# Chapter 1

# Introduction

The thesis titled "Study of Dynamics of Fluid in Porous Media" confirms that here the mathematical models describing the transport of solute concentration in groundwater through the porous media have been examined. In this scientific work, mainly, drives have been developed under prescribed initial and boundary conditions to deal with those mathematical transport models numerically. While the numerical computations the known and existing drives are taken and those are extended in accordance to the concerned mathematical models for various fluid transport phenomena. Scientists and researchers seek the attention of the problems of groundwater contamination nowadays. The recent studies and results works on groundwater contamination problems have motivated the author to examine the transport models of solute concentration.

## 1.1 Groundwater Contamination

Groundwater is an important source of freshwater in forming, industries, and drinking water for humanities. Major part of populations get their drinking water through groundwater. Big problems occur nowadays for drinking water as it is getting polluted by many sources from humans and nature. Groundwater pollution (also called groundwater contamination) occurs when pollutants are released to the ground and make their way down into groundwater. This type of water pollution can also occur naturally due to the presence of a minor and unwanted constituent, contaminant or impurity in the groundwater, in which case it is more likely referred to as contamination rather than pollution. Pollution can occur from on-site sanitation systems, landfills, effluent from waste water treatment plants, leaking sewers, petrol filling stations or from over applications of fertilizers in agriculture

[1, 2, 3, 4] (see Fig. 1.1). Pollution (or contamination) can also occur from naturally occurring contaminants, such as arsenic or fluoride. Using polluted groundwater causes hazards to public health through poisoning or the spread of diseases.

Different mechanisms have influenced on the transport of pollutants, e.g., diffusion, adsorption, precipitation, decay, in the groundwater. The interaction of groundwater contamination with surface waters is analyzed by use of hydrology transport models.

