

Chapter 1

Introduction

The partial diffusion equations describe many physical phenomena but finding their exact solutions are not always possible, so developing the numerical method that can solve those equations accurately is a significant challenge. From the thesis title “**Behavior of solute concentration in porous media**”, it is very much clear that the work is mainly focused on solving the diffusion equations arising in porous media and observe the behavior of solute concentration due to change in different parameters of the diffusion models. The author has not only focused on solving unsolved porous media models but also on developing numerical methods that can perform better than previously existing numerical methods. Before the starting of discussion about solving the diffusion model, it needs to discuss some of the basic terms used in the thesis.

1.1 Porous Media

Porous media is nothing but a domain with partially occupied with solid matrix, and the remaining parts of the domain are referred to as pore or void. The term ‘solid’ here represents the wider spectrum than its strict definition describes. Thus crystalline substance, manufactured polymers, rubber, and organic materials, such as the tissue matrix of lungs and kidneys, are also regarded as ‘solid’. The remaining part, i.e., the void space, is filled with one or more fluid phases like gas or liquid. The solid phase and void space should be uniformly distributed throughout the medium. This solid phase of the medium dictates the flow of fluid in the porous medium. At least some of the pores should be interconnected and sometimes called as effective pore space. The unconnected pores may be taken as part of the solid matrix. If we look around, we can observe that there are various types

of porous media those are present around us, viz. sand, fissured rock, fractured porous rock, cemented sandstone, and Karstic limestone, etc., are naturally accruing porous media. In the natural porous media, the distribution of pores with respect to shape and size is irregular. Paper, ceramics, foam rubber, bread, and filter, etc., are manufactured porous media, and bones, lungs and kidneys, etc., are organic porous media. From Figure 1.1, we can visualize some of the porous media. The porous media domain is used in a large number of industrial and engineering disciplines, viz., paper and diaper industries, petroleum reservoir engineering, hydrogeology, chemical engineering, and biomedical engineering. Soil- water problem in civil engineering is described on the basis of the theory of porous media.

