Chapter 1

Introduction

From the title of the thesis "Study of Some Transport Phenomena Problems in Porous Media", it is clear that the transport models appear in porous media are studied here. For that reason, the models that describe the solute movement in groundwater are considered. Mainly, a drive has been taken to solve these models numerically subject to initial and boundary conditions. During numerical computation, the existing spectral approach is considered and the extension of the approach is made according to the considered problems. Due to the seriousness of groundwater contamination problems, it seeks the attention of a lot of scientists and researchers in the last few decades. It has motivated the author to choose a solute transport model for study. The seriousness of the groundwater contamination is discussed in the next section.

1.1 Groundwater Contamination

It is known that water is one of the primary elements for life on earth with two-thirds of the earth's surface is covered by water and the human body consisting of 75% of the same. The water on the earth presents itself in two forms viz., surface water and groundwater, of which only 2.5% is fresh water. More than two third of this fresh water is covered by the glacier and ice caps (see Fig 1.1). So the groundwater is one of the most important sources of freshwater towards the fulfillment of basic needs like agriculture, industries and also as an important source of drinking water in both urban and rural areas. For drinking water half of the population of the United States depends on groundwater. Ninety-seven percent of the freshwater comes from groundwater, so it is important compared to surface water.

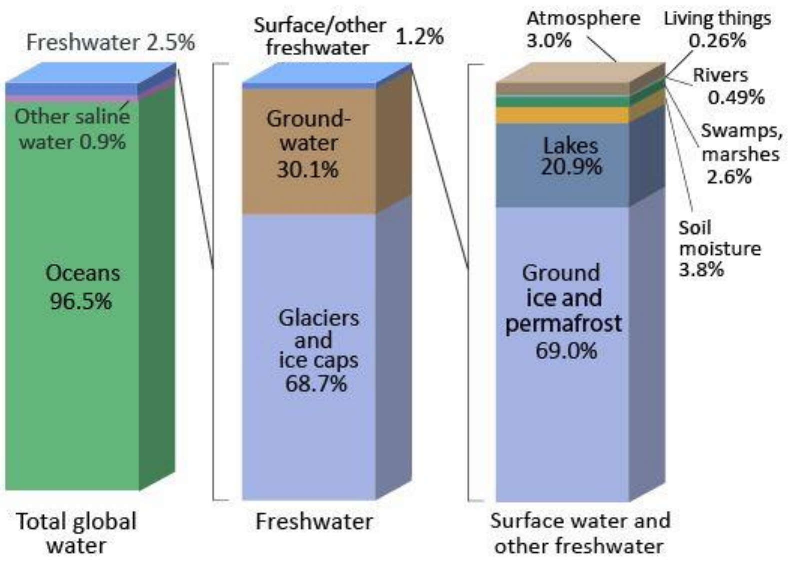

Fig 1.1 Distribution of earth's water, taken from the USGS, USA site (https://water.usgs.gov/edu/watercycle.html)

Unfortunately, it is getting polluted every day due to various reasons. The source of groundwater contaminations can be natural or human activities. This form of environmental degradation occurs when pollutants are directly or indirectly discharged into the water bodies. Our country is one of the worst affected countries in terms of contaminated water due to factors like urbanization, industrialization and agriculture which play crucial roles. The natural contamination depends on material through which the groundwater moves. During movement, it may pick up a wide range of compounds such as magnesium, calcium and chlorides. Naturally occurring minerals and metallic deposits in rock and soil also create groundwater contamination. Very often, neighborhood ponds, streams, rivers get polluted due to industries. Moreover infiltrated the chemical ingredients of the industries get mingled with the groundwater and create contamination. Humanmade products like gasoline, oil, road salts and chemicals get mingled with groundwater and create groundwater contamination (See Fig. 1.2). Due to increase of population it is overexploited and become thus contaminated by various point and non-point sources like storage tank, disposal sites, industry waste disposal sites, accidental spills, leaking gasolines, landfills, fertilizers, pesticides and herbicides (Fried (1975); USEPA (1989, 1990); Anderson and Woessner (1992); Charbeneau (2000); Kebew (2001); Sharma and Reddy (2004); Rai (2004); Rausch et al. (2005); Thangarajan (2006)).