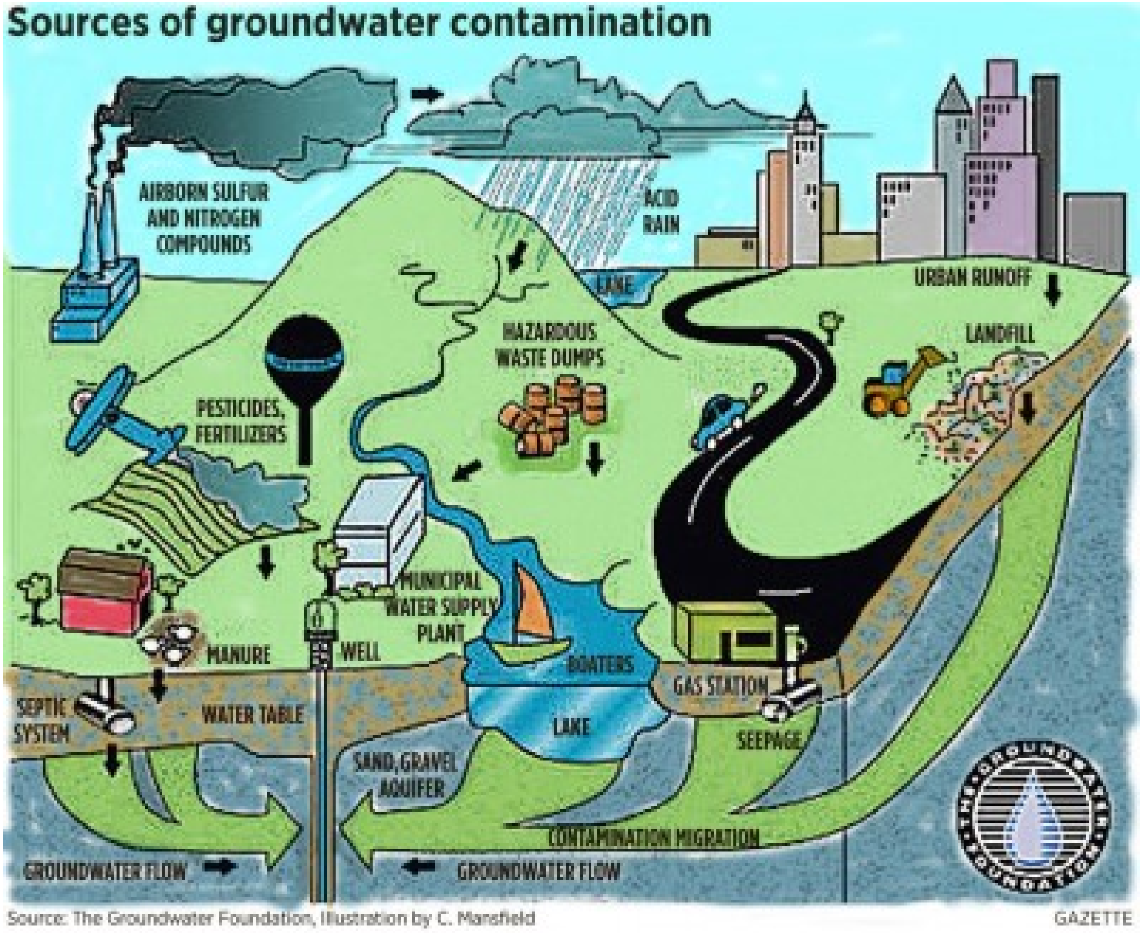


FIGURE 1.1: Various sources of groundwater contamination
(Source: The Groundwater Foundation)

The prediction of contaminant transportation in the subsurface is very difficult and complex. The nature of reaction with geologic substances is different for different contaminants. Percolation through soils is the most common process of contaminant transportation. Dispersion and advection are the main processes for the transport of dissolved solutes. Solubility is a significant characteristic of contaminant for the groundwater contamination (Fig. 1.2).

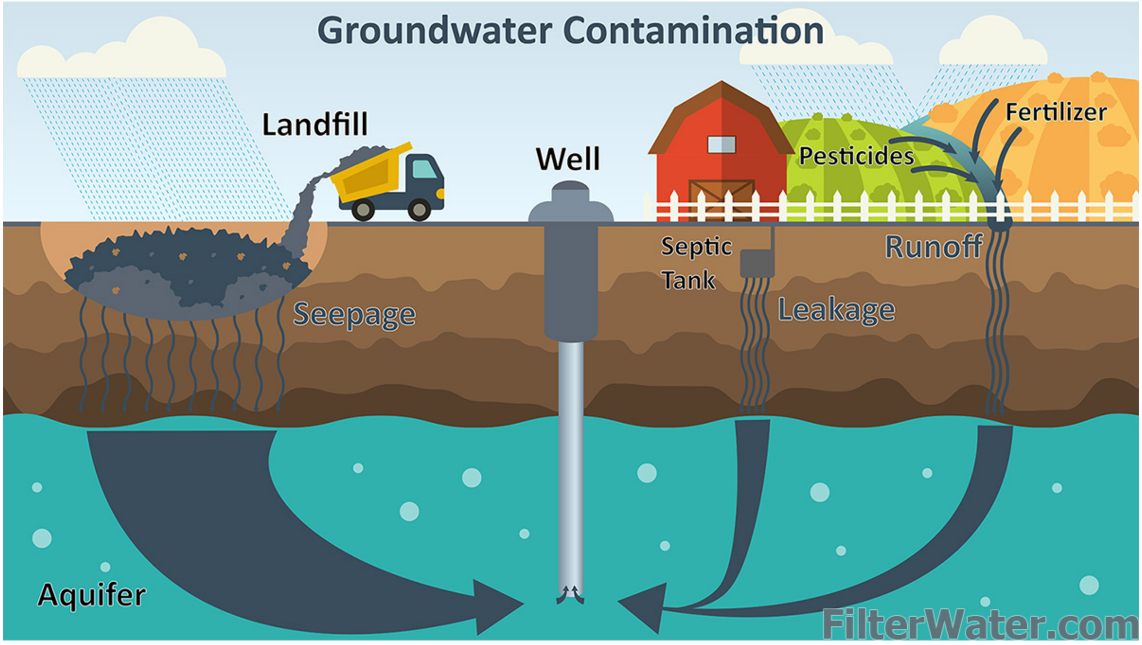


FIGURE 1.2: Plot of groundwater contamination

## 1.2 Porous Media

Generally, a porous medium or a porous material is a material containing pores (voids). The pores are typically filled with a fluid (liquid or gas). But it is not sufficient to describe the flow through the porous media. One may try to improve the definitions by stipulating that the pores are interconnected, with at least several continuous paths from one side of the medium to other. Also the Mass conservation of fluid across the porous medium involves the basic principle that mass 'flux in' minus mass 'flux out' equals to the increase in amount stored by a medium. This means that total mass of the fluid is always conserved.