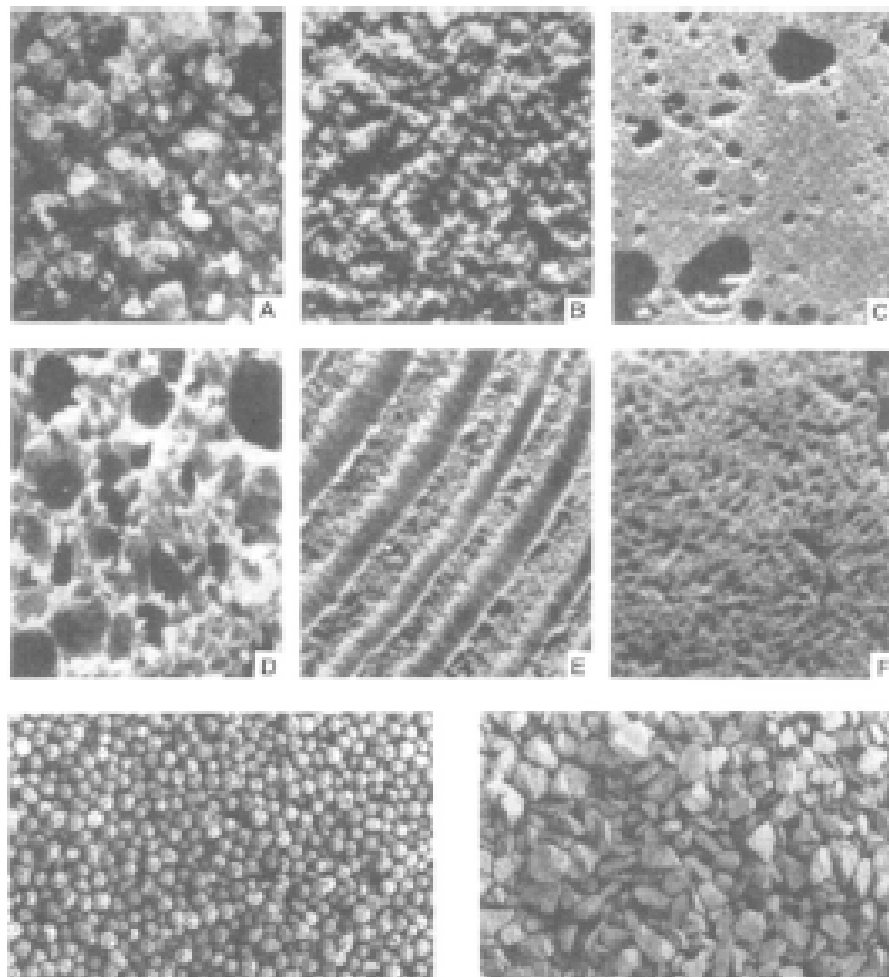


FIGURE 1.1: Top: Examples of natural and organic porous materials: (a) beach sand, (b) sandstone, (c) limestone, (d) rye bread, (e) wood, and (f) human lung. Bottom: Granular porous materials used in the construction industry, 0.5-cm-diameter Liapor® spheres (left), and 1-cm-size crushed limestone(right) [1]

In the 18th and 19th centuries, the essential parts of porous media theory were formulated viz. the geometry of porous bodies, fundamental principles of mechanics and volume fraction concept, etc. It is worth to mention that Leonhard Euler in 1762 made a remark on porous bodies in the published work "Anleitung zur Naturlehre". After that, Euler did not contribute directly to porous media theory, but he was involved indirectly. Some of the important axioms of continuum mechanics were created and formulated by Euler viz. cut principle, the balance of mass, the balance of moment, the balance of moment of momentum. Reinhard Woltman(1754-1837), who was an excellent engineer and scientist, made an outstanding contribution to the porous media theory. He wrote his idea on soil mechanics, and porous media in the third volume of "Beytrage zur Hydraulischen Architektur" [2]. He further introduced the concept of volume friction. He was probably the first scientist to use this concept. Unfortunately, he did not continue his work on porous bodies, but his concept of volume frictions related to volume elements of the water-saturated porous body played a very important role in the development of porous media theory. Delesse [3] in 1848, developed a concept related to the surface element of a saturated porous body. He successfully proved that under certain conditions, surface friction is equal to volume friction. At the beginning of the development of the theory of porous media, the reflection principle of Delesse played an important role. In the 19th century, the development of a second important branch of porous media theory started, viz. the development of the mixture theory. In 1855, Fick [4], made the first attempt to create the theory of mixture while studying the problem related to diffusion. Later, Stefan [5] in the year 1871 successfully created the theory of mixture for two gases. Darcy [6] in 1865, gave a result through an experiment by observing the loss of pressure and total volume of running water through the saturated sand. His results are very essential for mechanical treatment of the motion of liquid through porous media. Till the 19th century, there was enough background materials to treat empty or fluid-saturated porous media viz. main principles of mechanics by Euler, the concept of volume friction by R. Woltman, some of the import laws by A. Delesse, A. Fick and Darcy, and mixture theory by Stefan. Apart from them, many other scientists were contributed to the development of porous media theory. Gibbs published many articles during the years 1876-1878 to interpret the chemo-physical phenomenon with the help of thermodynamical methods and established the entire field of physical chemistry, which is part of modern porous media approach. Jaumann [7] in the year 1911, worked on continuum mechanics and mixture theory which later become the pillars of the modern theory of porous media. Fillunger [8] in 1913, published his first article related to buoyancy force in the gravity dams, which became a