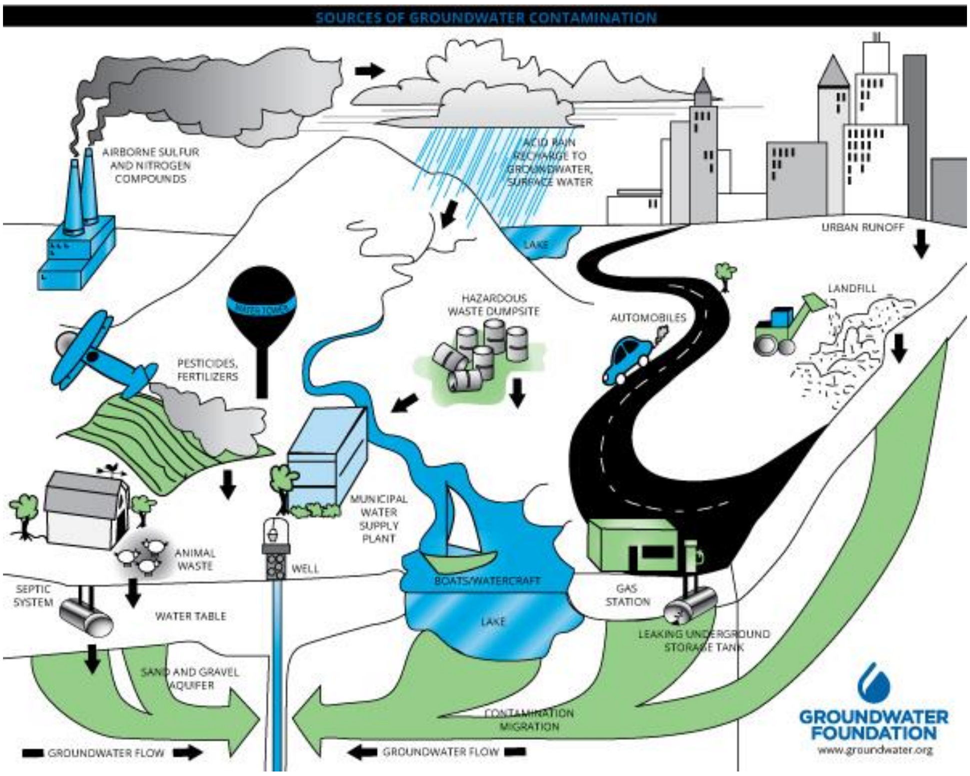

Fig. 1.2 Sources of groundwater contamination, taken from the site of groundwater foundation 2018 (www.groundwater.org)

Near the coast, a vacuum is created by overpumping an aquifer which can quickly be filled up with salty sea water due to which water supply may become undrinkable and useless for irrigation. Groundwater pumping has exceeded the rate of replenishment. In our country the contamination of groundwater is caused by human activities such as sewage disposal, refuse disposal, pesticides and use of fertilizers, industrial discharges, and toxic waste disposal. Improper management of groundwater resources is also a major issue leading to increase in the problem of drinking water and as a result, the water level is getting down fast in several parts of India because of excessive extraction of groundwater as reported by National water policy (1987). Since non-point source materials are used over a large area, hence it can have a large impact on the water in an aquifer compared to point-source. Contaminated groundwater is very harmful for the environment, human health and widely affect the wildlife. It may not damage human and animal health immediately but can be harmful after long-term exposure. Groundwater contamination through septic tank waste can have serious effects on human health. Various diseases like cancer, hepatitis and dysentery may be caused by polluted water. Different actions are being taken by different countries to remediate the surface and groundwater. Compared to surface water, groundwater contamination is more difficult to abate because it can move very large distance in unseen aquifers.

If groundwater is contaminated overall, then the rehabilitation is deemed to be too difficult and expensive. As a result, it may become unusable for decades. Then finding the other source of water is the only option which is seen as impossible. So it is important to develop a mathematical model that predicts the solute movement in aquifers and its effect on human health and the environment. To accomplish this, a thorough understanding of the physical, chemical and biological processes that control the transport of solute in groundwater is necessary at the outset. Careful attention is very much required for describing the problem domain, boundary conditions and modelparameters for creating the numerical groundwater models of field problems.

Solute transport through the groundwater is topic encountered in the interdisciplinary branch of science and engineering, called hydrogeology. The word hydrogeology is the combination of three words hydro meaning water; geo means earth and logy means study. This branch of science is the combination of two separate branches viz., hydrology where one study about water and the geology where one study about the earth. In hydrology, basically water movement, distribution and quality of water present in the earth and other planets are studied. This branch is also subdivided into many branches like chemical hydrology, echo hydrology, surface hydrology, hydrogeology, hydro informatics, hydrometeorology and isotope hydrology. In geology, the study is concerned about the earth structure, beneath, rocks of which it is composed and the processes by which those are changed over time. From this, we get the knowledge about the age of the earth, the history of the earth and also the properties of materials of which earth is composed. In practical terms, geology is important for minerals and hydrocarbon exploration and exploitation, evaluating water resources, understanding the natural hazards, the remediation of environmental problems and providing insights into past climate change. Both the fields, hydrology and geology, have their own historical background. In hydrogeology, we mainly study about the water and solute that moves into a beneath of earth. The water that moves below the earth surface is called groundwater and the area where it moves generally called aquifer. In throughout the study, I have considered porous aquifer.

In science, as in all other departments of human knowledge and inquiry, no thorough grasp of a subject can be gained, unless the history of its development is appreciated. History provides a window through which the rise and decline of any aspect of the society can be seen. So in the next two sections, the history of "Hydrogeology" and "Theory of porous media" are discussed.

1.2 History of Hydrogeology

The modern science of hydrogeology is considered, to begin with, measurements of rainfall, evaporation, and river discharge by area-velocity method etc. But the concept of the hydrological cycle (see Fig. 1.3) was given by many philosophers from over the years.