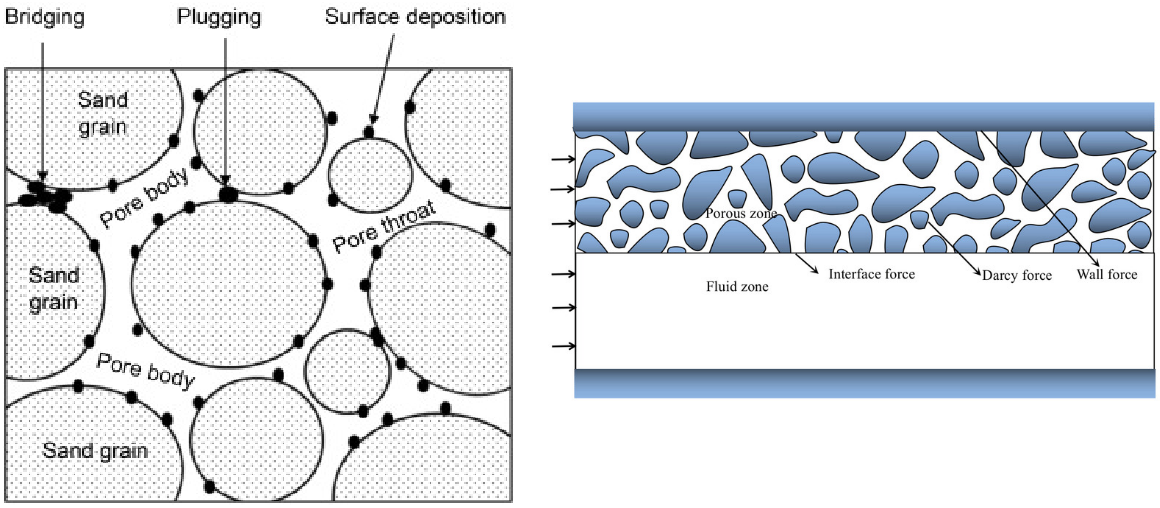


FIGURE 1.3: Pictorial form of some porous media

Membranes, pigments, electrodes, ceramics, catalysts, sensors, etc., are few useful porous materials used in various industries. Due to wide applications of porous materials in industries and many types of porous structure, there have been many experiments performed to analyze the characteristic of porous solid. There are many useful definitions given in order to characterize porous solid.

**True Density:** It is the density of solid network present in porous material i.e., density of porous material except interparticle voids and pores.

**Apparent Density:** It is the density of porous material including inaccessible and closed pores.

**Bulk Density:** It is the density of the porous material which also includes interparticle voids and pores.

**Pore Volume:** It is the total volume of pores present in the porous material.

**Pore Size (Pore Diameter/Width):** It is the distance between two opposite walls of pore.

**Porosity:** It is the ratio of pore volume to the apparent volume of the porous material.

**Surface Area:** It is the total detectable (accessible) of solid surface per unit mass of the porous material.

The history and development of applications of porous media have already been discussed and analyzed by many scientists and engineers in their research articles and monographs [5, 6, 7]. Based on their research, the study of porous media which is basically a macroscopic continuum mechanical approach was evolved in three main phases. The study of principles of mechanics, theory of mixtures and concept of volume fraction during the early 19th century is considered as the first phase of evolution of porous media. Later on the study of interactions of solid rigid porous materials, gases and liquids between 1910 and 1960, and the study of theory of immiscible mixtures between 1970 and 1980 are considered as second and third phases of evolution of porous media.

The authors of [8] have explained that the problem containing fluid flow through a porous material is mainly depends on the scale consideration. For the macro scale (large scale) there are a large number of void/pore spaces in the field of vision and in these types of scale they have used a volume continuum (averaging) approach because the complication in fluid flow paths and the need to mention the complex spatial resolution of the porous material reduce the possibility of applications of conventional fluid mechanics approach. The micro scale (small scale) there are only few small pores visible and to analyze the fluid flow processes in the fluid filled pores. In this case, they have used conventional fluid mechanics approach.

### 1.2.1 Local Thermodynamic Equilibrium in Porous Media

In porous media, the local thermodynamic equilibrium mainly counts the chemical equilibrium, mechanical equilibrium and thermal equilibrium. These equilibrium system is defined as follows.

**Chemical Equilibrium:** In a chemical equilibrium, the potential to exchange the chemical components within a particular phase or across different phases is zero. Particularly, no exchange of chemical components between different phases or within a particular phase.

**Mechanical Equilibrium:** In a mechanical equilibrium, there are equal pressure present on both sides of the phase boundary for multi fluid phase systems. For fluid flow in porous media there may be pressure jump due to capillarity on the boundaries of fluid phase [9].

**Thermal Equilibrium:** In a thermal equilibrium, all phases of the system are at same temperature at any point of the system.

### 1.2.2 Darcy's Law

The basic law governing the flow of fluids through porous media is Darcy's Law, which was formulated by the Henry Darcy in 1856 based on his experiment (Fig. 1.4) on vertical water filtration through sand beds [10]. This law can be expressed by the following expression as

$$N \cdot W = -K \cdot gradH. \tag{1.1}$$

In this expression, the pressure head is given by $gradH, K$ is the hydraulic conductivity also known as Darcy permeability, fluid volume fraction is given by $N, W$ is the seepage velocity, and their product $N \cdot W$ is called as filter velocity.