masterpiece when the problem is taken in two interacting continua soil and water. Unfortunately, there was a slight mistake in Fillunger's concept, which was later pointed by Terzaghi. Many scientists have continued the basic work done by Fillunger and Terzaghi on porous media viz., Heinrich [9] in 1938, who follow the idea of Fillunger and published work related to the settlement of clay layers. Biot [10, 11] in 1935 and 1941 published his articles intuitively based treaties by following the basic ideas of Terzaghi, although he became famous for his work in the years 1955 and 1956 [12, 13, 14]. Boer and Ehlers [15] in 1988, published the reviewing the history of porous media firstly. R. D. Boer is also known for recovering the lost article written by Heinrich and Desoyer [9, 16]. Modern era of porous media theories is started when Truesdell-III entered in this field and brought the Jaumann [7] work on continuum mechanics into light again. His works originated the modern view on mixture theory, and continuum [17] and thermodynamics [18], but some of the assumptions considered by Truesdell were wrong. Later Kelly [19] generalized Truesdell's mixture theory in 1964. Adkins [20, 21, 22] and Green and Adkins [23] developed the first mechanically motivated approach for single and mixture fluid and elastic solid, which was literally based on Truesdell's mixture theory. Bowen [24] in 1967, came up with own version of constitutive equations of mixtures based on the tensor of chemical potential. He believes that there are mistakes in the existing theories as those are based on partial stress instead of chemical potential, and thus those describe only ideal mixtures. A. E. Green and P. M. Naghadi showed that taking tensors of chemical potential instead of partial stress would not lead us to a different theory which was later accepted by Bowen [25] in 1969. Truesdell [17] in 1968 developed his own version of mixture theory which was later called as Bowen-Truesdell form, because of the results of Bowen and Truesdell were identical. Bowen [26, 27] published two models for incompressible and compressible porous media in the years 1980 and 1982 respectively, which are based on his own famous theory of mixture [28]. Porous media theories split into two different directions after Bowen's article. One was following the Terzaghi-Biot line, and another was following Bowen's line. In the year 1989, a new concept related to the component of porous media was introduced by the Ehlers [29] named phase separation to overcome the confusion related to the grading of material. In recent times, the theory of porous media is being used in many fields viz. to measure the stability behavior of partially and fully saturated soils and also to construct the dams, embankments, electronics cooling, catalytic reactor, tissue engineering, nuclear waste repository, etc.

1.2 Fractional Calculus

We all are familiar with differential calculus and clearly understood the notation of n th order derivative, that is, applying the differential operator n -times in succession. Later in 1695, G. de L'Hospital and G. W. Leibniz discussed the possibility of n to be other than integers through the letters. That was the day when fractional calculus was born. From that day to date, the question raised by G. de L'Hospital and G. W. Leibniz became the topic of research for many researchers. Many renowned mathematicians like Leonhard Euler, Lagrange, Laplace, S.F. Lacroix, J. Fourier, N.H. Abel, J. Liouville, O. Heaviside, B. Riemann, H. Weyl, G. Leibniz, A. K. Grunwald, and A.V. Letnikov have their valuable contributions in the field of fractional calculus.

Although G. de L'Hospital and G. W. Leibniz discussed about fractional-order derivative in 1695 but no literature is found from 17th-century to 18th-century related to arbitrary order derivative. Leonhard Euler and Joseph Fourier mentioned about the derivative of arbitrary order, but they did not consider it in their further work. In the second decade of the 19-th-century, S. F. Lacroix defined the derivative of arbitrary order of x^m in 1819 by using Gamma function as

$$D^\alpha x^m = \frac{\Gamma(m)}{\Gamma(m-\alpha)} x^{m-\alpha}, \quad (1.1)$$

where $\Gamma(m)$ is the Gamma function defined by

$$\Gamma(m) = \int_0^\infty e^{-t} t^{m-1} dt.$$

In the book written by Ross [30], it is discussed that how the fractional calculus evolved and how the researchers used the fractional calculus to solve their problem. It is mentioned that N. H. Abel in 1823, used fractional derivative to solve the Tautochrone problem. This attracts J. Liouville, and in 1832, he made the first major attempt to give the logical definition of the fractional-order derivative of any arbitrary function by expanding it in series of exponential. He started his theoretical development with the well-known result of derivatives of integer order n as