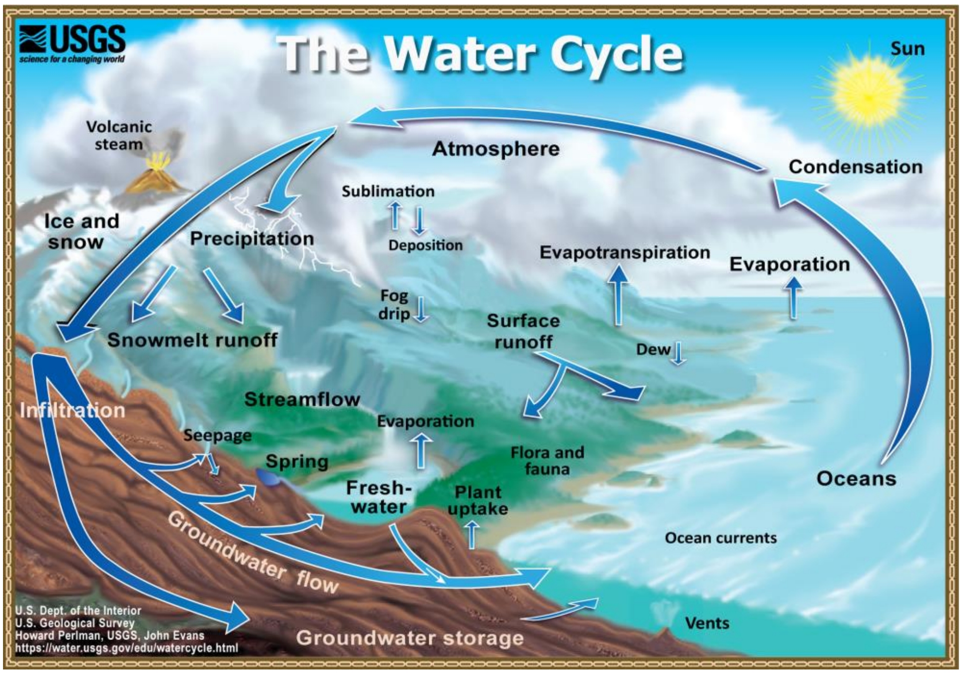

Fig 1.3 The Water Cycle, taken from the USGS, USA site (https://water.usgs.gov/edu/watercycle.html)

If one looks towards the literature to know how the science of hydrogeology was developed, various research articles and books can be found on that in which the various eminent researchers mainly hydro-geologists have talked about the historical development of hydrogeology. Since it is an interdisciplinary branch of science, therefore it has contributions on other branches of science like earth science, fracture mechanics, porous media etc. In the research article by American hydro-geologists O. E. Meinzer (1934) who is also known as “Father of Hydrogeology” documented the history and development of groundwater hydrology where he has documented the contribution made by French, German, Italian and British geologists and drillers. James E. Hackett (1952) summarized the birth and development of groundwater hydrology in his article based on the works of Adams (1938), Baker and Horton (1936), and Meinzer (1934). E. Hackett summarized this theory in four parts. First one, the origin of underground water, where he started a discussion with the pluvial cycle, then talked about original hydrology cycle by Greek philosophers and lastly discussed the experimental works by two Frenchmen Perrault and Mariotte in 17th-century who laid the foundation of further investigation and the modern concept of the hydrologic cycle. The second one, the occurrence of underground water where he talked about the fundamental principle of geology which has been established at the beginning of the 19th-century. The third one is the movement of underground water, where he talked about Darcy’s law. The last one is the development of groundwater hydrology, where he talked about the work of Gunther Theim in 1906 in the United States. In the book “200 Years of British Hydrogeology” edited by J. D. Mather (2004), it is found the historical development of the British hydrogeology in which the editor included many research articles to clear how the British hydrogeology developed during 1800 to 1975. The historical development of the hydrogeology of different countries have been collectively illustrated in the book titled “History of Hydrogeology” by Howden and Mather (2013) in which the authors included history of hydrogeology of different centuries like Australia, Island, China, Czech Republic, French, Central Europe, Hungarian, India, Japan, Netherlands, Norway, Poland, Romanian, Russia, Serbia, South Africa, Spain, Sweden and Britain in 21 separate chapters. Review of this book had been done by Li Peiyue (2015). Regarding the development of Indian hydrogeology, one should go through the work titled “A brief history of Indian hydrogeology” by Dr. Shrikant D. Limaye, which was also included in the monograph of Howden and Mather (2013).

Regarding the overall development of the science of hydrogeology, it is found that up to 14th-century the concepts on hydrology were confined to constructions of hydraulic structure and up to 16th-century, it was confined to observations. Leonardo da Vinci gave the better understanding of flow in open channels and later Palissy stated that rainfall was the only source of water of spring and rivers. In the 17th-century many developments have occurred of which notable work has been contributed by Pierre Perrault and Edme Mariotte. In the 18th-century, a number of hydraulic experiments have been done and on the basis of those many principles of hydrology were developed viz., Bernoulli's piezometer, the Borda tube, the Pitot tube, Bernoulli’s theorem, Chezy’s formula etc., which vastly contributed towards taking up of quantitative hydrologic studies. It is the 19th-century when famous Darcy’s law of groundwater flow given by French civil engineer Henry Darcy which accelerated the research work in the field of hydrogeology. Simultaneously, many modernized experimental studies have been done and the results of those are Dupit’s well formula, Hagen-Poiseuille’s equation of capillary flow, Francis weir discharge formula, Manning’s flow formula, development of price current-meter, Dalton’s law etc. Up to the end of the 19th-century, the science of hydrogeology was largely empirical and the work in first three decades of the 20th-century was responsible for the advancement of the science of hydrogeology. It is mid of 20th-century when many theoretical investigations have been considered in this field. After that, the dependency of living things and the ecosystem on groundwater and the degradation of groundwater by pollution landed wings the research in the field of hydrogeology. After the advent of high-speed computers, the solutions of complicated mathematical hydrogeological theories are current states of research and as a result, this area is still a very active area of research.