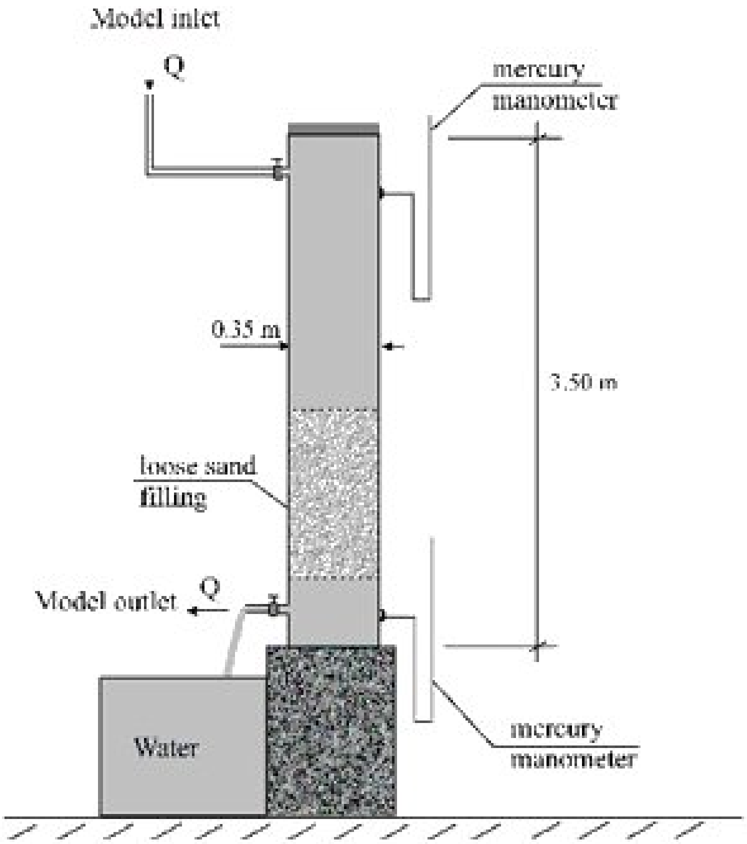


FIGURE 1.4: Darcy's apparatus.

The problem of diffusion in the theory of mixtures is first discussed by Adolf Fick. In his first law, he states that the concentration flow of particles (diffusion flux) in a two component mixtures is directly proportional to the concentration gradient. The mass conservation equation with the Fick's first law provides us the following equation known as Fick's second law.

$$\frac{\partial C}{\partial t} = d \cdot div(gradC). \tag{1.2}$$

Here $C$ is the particle concentration and $d$ is the diffusion coefficient.

The Darcy's law is derived from the famous Navier-Stokes equation. Darcy in 1856 based on his experiment states that the flow rate of particles in the medium is directly proportional to the applied pressure difference and it is similar to Ohm's law, Fourier's law and Fick's law in electric field, heat conduction and diffusion processes, respectively. For transient processes in which the flux varies from point to-point, the following differential form of Darcy's law is used.

$$Q = -\frac{KA}{\mu}\frac{dp}{dx}, \tag{1.3}$$

where $Q$ is volumetric flow rate, $p$ is pressure across medium, $A$ is cross-sectional area of porous medium, $\mu$ is fluid viscosity , $K$ is permeability is a function of material type, $L$ is the length of sample. Darcy's law is valid for situation where the porous material is already saturated with the fluid.

## 1.3 Mathematical Modeling of Solute Transport

Flow of the fluid through porous medium is an important topic which is encountered in reservoir engineering, soil mechanics, ground water hydrology etc. The problems of ground water contamination and declination seek the attention of lots of environmentalists, mathematicians, soil and agriculture scientists, hydrologists and chemical engineers [11, 12]. The contaminants in aquifers form a contaminant plume which widely spreads because of water movements and diffusion. The study of movement of contaminant plumes can be done through a mathematical modeling of solute transport in porous media. Problems on the contamination of groundwater have been solved by many efficient techniques developed by scientists and engineers [13, 14, 15].

When the groundwater is mostly adulterate, then the resuscitate is considered to be very difficult and more expensive. A very careful approach and attention are very much necessary for describing the boundary conditions, problem domain and model parameters for using the numerical approach of groundwater model of the field problems. Hydrology is an interdisciplinary part of science and engineering, in which the topic of solute transport through the groundwater is included.