$$D_x^n = a^n e^{ax}. \quad (1.2)$$

He generalized the above equation for non-integer order as

$$D_x^\beta = a^\beta e^{ax}. \quad (1.3)$$

He wrote any arbitrary function $f(x)$ in series form as

$$f(x) = \sum_{n=0}^{\infty} c_n e^{a_n x}, \quad (1.4)$$

and the derivative of $f(x)$ on any arbitrary order β as

$$D^\beta f(x) = \sum_{n=0}^{\infty} c_n a_n^\beta e^{a_n x}. \quad (1.5)$$

This formula is known as Liouville's first definition, and obviously, it had some disadvantages, but it was the first milestone in fractional calculus. To overcome with the disadvantages, Liouville produced a second definition by transforming an integral to the gamma function and derived the following formula for arbitrary order derivative

$$D_x^\beta x^{-\alpha} = (-1)^\beta \frac{\Gamma(\beta + \alpha)}{\Gamma(\alpha)} x^{-\alpha - \beta}. \quad (1.6)$$

Later, between the years 1835 to 1850, there were many controversies between the mathematicians regarding the definitions of fractional-order derivatives. The most useful advancement in the fractional calculus was due to the article written by G. F. Bernhard Riemann during his student days when he was seeking to generalize a Taylor series in 1853. Riemann gave a different definition that involved the definite integral as

$$D_c^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_c^x (x-t)^{\alpha-1} f(t) dt + \psi(x), \quad (1.7)$$

where $\psi(x)$ is the Riemann's complementary function. He added a complementary function due to ambiguity in the lower limit of the integration. The present days' definition of fractional integration is the same as above but doesn't contain a complementary function. Since neither Riemann nor Liouville solved the problem of complementary function, it will be of greater interest how today's Riemann-Liouville finally looks like. In 1869, Sonin [31] did the work which leads us to today's Riemann-Liouville differentiation of arbitrary order. Sonin started with Cauchy's integral formula to define the differentiation with arbitrary order. In a very short period of time, Letnikov [32] in the year 1872 extended the idea of Sonin. Both tried to define fractional derivative by utilizing a closed contour, but we all know that Cauchy's integral formula contains a branch point, which means appropriate

contour will be required for branch cut, which was not included in the work of Sonin and Letnikov. Later, Laurent [33] has developed today's Riemann-Liouville fractional integral by using an open circuit instead of a closed circuit. Nearly simultaneously, Grunwald and Letnikov [34] have provided another definition of fractional order derivative, which is also frequently used today. Later in 1927, Marchaud [35] developed an integral version of Grunwald and Letnikov's definition. M. Caputo made the most significant contribution to the fractional calculus in the modern era in 1967 to deal with the main drawback of Riemann-Liouville's definition of fractional derivative. In the next section, we will discuss various properties, drawbacks, and relation between Riemann-Liouville and Caputo derivatives. The first conference on fractional calculus with the name "The First Conference on Fractional Calculus and its Applications" was held in 1974 in New Haven. In the same year, the first book on fractional calculus was published by Oldham and Spanier [36]. This seeks the attention of researchers from different background and they have published a number of book on fractional calculus afterward viz., Nishimoto [37], Miller and Ross [38], Kiryakova [39], Rubin [40], Podlubny [41], Hilfer [42], Kilbas et al. [43], etc.

1.3 Definitions of fractional order derivative and integral

There are various versions of the definition of fractional order derivative and integral. In this section, the author has discussed only those definitions which have been used in the forthcoming chapters.

1.3.1 Riemann-Liouville Arbitrary Order Integral

Let $f(x)$ be the locally integrable function. The Riemann-Liouville integral of arbitrary order $\beta \geq 0$ is defined by

$${}_a D_t^{-\beta} f(x) = \begin{cases} f(x), & \beta = 0, \\ \frac{1}{\Gamma(\beta)} \int_c^t (t - \tau)^{\beta-1} f(\tau) d\tau, & \beta > 0, \end{cases} \quad (1.8)$$

where $t > c$, $t, c, \beta \in \mathbb{R}$ and $\Gamma(\cdot)$ is the gamma function.