1.3 History of Porous Media Theory

When it is looked the literature to know how the theory of porous media was developed, it is found that there are many books and research articles in which development of that had already discussed. Mainly the research articles and books of German engineer scientist of mechanics Reint de Boer and his doctoral candidate Wolfgang Ehlers, in which the development of porous media theory are discussed in details. Contents of further discussion have been taken from the research articles of Reint de Boer (1998) titled “Theory of Porous Media- Past and Present” and also from the Wolfgang Ehlers article titled “Porous Media in the Light of History” included in the monograph titled “The History of Theoretical, Material and Computational Mechanics” edited by Stein (2014).

According to them the theory of porous media which is a macroscopic continuum mechanical approach was developed in three phases. The first phase was the phase when the fundamental principles of mechanics, the concept of volume fraction and the theory of mixtures were developed which have been done at the end of 18th-century and early days of 19th-century. The second phase was between 1910 and 1960 when the mechanical interaction of liquids, gases and rigid porous solids had been clarified the first time and deformable saturated porous solids had been treated. The third phase was between 1970 and 1980 when the theories of immiscible mixtures were developed.

This theory starts with Leonhard Euler in 1762 when he described the geometry of the porous bodies and his remarks on the porous bodies are interesting. Later he did not use the porous solid in his further work, but he was indirectly participated in creating a sequent porous media theory. Also, he developed the axioms of continuum mechanics, namely the cut principle, the balance of mass, the balance of momentum and the balance of moment of momentum.

At the end of 18th-century, porous media theory was initiated through the physical problems viz., coupled water-solid problems and the dike construction problems. At that time, Reinhard Woltman proposed the essential part of the porous media theory, i.e., the concept of volume fraction as the ratio of the volumetric portions of the soil and the pore water components of any dike construction which was not noticed earlier. He attentively observed totally water-saturated mud and introduced the concept of volume fraction. With Woltman’s concept of volume fraction for volume elements of a saturated body, the theory of porous media was already developed in the early days of the history of mechanics. However, to evaluate the balance of momentum, it is necessary to develop the same concept for surface elements of a saturated body.
Achille Ernest Oscar Joseph Delesse was the person who created such a concept when he was working on a totally different problem. He started a career as a mining engineer and became a renowned scientist. He was working on a problem to distinguish between the portions of the minerals in mine and observed that the area fraction of the minerals is the same as the volume fraction. In the year 1848, by statistical investigation of various slices of minerals conglomerates, he found that the area fractions and volume fractions are equivalent which leads to

$$n^{\alpha} = \frac{dv^{\alpha}}{dv} = \frac{da^{\alpha}}{da}, \tag{1.1}$$

where n^{α} is the volume fraction, obtained by relating the local volume or the local area element of the $\alpha - th$ constituent to the overall volume element dv or the overall area element da.

At the same time, Henry Philibert Gaspard Darcy was working as a hydraulic engineer, who published a very famous law which is known as Darcy’s law (1856), which is given by

$$n^F w^F = -k^F grad \;\; h, \tag{1.2}$$

where n^F is the fluid volume fraction, w^F is the seepage velocity and the product of that $n^F w^F$ known as the filter velocity. k^F is the Darcy permeability or the hydraulic conductivity and $gradh$ is the pressure head. Although his investigations were of purely experimental nature, his results are essential for a mechanical continuum treatment of the motion of a liquid in a porous solid. It seems that only Darcy's law justifies the creation of a partial fluid body in the porous media theory. The interaction of different constituents in a multiphase continuum - a binary model consisting of a rigid porous solid and a liquid in motion was first studied by him which can be found in Darcy (1856). Nowadays this law seems like a combination of a constitutive equation for the direct momentum production term and the momentum balance of the liquid component of a binary system of solid and fluid and widely used in hydraulic engineering. The Darcy's law is considered as the basic constitutive relation for the problem of running water through a filter bed. The aforementioned Darcy's law is not valid in all cases. It discussed later in details in Section 1.12.

In the 19th-century, the development of mixture theory started, which is the second important branch of porous media theory. Adolf Eugen Fick gave the phenomenological theory of mixtures, who first studied the problem of diffusion. According to the development of the Fourier equation of the heat propagation, he arrived by an analogy procedure at the differential equation of the diffusion stream, from where Fick's second law of diffusion arrived. In this article, he did not give any hint for constitutive equations for diffusive flux vector which is known as Fick's first law. Fick's first law states that the concentration flow of a species in a mixture of two components is proportional to its concentration gradient and this law with the mass conservation equation gives Fick's second law as

$$\frac{\partial c}{\partial t} = D\, div\, grad\, c, \tag{1.3}$$

where c is the species concentration, D the diffusion coefficient.

All investigations and findings by R. Woltman, A.E.O.J. Delesse, H.P.G. Darcy and A.E. Fick were based on experimental observations and conclusions from other scientific laws. It is seen from the literature survey that Fick did not proceed from ensured mechanical principles. This was done by Josef Stefan in 1871, who introduced the main assumption concerning the interaction forces between the constituents. He was the first who studied the diffusion behavior in the sense of continuum mechanics. He enhanced Fick's diffusion laws through investigation of mixtures of three components and extended his findings to the diffusion of gases across porous walls. J. Stefan described the gas diffusion through rigid membranes. The relation of the effective (free) gas pressure compared to the partial pressure of the pore gas in the porous wall was described on the basis of the porosity of the porous solid. Thus he was the first who included the concept of volume fractions into a continuum theory of porous media and created the mixture theory consequently treating the different phases as individual constituents considering the interaction forces. However, his investigations were restricted to the description of the purely mechanical behavior of the constituents. The thermal effects had been incorporated in the second half of the 19th-century.