In the process of mathematical modeling of many physical complex problems, a lot of common basic assumptions are used like constant dispersion coefficient, steady seepage flow velocity and homogeneity of porous material with constant pores. Ebach and White [16] have studied the problem of longitudinal dispersion with periodically varying input concentration. In heterogeneous aquifer with non-uniform seepage flow, Hunt [17] has applied the perturbation method to the problems of lateral and longitudinal dispersions. To find the solutions of Burgers' equations in the phenomena of longitudinal dispersion which occur in miscible phase flow through porous medium, an analytical approach has been applied by Joshi et al. [18].

The generalized solute transport model in the porous media is the well known reaction-advection-dispersion equation (RADE) [19, 20]. This equation has the combined effects of advection, reaction and dispersion process due to which the concentration of the solute is dispersed while transported down along the stream and sometimes it reacts with the medium through which it moves. From the mass balance principles, the advection-dispersion equation can be easily derived. The modeling of solute transport is very helpful for the prediction of solute concentration in rivers, streams, aquifers and lakes, which can be represented mathematically as

$$\frac{\partial u}{\partial t} = \nabla \cdot (d\nabla u) - \nabla(\nu u) + R, \tag{1.4}$$

where $R$ denotes the reaction term of the species $u$, and the symbol $\nabla$ is defined in $\mathbb{R}^n$ in terms of partial derivative operators as $\nabla = (\frac{\partial}{\partial x_1}, \cdots, \frac{\partial}{\partial x_n})$.
In the right-hand side of the equation (1.4), the first term describes the dispersion phenomena, the second term represents the advection process and the last term is for the reaction kinetics. If there is no reaction between the solute and the medium through which the solute moves, and also there is no kind of radioactive decay then this type of system is called as conservative system, otherwise it is non-conservative. In the case of non-conservative system, the last term of the equation (1.4) is encountered. If there is only diffusion process which is responsible for the movement of the solute concentration, then the above equation is known as diffusion equation.

To understand the physical behavior of problem of ground water pollution and its future effect on human beings and environment, many physical problems are models in the form of mathematical models viz., convection model, diffusion model, reaction-convection diffusion model, convection-diffusion model etc., which analyze the solute flow in aquifer. PDEs are the fundamental equations which describe kinematic and dynamic relationships among flow parameters, fluid and medium at an arbitrary point inside a considered flow domain. Nonlinear PDEs viz., Fisher equation, Burgers' equation, Huxley equation play vital roles to understand the physics of solute transport in porous media. Many researchers have performed experiments in laboratory concerning one dimensional fluid flow where a uniform pressure was already applied to the lower boundary of column to determine the fluid flow rate in uniformly length column filled in a particular porous medium [21].

In recent years, many researchers seek their attention in the field of solute transport in the artificial or natural porous medium due to declination of the groundwater. One of the most omnipresent natural phenomena is diffusion process. The ubiquity of diffusion processes matches to the porous medium. The initial studies and reports of diffusion are mainly based on diffusion processes in porous medium. Due to wide range of applications of reactive-diffusive transport of solutes in porous medium, it has been become interesting area by many of research during last few decades. The PDEs of reaction-diffusion types have been studied in wider range in mathematical modeling of physical phenomena arises in porous media. The concentration of solute profile in reaction-diffusion processes in porous media is modeled by a special type of partial differential equations known as reaction-diffusion equation.

The reaction-diffusion equation is most general solute transport model as it contains the joint effects and variations of reaction and diffusion processes. Because of these processes solute concentrations are transported down with the stream along the flow in porous medium and get diffused/dispersed. Some times the solute also reacts with the medium then these systems are called as non-conservative systems other wise conservative systems. The general reaction-diffusion type PDE mainly contains two terms viz., reaction rate and diffusion term. The reaction-diffusion equations govern the species's population density, evolution of solute concentration w.r.to time at different locations. The diffusion term in these types of mathematical modelings is given by Laplace operator on solute concentration w.r.to spatial variables and the reaction term is given by some additive terms which represent per unit change in solute concentration through some reaction rate. The law of mass action is being used for the derivation of reaction rate equations in well mixed systems.