1.3.2 Riemann-Liouville Arbitrary Order derivative

The Riemann-Liouville derivative of arbitrary order $\alpha \geq 0$ of the function $f(x)$ is defined by

$${}_a D_t^\alpha f(x) = \begin{cases} f(x), & \alpha = 0, \\ \frac{1}{\Gamma(k-\alpha)} \frac{d^k}{dt^k} \int_c^t (t-\tau)^{k-\alpha-1} f(\tau) d\tau, & \alpha > 0, \end{cases} \quad (1.9)$$

where, $t > a$, $t, a, \alpha \in \mathbb{R}$, $k-1 \leq \alpha < k$.

1.3.3 Caputo Arbitrary Order Derivative

The fractional order derivative of function $f(x)$ in Caputo sense of order α is

$${}_a^C D_t^\alpha = \begin{cases} f(t), & \alpha = 0, \\ \frac{1}{\Gamma(\alpha-n)} \int_a^t \frac{f^{(n)}(\tau)}{(t-\tau)^{\alpha+1-n}} d\tau, & \alpha > 0, \end{cases} \quad (1.10)$$

where $t > a$, $t, a, \alpha \in \mathbb{R}$, $k-1 \leq \alpha < k$.

1.3.4 Some properties of Fractional operators

1. ${}_a D_t^{-\alpha} ({}_a D_t^{-\beta} f(t)) = {}_a D_t^{-\beta} ({}_a D_t^{-\alpha} f(t)) = {}_a D_t^{-\alpha-\beta} f(t)$,
2. ${}_a D_t^\alpha ({}_a D_t^\beta f(t)) = {}_a D_t^\beta ({}_a D_t^\alpha f(t)) = {}_a D_t^{\alpha+\beta} f(t)$,
3. ${}_a D_t^\alpha ({}_a D_t^{-\alpha} f(t)) = f(t)$,
4. ${}_a D_t^{-\alpha} ({}_a D_t^\alpha f(t)) = f(t) - \sum_{j=1}^k [{}_a D_t^{\alpha-j} f(t)]_{t=a} \frac{(t-a)^{\alpha-j}}{\Gamma(\alpha-j+1)}$, $k-1 \leq \alpha < k$,
5. ${}_a D_t^{-\alpha} ((t-a)^v) = \frac{\Gamma(1+v)}{\Gamma(1+v-\alpha)} (t-a)^{v+\alpha}$
6. ${}_a D_t^\alpha ((t-a)^v) = {}_a^C D_t^\alpha ((t-a)^v) = \begin{cases} 0, & v \in 0, 1, 2, \dots, [\alpha] - 1, \\ \frac{\Gamma(1+v)}{\Gamma(1+v-\alpha)} (t-a)^{v-\alpha}, & v \geq [\alpha]. \end{cases}$
7. ${}_0 D_t^\alpha A = \frac{At^{-\alpha}}{\Gamma(1-\alpha)}$
8. ${}_a^C D_t^\alpha A = 0$
9. ${}_a^C D_t^\alpha (\lambda f(x) + \mu g(x)) = \lambda ({}_a^C D_t^\alpha f(x)) + \mu ({}_a^C D_t^\alpha g(x))$

1.4 Fibonacci Polynomial

In almost every chapter of the thesis, the Fibonacci polynomial has been used to develop the numerical method, so it will be fairly good to discuss something about it here. Fibonacci polynomials are a natural extension of k -Fibonacci numbers. For any positive real number k , the K -Fibonacci numbers are defined as

$$F_{k,n+1} = kF_{k,n} + F_{k,n-1}, \quad \text{for } n \geq 1, \quad (1.11)$$

with initial conditions $F_{k,0} = 0$ and $F_{k,1} = 1$. Now if we consider k as the real variable x then the Fibonacci polynomial will be defined as

$$F_{n+1}(x) = \begin{cases} 1, & \text{if } n = 0, \\ x, & \text{if } n = 1, \\ xF_n(x) + F_{n-1}(x), & \text{if } n > 1. \end{cases} \quad (1.12)$$

Fibonacci polynomials are known for a long time but in recent years it has gained the attention of researchers. From the above relation (1.12), the explicit form of the series is obtained as

$$F_n(x) = \sum_{r=0}^{\lfloor \frac{n-1}{2} \rfloor} \binom{n-r-1}{r} x^{n-2r-1}, \quad (1.13)$$

where $\lfloor \cdot \rfloor$ denotes the floor function.