Thus the basic background of porous media theory was developed by Woltman, Delesse, Darcy, Fick and Stefan. Apart from them a lot of scientists contributed to developing the porous media theory in 19th-century. The Scottish scientist William John Macquorn Rankine contributed to the evolution of thermodynamics. Rankine (1857) was involved in the field of soil mechanics. The work of Rudolf Julius Emanuel Clausius had important contribution to merge the continuum mechanics and thermodynamics. A series of articles published between 1876 and 1878 by Josiah Willard Gibbs, who used thermodynamical methods to interpret chemo-physical phenomena. Gibbs is not only be considered as the father of vector calculus but, together with Hermann Ludwig Ferdinand von Helmholtz, he established the entire field of physical chemistry which is also part of modern porous media approaches.

In 1911, Gustav Jaumann worked on continuum mechanics of the complex system and included the “Jaumaan derivative” which is still in use in various plasticity approaches. Based on previous work of Gibbs, he was the first who used the tensor calculus extensively which was called dyade calculations. He is known as the pioneer of continuum mechanics and mixture theories as the bearing pillar of the modern theory of Porous Media.

At the end of 19th-century, the basic theory of porous media was developed to treat empty and saturated porous solids and it is established in 20th-century with the contributions of many scientists. Now the geotechnical problems seek the attention of geotechnical experts like Terzaghi and Biot in this field. In 1912, Civil engineer Karl von Terzaghi visited dam construction sites in the USA because of his deep interest in geotechnical problems. Though he was aware of the complexity of soil as a binary medium of solid grains and water, but he was not an expert in the theoretical description of porous-media problems. However, Terzaghi, an engineer always tried to combine theory and practice. Thus, Terzaghi's work led to scientific oppositions.

In 1913, P. Fillunger published a scientific article on buoyancy forces in gravity dams, where he considered the problem as a binary medium of two interacting continua, soil and water. From this point of view, Fillunger can be regarded as the pioneer of the modern Theory of Porous Media. However, there is a tragedy of Fillunger's work, which his buoyancy equation included a mistake by presenting the buoyancy force as a linear function of the difference between the volume and the surface porosity. This mistake was recognized by Terzaghi, which was supported by a scientific commission of the Technical University of Vienna, who concluded that Fillunger was wrong (Boer (2004)).

The geotechnically-based porous media work of Fillunger's and Terzaghi's have been continued by a lot of scientists, namely Belgian-American applied physicist Maurice Anthony Biot, the Austrian Gerhard Heinrich etc. This dissociation of the porous-media society is, by the way, still active. While the procedure of Terzaghi and Terzaghi and Fröhlich is, from a modern point of view, more or less unsatisfactory, Fillunger's approach is still modern, because he started with the balance equations of two overlaying constituents, soil and water, and treated this aggregate in the sense of a mixture with immiscible but interacting constituents. The research work of Biot (1935,

1941) are based on the basic ideas of Terzaghi's and his very famous works (1955, 1956) are still highly cited by young researchers for basic materials to solve the porous media problems. Only Reint de Boer recovered these articles during his visits in Vienna in 1987 and later. The detailed review of the history of porous media theory can found in Boer and Ehlers (1988).

The modern era of porous media theory was started in 1950 when US-American scientist Clifford Ambrose Truesdell III entered in this field by considering the work of Jaumann on continuum mechanics and recovered the continuum mechanics after 46 years elapsed. However, in those days without powerful computers, researchers would prefer the simple numerical computational methods to handle the complex continuum-mechanical equations. C. A. Truesdell originated the modern view on continuum mechanics and thermodynamics including mixture theories. His early work has attracted a variety of young researchers namely Richard Toupin, Walter Noll etc. His work with Toupin (1960) and Noll (1965) included in the famous book "Handbuch der Physik" which contained the complete continuum-mechanical knowledge.

In 1957, C. Truesdell described a closed mixture system where the single component behaves like open system on the basis of his work where local balances of mass, momentum and energy for arbitrarily constituted mixtures are presented.

However, in Truesdell's description of mixtures, there was no relation for a balance of moment of momentum for the mixture constituents. Moreover, an entropy inequality was also missing, although the entropy principle of Clausius was part of the description of standard single-phasic materials for a long time. Without raising their hypothesis to a principle, Truesdell and Toupin summarised that the entropy inequality of heterogeneous media would basically be the same as that of a single-component medium. However, this assumption turned out to be wrong later.

In 1964, Truesdell's mixture theory was generalized by Kelly (1964). He derived the balance equations for the multi-component system on the basis of so-called fundamental balance law and formulated angular-momentum balances for the components. Thus, the partial stress tensors of the components turned out to be non-symmetric, whereas the overall stress obtained from the partial stresses was symmetric. Due to the contribution of Kelly, the continuum-mechanical frame of mixtures was built apart from the formulation of a sound version of the entropy inequality.

The inclusion of an angular-momentum production yielding non-symmetric partial stresses in the sense of the contributions made by Cosserat brothers between 1907 and 1909, is somehow contradictory to the fact that the whole system has symmetric stresses in the sense of a standard Cauchy continuum.

Based on Truesdell's mixture theory, Adkins (1963, 1964) and Green and Adkins (1964) developed purely mechanically motivated approaches for mixtures of fluids, and for a mixture of a single fluid and an elastic solid. Although these models have been subjected to certain invariance criteria obtained from the "principle of objectivity", a thermodynamic investigation of the constitutive equations for mixtures was missing and had only been introduced to standard continua by Coleman and Noll (1963).