### 1.3.1 Diffusion

Einstein's theory of Brownian motion reveals that the mean square displacement (MSD) of a particle moving randomly is proportional to time, which also can be justified for the case of a simple integer order linear diffusion equation. But as the research on fractional calculus progresses, it is found that the MSD for the anomalous case i.e., for time fractional diffusion equation, increases slowly with time. For the linear time fractional diffusion equation $\frac{\partial^\alpha u}{\partial t^\alpha} = \frac{\partial^2 u}{\partial x^2}$, the MSD is $\langle X^2(t)\rangle \sim t^\alpha$, where $0 < \alpha < 1$ is the anomalous diffusion exponent. The equation represents an evolution equation which generates the fractional Brownian motion, a generalization of Brownian motion. Thus it is seen that for the diffusion model, if the integer order time derivative is replaced by the fractional order time derivative, it changes the fundamental concept of evolution of foundation of physics. The physical meaning of the fractional order time derivative related to the statistics is the waiting time in accordance with the Montroll-Weiss theory. Hilfer and Anton [22] have showed that Montroll-Weiss continuous time random walk (CTRW) with a Mittag-Leffler waiting time density is equivalent to a fractional order master equation. Later, Hilfer [23] explained that this underlying CTRW of the model is connected to the time fractional diffusion equation in the asymptotic sense of long time and large distance. Thus random walk approach is needed to simulate diffusive phenomena of a fractional order equation. Gorenflo et al. [24] stated that the time fractional order diffusion equation generates a class of symmetric densities whose moments of order $2m$ are proportional to the $m\alpha$ power of time. Thus classes of non-Markovian stochastic processes can be obtained, which exhibit slow anomalous diffusions. By using fractional order Fokker-Plank equation approach, Metzler et al. [25] have shown that anomalous diffusion is based upon the Boltzman statistics. Many researchers have used fractional equations during description of Levy flights or diverging diffusion. The tool is very powerful in modeling multi scale problems, characterized by wide time or length scale. The fractional order differential operator has the characteristic of non-local property, which states that the future state not only depends upon the present state but also upon all of the history of its previous states. Due to the greater flexibilities, the fractional order models have gained popularity to investigate the dynamical system. Also, Contaminant in groundwater moves from more concentrated place to less concentrated place through the process of diffusion. The process of diffusion occurs as long as the concentration gradient exists in groundwater regardless of fluid movement.

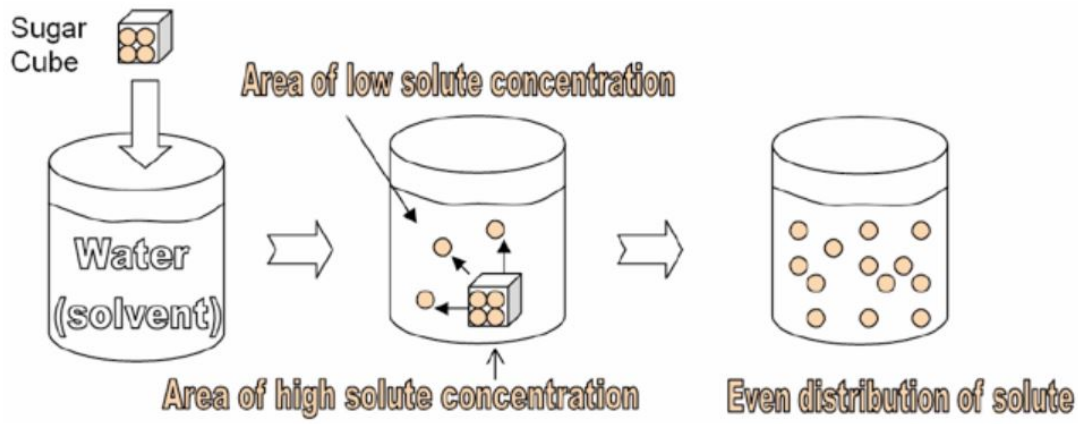


FIGURE 1.5: Diffusion process

The anomalous diffusion process seeks the attention of many researchers [26, 27, 28]. Anomalous diffusion can be easily seen within complex systems like diffusion process in porous media. The fluid particles undergo in sub-diffusion process if $\alpha < 1$. A subclass of anomalous diffusive system is the fractional sub-diffusion equation (FSDE), which can be illustrated from the standard parabolic PDE by replacing the first-order time derivative with a fractional derivative of order $\alpha$, $0 < \alpha < 1$ (Moodie and Tait [29]).

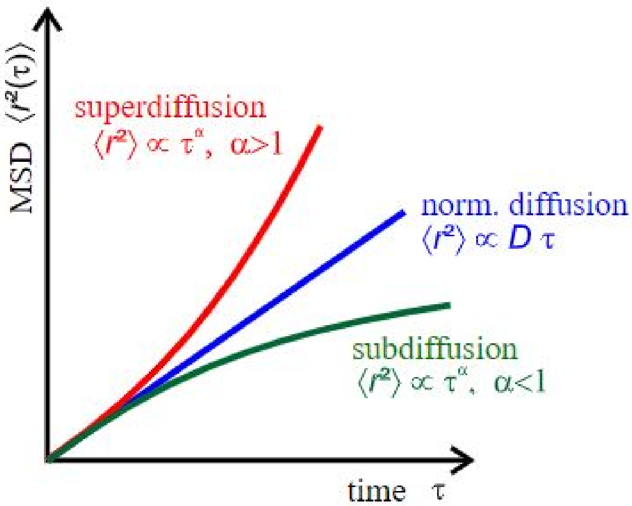


FIGURE 1.6: Plot of MSD vs. time for different kinds of anomalous diffusion.

