), the unknown function $u(x)$ of the diffential equation (1.3.1) is defined by an infinite series as:

$$u(x)=\sum_{i=0}^{\infty}u_i(x)\,. \qquad (1.3.9)$$

The nonlinear term $N(u)$ of equation (1.3.1) is decomposed into an infinite series as:

$$N(u) = \sum_{n=0}^{\infty} A_n , \qquad (1.3.10)$$

where A_n are the Adomian polynomials which are defined as:

$$A_n = \frac{1}{n!} \frac{d^n}{d s^n} N\left[\left(\sum_{i=0}^{\infty} s^i u_i\right)\right]_{x=s_0}, \; n = 0, 1, 2, \cdots . \qquad (1.3.11)$$

Equation (1.3.11) gives

$$A_0 = N(u_0), \qquad (1.3.12)$$

$$A_1 = u_1 N^{'}(u_0), \qquad (1.3.13)$$

$$A_2 = u_2 N^{'}(u_0) + \frac{1}{2} u_1^2 N^{''}(u_0), \qquad (1.3.14)$$

$$A_3 = u_3 N^{'}(u_0) + u_1 u_2 N^{''}(u_0) + \frac{1}{3} u_1^3 N^{'''}(u_0), \qquad (1.3.15)$$

$\vdots$

and so on.

From the equations (1.3.1), (1.3.9) and (1.3.10), we get

$$\sum_{i=0}^{\infty} u_i(x) = \varphi + L^{-1}(f(x)) - L^{-1}(L(\sum_{i=0}^{\infty} u_i(x))) - L^{-1}(\sum_{n=0}^{\infty} A_n), \qquad (1.3.16)$$

where φ is integration constant and inverse operator L^{-1} is one fold integral operator which is defined as:

$$L^{-1}(.) = \int_0^t (.) d\tau . \qquad (1.3.17)$$

Equation (1.3.16) gives

$$u_0(t) = \varphi + L^{-1}(f(x)), \qquad (1.3.18)$$

$$u_{n+1}(t) = -L^{-1}(L(u_n(t))) - L^{-1}A_n(u_0, u_1, u_2, u_3, \cdots, u_n). \tag{1.3.19}$$

The approximate solution of (1.3.1) is given by

$$\varphi_k = \sum_{i=0}^{k-1} u_i(t). \tag{1.3.20}$$

Generally, this series converges quickly. Therefore, few terms of the series give sufficiently accurate result.

(III) Optimal Homotopy Asymptotic Method (OHAM)

We consider the following differential equation:

$$L(u(x)) + f(x) + N(u(x)) = 0, \tag{1.3.21}$$

with

$$B\left(u, \frac{du}{dx}\right) = 0\ , \tag{1.3.22}$$

where L is a linear operator, N is nonlinear operator, x is independent variable $u(x)$ is an unknown function, $f(x)$ is a known function, and B is a boundary operator. According to optimal homotopy asymptotic method (Marinca and Herisanu (2008, 2010), Iqbal et al. (2010)), we construct homotopy as follows:

$$(1-p)[L(\Phi(x,p)) + f(x)] = H(p)[L(\Phi(x,p)) + f(x) + N(\Phi(x,p))], \tag{1.2.23}$$

$$B\left(\Phi(x,p), \frac{d\Phi(x,p)}{dx}\right) = 0, \tag{1.2.24}$$

where $x \in R,\ p \in [0,1]$ is an embedding parameter, $H(p)$ is non zero auxiliary function for $p \neq 0,\ H(0) = 0$ and $\Phi(x,p)$ is an unknown function. Moreover, $\Phi(x,0) = u_0(x)$ and $\Phi(x,1) = u(x)$.

It is clear that as p varies from 0 to 1, the solution $\Phi(x,p)$ changes from $u_0(x)$ to $u(x)$.

We choose the auxiliary function $H(p)$ in following form:

$$H(p)=\sum_{i=1}^{m} p^i c_i\,, \tag{1.3.25}$$

where c_0, c_1, c_2........... are constants which are to be determined latter.

In order to get solution, expanding $\Phi(x,p,c_i)$ in Taylor's series about p as:

$$\Phi(x,p,c_i)=u_0(x)+\sum_{m=1}^{\infty} u_m(x,c_1,c_2.......c_m)p^m\,, \tag{1.3.26}$$

and $N(\Phi(x,p,c_i))$ about the embedding parameter p as:

$$N(\Phi(x,p,c_i))=N_0(u_0(x))+\sum_{m=1}^{\infty} N_m(u_1,u_2.......u_m)p^m\,. \tag{1.3.27}$$

Now, substituting Eqs. (1.3.26 – 1.3.28) into Eq. (1.3.23) and equating the coefficient of like power of p, the following equations can be obtained:

$$L(u_0(x))+f(x)=0, \qquad B\left(u_0,\frac{du_0}{dx}\right)=0\,, \tag{1.3.28}$$

$$L(u_1(x))=c_1N_0(u_0(x)),\ B\left(u_1,\frac{du_1}{dx}\right)=0\,, \tag{1.3.29}$$

$$\begin{aligned}L(u_2(x))-L(u_1(x))&=c_2N_0(u_0(x))\\&\quad+c_1[L(u_1(x))+N_1(u_0(x),u_1(x))], \quad B\left(u_2,\frac{du_2}{dx}\right)=0\end{aligned} \tag{1.3.30}$$

and so on.