Furthermore, the polynomial x^m in terms of Fibonacci polynomial is [44]

$$x^m = \sum_{i=0}^{\lfloor \frac{m-1}{2} \rfloor} (-1)^i \left[\binom{m}{i} - \binom{m}{i-1} \right] F_{m-2i+1}(x), \quad m \geq 0. \quad (1.14)$$

Now equations (1.13) and (1.14) can be rewritten as

$$F_i(x) = \sum_{\substack{j=0 \\ (j+i)=\text{odd}}}^i \frac{\binom{i+j-1}{\frac{i+j-1}{2}}!}{j! \binom{i-j-1}{\frac{i-j-1}{2}}!} x^j, \quad i \geq 0 \quad (1.15)$$

and

$$x^m = m! \sum_{\substack{j=1 \\ (j+m)=\text{odd}}}^{m+1} \frac{(-1)^{\frac{i+j-1}{2}} j}{\binom{m-j+1}{\frac{m-j+1}{2}}! \binom{m+j+1}{\frac{m+j+1}{2}}!} F_j(x), \quad m \geq 0, \quad (1.16)$$

respectively.

A square integrable function $f(x)$ can be expressed in terms of Fibonacci polynomial as [45]

$$f(x) = \sum_{k=1}^{\infty} c_k F_k, \quad (1.17)$$

where

$$c_k = \sum_{j=0}^{\infty} \frac{k(-1)^j f^{(2j+k-1)}(0)}{2^{(2j+k-1)} j!(j+k)!}.$$

1.5 Advection Reaction-Diffusion Equation in Porous Media

The present work is focused on solving the advection-reaction-diffusion equations. Let us talk about all the terms of the advection reaction-diffusion equation. The general form of the equation for $u(x, t)$ is written as

$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u) - \nabla \cdot (vu) + ku. \quad (1.18)$$

The above equation (1.18) governs the concentration of the solute particle u in the medium (fluid). The first term from the right-hand side of the equation (1.18) represents the diffusion term, and D is the diffusion coefficient. The second term from the right-hand side of the equation (1.18) represents the advection term, and v represents the velocity of the medium. The last term represents the reaction term. The value of k is dependent on the medium and could be positive, negative, and zero for source, sink, and conservative medium, respectively. The change in the concentration of the solute particle in the medium mainly depends on transport and transformation. The two primary modes of transport of solute particles are diffusion (the transport associated with the random motion of the solute particle within the medium) and advection (transport associated with the flow of the medium). Transformation refers to those processes that change a substance of interest into another substance. The two primary modes of transformation are physical (transformations caused by physical laws, such as radioactive decay) and chemical (transformations caused by chemical or biological reactions, such as dissolution). The transformation governs with the reaction term.

The term Diffusion comes from the Latin language, which means “to spread out”. Diffusion is a fundamental process that results from the random collision of solute molecules and produces a flux of solute particles from areas of higher to lower solute concentration. One can understand the diffusion process more accurately by an example, consider a bottle of perfume is opened in an empty room and allowed to evaporate into the air, soon the whole room will be scented. We also know from experience that the scent will be stronger near the source and weaker as we move away, but fragrance molecules will have wandered throughout the room due to random molecular and turbulent motions. Thus diffusion has two primary properties, it is random in nature, and transport is from regions of high concentration to low concentration, with an equilibrium state of uniform concentration. If only the diffusion process is responsible for the movement of the solute particle, then equation (1.18) is called a diffusion equation and will be reduced into the following form