In the real world problems, the FSDE has been widely applied in several fields of research [30, 31, 32]. So finding the solutions of these equations have become increasingly interesting and popular. The authors of [33, 34, 35] have provided a typical explanation of the anomalous diffusion process based on the continuous time random walk. The process of anomalous diffusion for real complex physical systems can be well explained by fractional order diffusion models.

## 1.4 History of Fractional Calculus

The origin of fractional calculus can be traced in the end of 17th century from few letter exchanged between Leibniz and L'Hospital. The questions and ideas raised between their letters have became an interesting topic for more than three century. Many revered mathematicians like Neils Abel, J.B.J. Fourier, P.S.M. de Laplace, Leonhard Euler, J.L. Lagrange, Joseph Liouville, Oliver Heaviside, G.W. Leibniz, etc., have done great works in this field. The definition of fractional integration was first given by G.F.B. Riemann in 1847.

It is not justified to categorize the fractional calculus theory as a young science. The origin of fractional calculus is as old as classical calculus itself. During the past few decades it has become the focus of interest of many disciplines of science and technology which provides an excellent and efficient tool for modeling and describing various scientific and complex engineering phenomena such as aerodynamics, polymer rheology, electrodynamics of complex medium, fluid-dynamic traffic model [36, 37, 38, 39, 40]. In the last few decades there have been a lot of research on the applications of fractional calculus theory to various scientific fields ranging from the physics of diffusion and advection phenomena to control system of finance and economics.

Fractional differentiation has a lot of advantages on the simulation of dynamical systems and physical phenomena as compared to integer order differentiation, due to its non-Markovian and non-local behaviors [41, 42]. In many cases it is not possible to model the known equations in fractional order forms. For this some basic physical postulates are to be satisfied before giving its shape into fractional order system. Therefore every equation can not be generalised simply by replacing the integer order derivative by fractional order derivative.

The fractional calculus theory is a very important tool to analyze many complex realistic processes. Nowadays a more generalized form of fractional order derivative is a hot topic for researchers viz., differential equations with variable order arising in different processes in porous media [43, 44]. The concepts of generalized calculus theory were first introduced by Neils Abel and Joseph Liouville. The calculus theory in which the concept of any arbitrary order differentiation and integration is discussed that can be a generalization of classical calculus theory. This generalized calculus theory (fractional calculus) has diverse and widely spread in applied mathematical sciences, engineering, fluid mechanics, electromagnetic, etc., and increasingly applied to mathematical modeling of several complex physical phenomena viz., fluid flow, viscoelasticity, dynamical systems, control, groundwater contamination, transports of molecules via pores, etc. Due to its wide application and feasibility, fractional calculus seeks the attention of many researchers, scientists, engineers, and applied mathematicians.

From literature survey, it is seen that the fundamental ideas of the algorithms are correlated to the ideas proposed by authors of [45, 46] and Bhrawy [47], which have been used to develop the efficient and accurate algorithms for the purpose of solving partial differential equations [48]. Additionally, for finding the numerical solutions of linear fractional differential equations (FDEs), Bhrawy et al. [49] have developed an operational matrix with the popular Laguerre polynomials for the fractional order integration and have revised the generalized Laguerre polynomials on the semi-infinite intervals. In [50], the authors have introduced an operational matrix for the fractional order derivative for solving the linear and non-linear FDEs with given initial conditions.

Diverse application of generalized fractional calculus theory leads us to deal with the fractional differential and partial differential equations [51]. The analytical solution of many fractional PDEs is very tough to find. To overcome the lack of exact solution many researchers have developed various techniques to compute the approximate analytical solution of such types of fractional systems. The authors of [52] have introduced a numerical scheme based on meshless approach for time fractional PDEs. Zada et al. [53] used Haar wavelet for finding the solution of FPDEs. Other well-known methods for numerical solution of FPDEs are reproducing kernel discretization method [54], Chebyshev cardinal functions [55], Laplace transform method [56], residual power series method [57], Hierarchical matrix approximations [58], etc. Some of these numerical techniques can also be used to find the numerical solutions of integro-differential equations and integral equations [59, 60]. Few operational matrices are developed on polynomials such as Genocchi polynomial [32], Chebyshev polynomial [61], Laguerre polynomial [62], Fibonacci polynomials [63], etc.