The value of $u_0(x)$ can be obtained from Eq. (1.2.28) and this is known as zeroth order problem. Eqs. (1.3.29) and (1.3.30) are the first and second order problems, respectively.

The general equation of $u_m(x)$ is given by:

$$L(u_m(x)) - L(u_{m-1}(x)) = c_m N_0(u_0(x)) + \sum_{i=1}^{m-1} c_i [L(u_{m-i}(x)) + N_{m-i}(u_0(x), u_1(x), .. u_{m-1}(x)], \quad (1.2.31)$$

$$B\left(u_m, \frac{du_m}{dx}\right) = 0; \quad (1.2.32)$$

where $m = 2, 3, \cdots$.

From the literature survey of OHAM, it is found that the convergence of series (1.3.27) depends on the constant $c_1, c_2 ....c_m$. If the series is convergent at $p = 1$ then approximate solution of $u(x)$ can be considered as:

$$\tilde{u}(x, c_1, c_2 ....c_m) = u_0(x) + \sum_{i=1}^{m} u_i(x, c_1, c_2 ....c_m). \quad (1.3.33)$$

From Eqs. (1.3.21) and (1.3.33), we define the following residual (as given by Iqbal et al. (2010)):

$$R(x, c_1, c_2 ....c_m) = L(\tilde{u}(x, c_1, c_2 ....c_m)) + f(x) + N(\tilde{u}(x, c_1, c_2 ....c_m)). \quad (1.3.34)$$

In order to obtain the values of c_i $(i = 1, 2, 3 \cdots, m)$, we first choose a and b for which optimum values of c_i exist. There are many methods like Galerkin method, Ritz method, collocation method to find the optimum value of constants. In this thesis, method of least square is used. In this method, a functional is constructed as given below:

$$J(c_1, c_2, ...c_m) = \int_a^b R^2(x, c_1, c_2, ...c_m)\, dx, \quad (1.3.35)$$

where $R(x, c_1, c_2 ....c_m)$ is residual as given in Eq. (1.3.34).

Optimum values of constants can be found by solving following equations:

$$\frac{\partial J}{\partial c_1} = 0, \frac{\partial J}{\partial c_2} = 0, \frac{\partial J}{\partial c_3} = 0, \cdots, \frac{\partial J}{\partial c_m} = 0. \quad (1.3.36)$$

With these constants, one can get the approximate solution of $u(x)$ of order *m*.

1.4 Caputo fractional derivative

In the literature of fractional derivatives, several definitions of fractional derivatives are available, like Riemann-Liouville, Caputo, Riesz , Grunwald-Letnikov, etc. In this thesis, Caputo fractional derivative is used in some mathematical models related to moving boundary problems. Caputo fractional derivative is the most convenient definition for real applications (Podlubny (1999), Rajeev et al. (2013)). The definition of Caputo fractional derivative (Podlubny (1999)) is proposed by M. Caputo.

Definition: Fractional derivative (D_t^{β}) of $f(t)$ in the Caputo's sense is defined as

$$
\begin{aligned}
{}_aD_t^{\beta} f(t) &= D_t^{\beta-n}[f^{(n)}(t)] \\
&= \frac{1}{\Gamma(n-\beta)} \int_a^t \frac{f^{(n)}(\tau)}{(t-\tau)^{\beta+1-n}} d\tau \qquad (n-1<\beta\le n,\ n\in N),
\end{aligned}
$$

and
$$
{}_aD_t^{-\beta} f(t) = \int_a^t \frac{(t-\tau)^{\beta-1}}{\Gamma(\beta)} f(\tau) d\tau \qquad (\beta>0).
$$

where $\Gamma(.)$ is the Euler gamma function which is defined as:

$$
\Gamma(\tau) = \int_0^{\infty} e^{-u} u^{\tau-1} d\tau \quad \text{for all} \quad \tau\in R,
$$

$$
\Gamma(\tau+1) = \tau\,\Gamma(\tau) \quad \text{when} \quad \tau\in N^{+}, \quad \Gamma(\tau) = (\tau-1)!\ .
$$

The following properties of Caputo fractional derivatives are used in this thesis:

(I) $D_t^{\beta} C = 0$, (C is constant)

(II) $D_t^{\beta} t^{\alpha} = \dfrac{\Gamma(1+\alpha)}{\Gamma(1+\alpha-\beta)} t^{\alpha-\beta}$, $(0\le m\le\beta<m+1, \alpha>m, m\in N)$.

(III) ${}_aD_t^{\beta}\left({}_aD_t^{m} f(t)\right) = {}_aD_t^{\beta+m} f(t)$, $(m=0,1,2,3\cdots;\ n-1<\beta<n)$.

In particular, if $\beta>0$

$$
D_t^{\beta} t^{\beta+1} = \Gamma(\beta+2) \text{ and } D_t^{\beta} t^{\beta} = \Gamma(\beta+1).
$$