In the research works of Eringen and Ingram (1965), and of Green and Naghdi (1965), the substantial theory of mixtures is used in the frame of thermodynamics. For this, it is necessary to transfer the entropy principle from single to heterogeneous media which was very difficult on those times. The basic procedure by Green and Naghdi in formulating only one single entropy inequality for the whole mixture proved to be right which used as a basic for the general theory of mixtures. The assumption of Eringen and Ingram which states that each constituent of a mixture with different constituent temperatures is associated with an individual entropy inequality, which cannot be accepted from a modern point of view. In 1969, Bowen and Wiese (1969) pointed out that the theory of Green and Naghdi lacked the free-energy transport produced by the diffusion process.

R. M. Bowen formulated his version of a mixture theory on the basis of so-called tensors of chemical potentials, thus extended the notion “chemical potential”, originally introduced by Gibbs as a scalar. The entropy inequality formulated by Bowen later was proved as the first fully correct version of an entropy inequality for mixtures. His work was criticized by Green and Naghdi with the argument that the introduction of tensors of chemical potentials instead of partial stresses would not lead to a basically different theory. It was seen that Bowen’s entropy postulates were identical to Truesdell’s result, especially the entropy inequality of mixtures which was called as Bowen-Truesdell form.

Around 1970, the basis of a general “Theory of Mixtures” was found. The theory of mixture was given by Bowen (1976), based on which he published on incompressible and compressible porous media models, where he extended the “Theory of Mixtures” by the concept of volume fractions (Bowen (1980,1982)).

With Bowen’s articles, porous media theories were split into two directions, the first one following the Terzaghi-Biot line and the other one following Bowen’s line which was based on the old ideas of Fillunger and Heinrich. The works of Truesdell, Noll and Coleman led to some confusion when the components of the mixture were treated like standard first-grade materials. Later Müller (1968) stated that mixture components always have to be treated as materials of second grade if one does not want to describe only simple mixtures. Although this concept is conductive, it leads to considerable confusion when complicated aggregates are investigated. To avoid this problem, Wolfgang Ehlers (1989) introduced the concept of phase separation.

In the present time, the theory of porous media is applied to various branches of science and engineering like civil engineering, environmental engineering, geoscience, geomechanics, biology etc. In geoscience, it has applied to investigate the deformation and stability behavior of fully and partially fluid-saturated soil constructions, such as dikes, embankments, railroad dams, or foundation and settlement problems. In mechanical engineering, this theory is applied when foamed materials and smart materials like electro-active polymers are taken under consideration. In biomechanics porous media play a dominant role because of the living tissues have more than 90% of fluids, interstitial fluid and blood, so to examine that this theory plays a dominant role.

This theory is even very important to solve the complex coupled problems of different areas like solid mechanics, fluid mechanics, thermodynamics, computational mechanics, etc.

1.4 Aquifer

The term aquifer came from the Latin language where ‘aqua’ means water and ‘fer’ i.e., ferre which means to bear. The aquifer is a geological formation that contains water and allows a significant amount of water to move through it under ordinary field conditions. The impervious formation of aquifer called aquiclude which contains water but does not allow to move through it under ordinary field conditions, for example, a clay layer. A semi-pervious formation is called aquitard (see Fig. 1.4) which allows the transmission of water at a very slow rate compared to the aquifer.

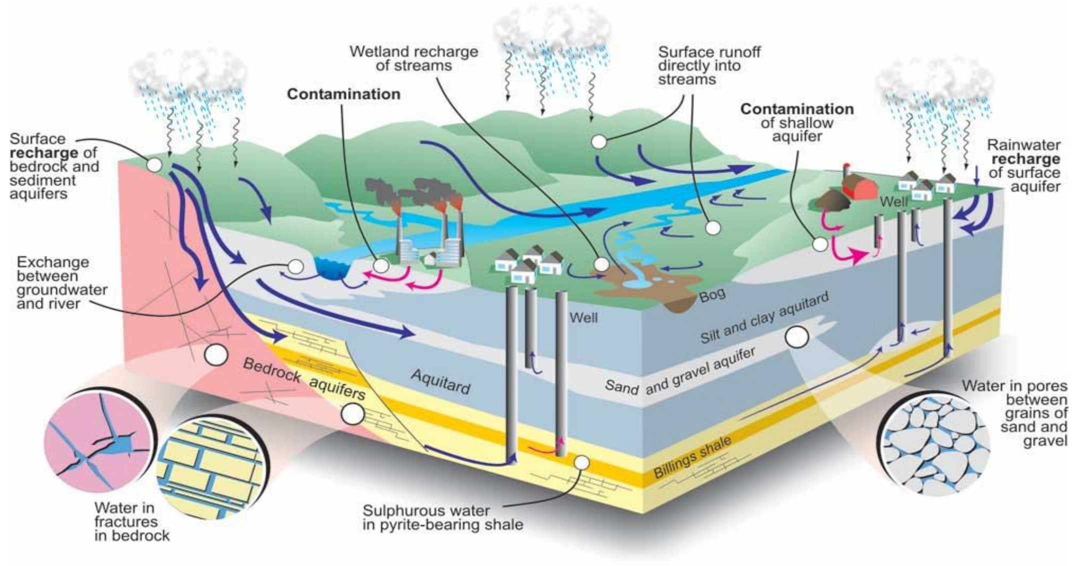

Fig. 1.4 The different types of aquifers, taken from the site of CEGN (www.cgenarchive.org)

However, over a large horizontal area, it may permit the passage of large amounts of water between adjacent aquifers, which are separated from each other and often known as a leaky formation. An aquifuge is an impervious formation that neither contains nor transmits water.