### 1.4.1 Fractional Integration and differentiation

In this section, some fundamental notations, definitions and some properties of the fractional order calculus theory have been given, which are necessary for establishing the results of the present work.

**Definition 1.** The Riemann-Liouville integration operator $J$ of given fractional order $\alpha \geq 0$ of a function $f(t)$ is defined by [64, 65]

$$(J^{\alpha}f)(t) = \begin{cases} \frac{1}{\Gamma(\alpha)}\int_0^t (t-\rho)^{\alpha-1}f(\rho)\,d\rho, & \text{if } \alpha > 0, \\ f(t) & \text{if } \alpha = 0. \end{cases} \tag{1.5}$$

In above expression $\mathit{\Gamma}(.)$ is the well known gamma function.

Some of the properties of $J^{\alpha}$ are as follows.

(i) $J^{\alpha}J^{\tau}f(t) = J^{\alpha+\tau}f(t)$,
(ii) $J^{\alpha}J^{\tau}f(t) = J^{\tau}J^{\alpha}f(t)$,
(iii) $J^{\alpha}t^{\vartheta} = \frac{\Gamma(\vartheta+1)}{\Gamma(\vartheta+\alpha+1)}t^{\vartheta+\alpha}$.

Now, the Riemann-Liouville fractional order derivative of a given order $\alpha > 0$ is normally defined by the following expression.

$$(D_l^{\alpha}f)(t) = (\frac{d}{dt})^m(J^{m-\alpha}f)(t), \ \ (\alpha > 0, \ \ m-1 < \alpha \leq m). \tag{1.6}$$

In the above expression $m$ be the integer number. Some of the properties of $D_l^{\alpha}$ are

(i) $D_l^{\alpha}(D_l^{-\tau}f(t))= D_l^{\alpha-\tau}f(t), \quad \alpha,\tau \in \mathbb{R}^+$ and $\alpha > \tau$.
(ii) $D_l^{\alpha}t^{\vartheta} = \frac{\Gamma(\vartheta+1)}{\Gamma(\vartheta-\alpha+1)}t^{\vartheta-\alpha}$.

As the Riemann-Liouville fractional derivative has some disadvantages, hence, an improved fractional order differential operator $D^{\alpha}$ is introduced, which is more reliable in many applications.

**Definition 2.** The fractional order derivative operator $D^{\alpha}$ of the given order $\alpha > 0$ in the Caputo sense is given by [64, 65]

$$(D^{\alpha}f)(t) = \begin{cases} \frac{d^m f(t)}{dx^m}, & \text{if } \alpha = m \in \mathbb{N}, \\ \frac{1}{\Gamma(m-\alpha)}\int_0^t (t-\rho)^{m-\alpha-1}f^{(m)}(\rho)\,d\rho, & \text{if } m-1 < \alpha < m. \end{cases} \tag{1.7}$$

In the above expression $m$ be the integer number. The Caputo definition of fractional order derivative has the following properties.

$$D^{\alpha}C = 0, \tag{1.8}$$

where $C$ is an arbitrary constant.

$$D^{\alpha}t^{\vartheta} = \begin{cases} 0, & \text{if } \vartheta \in \mathbb{N} \cup \{0\}, \vartheta < \lceil \alpha \rceil, \\ \frac{\Gamma(\vartheta+1)}{\Gamma(\vartheta-\alpha+1)} t^{\vartheta-\alpha}, & \text{if } \vartheta \in \mathbb{N} \cup \{0\}, \vartheta \geq \lceil \alpha \rceil \, or \, \vartheta \notin \mathbb{N}, \vartheta > \lfloor \alpha \rfloor, \end{cases} \tag{1.9}$$

where $\lceil \alpha \rceil$ be the ceiling function and $\lfloor \alpha \rfloor$ be the floor function and similar to the ordinary derivative, Caputo derivative is also linear i.e., for arbitrary constants $\phi, \varphi$, we have

$$D^{\alpha}(\phi p(x) + \varphi q(x)) = \phi D^{\alpha} p(x) + \varphi D^{\alpha} q(x). \tag{1.10}$$

A very useful relationship between the Riemann-Liouville operator and the Caputo operator is given by the following expressions for $m - 1 < \alpha \leq m$,

$$(D^{\alpha} J^{\alpha} f)(t) = f(t), \tag{1.11}$$

and

$$(J^{\alpha} D^{\alpha} f)(t) = -\sum_{\rho=0}^{m-1} f^{(\rho)}(0^{+}) \frac{t^{\rho}}{(\rho)!} + f(t), \;\; m - 1 < \alpha \leq m, \tag{1.12}$$

where $m$ be an integer number.