$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u). \quad (1.19)$$

We all know the above equation (1.19) is drawn with the help of Fick’s first law. Now, if in addition to diffusion, the solute particles are moving due to the flow of the medium, then the resulting equation will be called an advection-diffusion equation, and the equation (1.19) will be transformed into the following form

$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u) - \nabla(vu). \quad (1.20)$$

This added term is calculated with the help of Darcy’s law. Now, if the transformation of the solute particles is caused by any other reason in the medium, then the additional reaction term (R) will be added to the advection-diffusion equation and called advection reaction-diffusion equation and will take the form

$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u) - \nabla(vu) + R. \quad (1.21)$$

When the concept of fractional order derivatives into the picture, this gives advantage to the researchers to model any physical or chemical phenomenon more accurately, but advantage comes with the complexity of the model. The fractional-order general form of the above classical reaction-diffusion equation (1.21) in Caputo sense is of the form

$${}^C_0 D_t^\alpha u = {}^C_0 D_x^\beta (Du) - \nabla(vu) + R, \quad (1.22)$$

where $0 < \alpha \leq 1$ and $1 < \beta \leq 2$.

Experimental evidences suggest that the classical integer order diffusion equation may not accurately model many physical, biological phenomena, this is where the fractional type diffusion model comes in to the picture. Within the last two decades, many phenomena have been modeled with the help of fractional order diffusion equation viz. Baeumer et al. [46] modeled the contaminant transport, Gorenflo et al. [47] gave random walk model in the form of the fractional diffusion equation, Cartea and Negrete [48] developed a fractional order diffusion model to predict the option prices in markets with jumps, Magin et al. [49] modeled the porous biological tissues, Henry et al. [50] modeled the single processing in neuronal dendrites. Many researchers have modeled the cancer tumor cells with the help of fractional diffusion equation [51, 52, 53, 54, 55]. Although many phenomena can be modeled with fractional diffusion equation but finding the solution of that model is not always easy due to increase in complexity of the model. This becomes a challenging job to the researchers to develop an efficient method that can perform better on that type of complex model. Wang and Basu [56] developed a fast finite difference method to solve the space fractional diffusion model. Hanert and Piret [57] developed a numerical method with the help of Chebyshev polynomials and Galerkin method to solve temporal fractional diffusion equation. Cheng [58] developed an efficient Eulerian–Lagrangian control volume method to solve space-fractional diffusion equation. Li and Wu [59] have developed a numerical technique to solve distributed order fractional diffusion equation with the help of classical quadrature formula. Wei et al. [60] have used the local radial basis function to develop a method to solve variable-order fractional diffusion equation for the two-dimensional irregular domain. Zaky and Tenreiro [61] have developed a spectral tau scheme with Legendre polynomial to solve multi-dimensional fractional diffusion equation. Verma and Kumar [62] have solved the multi-dimensional fractional diffusion equation with two-step Adomian decomposition method.

Many researchers have developed efficient methods to solve fractional diffusion models related to some of the real-world phenomena. Jiang et al. [63] solved fractional diffusion model for non-local transport flow with finite Hankel integral and Laplace transformation. Jiang et al. [64] used the separation variables technique to solve the fractional diffusion model for fast desorption of methane in coal. Obembe et al. [65] solved variable order fractional diffusion model describing fluid flow in a heterogeneous porous medium with control volume finite difference approximations. Daihong Gu et al. [66] used Laplace transformation to solve the fractional diffusion model evaluating the performance of multiple fractured horizontal wells with stimulated reservoir volume in tight gas reservoirs. Bai et al. [67] used the finite difference method with L_2 formula to solve the fractional

diffusion model to measure the volatile organic compound concentrations of dry building materials. Obembe [68] solved fractional diffusion model of single-phase, single-well simulation in hydrocarbon reservoirs with block-centered finite-difference approximation method.

This thesis is an effort to fully explore the fractional diffusion model and develop the efficient and accurate numerical methods which perform better as compared to previously existing methods, to observe the behavior of diffusion models due to changes in different parameters of the models.