1.5 Groundwater

Water presents below the ground surface considered as groundwater. However, many scientists and engineers have their considerations, for example, the hydrologist uses the term groundwater for the water present in saturation zone and in the drainage of agriculture lands, the term groundwater is also used to denote the water in the partially saturated layers above the water table (see Fig. 1.5).

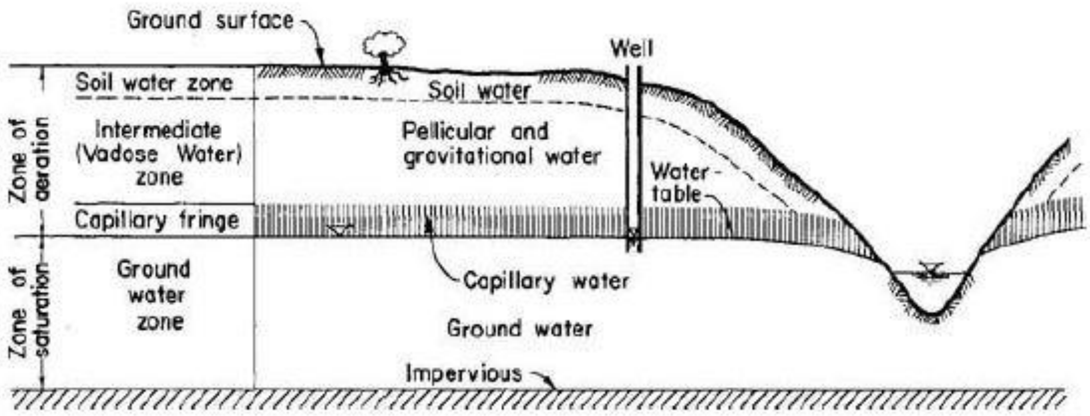

Fig. 1.5 The distribution of sub-surface water (Bear, 1992)

1.6 Void Space/ Pore Space/ Pores/ Interstices/ Fissures

The interstices of a rock can be grouped into two classes: original interstices, mainly in sedimentary and igneous rock, created by geological processes at the time the rock was formed, and secondary interstices, mainly in the form of fissures, joints and solution passages, developed after the rock was formed (see Fig. 1.6).

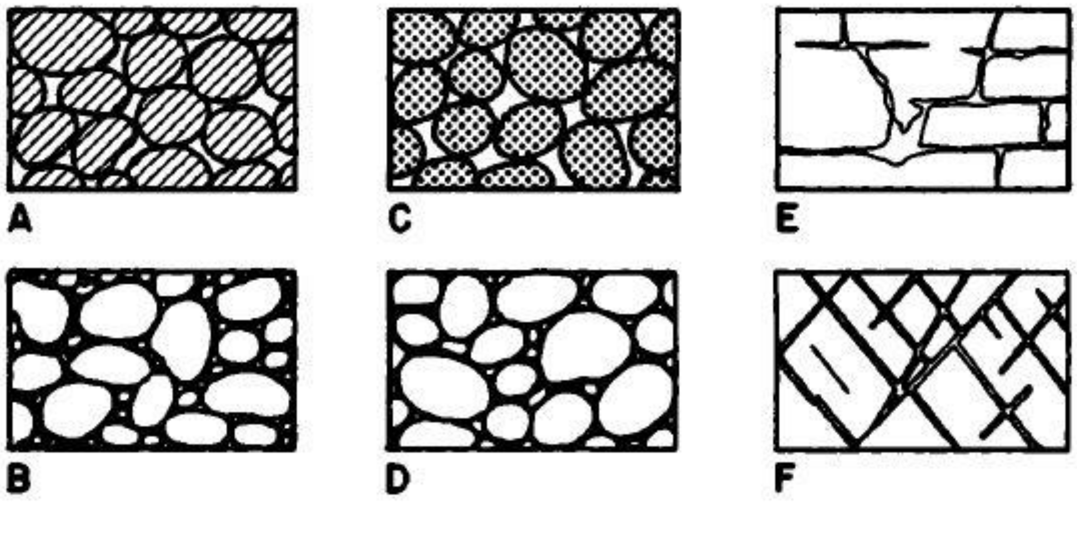

Fig. 1.6 Diagram showing several types of Rock Interstices. (A) well-sorted sedimentary deposit having high porosity; (B) Poorly sorted sedimentary deposit having low porosity; (C) Well-sorted sedimentary deposit consisting of pebbles that are themselves porous, so that the deposit as a whole has a very high porosity; (D) Well-sorted sedimentary deposit whose porosity has been diminished by the deposition of mineral matter in the interstices; (E) Rock rendered porous by solution; (F) Rock rendered porous by fracturing (Bear, 1972)

1.7 Porous

If something full of tiny holes or openings through which fluids can pass easily is called porous, the sponge is an example of it. If the border between countries is open for everyone to cross easily, it is also called porous. When potters make a mug, they use special glazes to seal the porous clay, which otherwise would absorb the liquid when it will be put in the mug. So porous can describe any barrier that allows easy passage in and out.

1.8 Porous Medium

By a porous medium, we mean a material consisting of a solid matrix with an interconnected void. The skeleton portion of the material is often called the matrix or frame. It is supposed that the matrix is either rigid or it undergoes small deformation. A structure like foams is often also usefully analyzed using the concept of porous media. The interconnectedness of the void allows the flow of one or more fluids through the material. The solid phase should be distributed throughout the porous medium within the domain occupied by a porous medium. An essential characteristic of a porous medium is that the specific surface of the solid matrix is relatively high. In many cases, this characteristic dictates the behavior of fluids in porous media. Another feature of a porous medium is that the various openings comprising the void space are relatively narrow. At least some of the pores comprising the void space should be interconnected. The interconnected pore space is sometimes termed as the effective pore space. As far as flow through porous media is concerned, unconnected pores may be considered as part of the solid matrix. Certain portions of the interconnected pore space may be ineffective as far as flow through the medium is concerned. For example, pores or channels with only a narrow single connection to the interconnected pore space, so that almost no flow occurs through them. Another way to define this porous medium characteristic is by requiring that any two points within the effective pore space may be connected by a curve that lies completely within it. Moreover, except for special cases, any two such points may be connected by many curves with an arbitrary maximal distance between any two of them. For a finite porous medium domain, this maximal distance is dictated by the domain's dimensions. In a natural porous medium, the distribution of pores with respect to shape and size is irregular. Examples of the natural porous medium are beach sand, sandstone, limestone, rye bread, soil (e.g., aquifers, petroleum reservoirs), wood and the human lung (see Fig. 1.7).

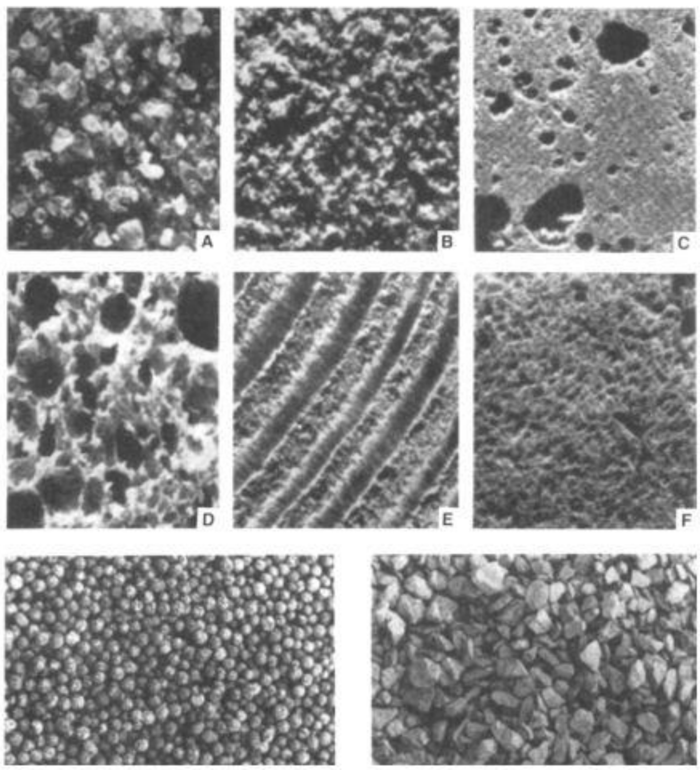

Fig. 1.7 Examples of natural porous materials: (A) beach sand, (B) sandstone, (C) limestone, (D) rye bread, (E) wood, and (F) human lung. Bottom: Granular porous materials used in the construction industry, 0.5-cm-diameter Liapor spheres (left), and 1-cm-size crushed limestone (right) (Nield and Bejan (2006))

The human-made materials such as cement and ceramics can be treated as a porous medium. When the pore space is completely full of water, then it is saturated, but if it contains both water and air, then it is unsaturated media. A porous medium most often characterized by its porosity.

1.9 Porosity

The porosity of the medium is defined as the fraction of the total volume of the medium that is occupied by void space. For an isotropic medium, the surface porosity (i.e., the fraction of void area to total area of a typical cross-section) will normally be equal to porosity. In defining porosity, one has to assume that all the void spaces are connected. If one has to deal with a medium in which some of the pores is disconnected from the remainder, then it is needed to introduce an "effective porosity", defined as the ratio of the connected void to the total volume. The value of porosity lies between 0 &1. For natural media, it does not normally exceed 0.6. For beds of solid spheres of uniform diameter, it can vary between the limit 0.2595 (rhombohedral packing) and 0.4764 (cubic packing). For humanmade materials such as metallic foams, it can approach the value 1.

1.10 Hydraulic Head

Hydraulic head or piezometric head is the combination of pressure head and elevation head. It is a specific measurement of liquid pressure above a geodetic datum. The gradient of the head is the change in hydraulic head per length of the flow path and proportional to the discharge, appears in Darcy's law. Therefore, it also called Darcy slope. In an aquifer, hydraulic head determines where the groundwater will flow.

1.11 Transport Through Porous Media

In science and engineering, transport through porous media is the manner in which transported species behave when transport through a porous medium. For example, when a fluid passes through a porous material, it is observed that some fluid flows through the media while some mass of the fluid is stored in the pores present in the media. Flow through porous media is a topic encountered in many branches of science and engineering, e.g., groundwater hydrology, reservoir engineering, soil science, soil mechanics, rock mechanics, acoustic, filtration, biology and biophysics, material science, chemical engineering, etc. On the pore scale, i.e., on a microscopic scale, the flow quantities will be clearly irregular. But in typical experiments, the quantities of interest are measured over areas that cross many pores, and such space-averaged (macroscopic) quantities change in a regular manner with respect to space and time, and hence are amenable to theoretical treatment.

Flow through a porous structure is largely a question of distance, the distance between the problem solver and the actual flow structure. When the distance is short, the observer sees only one or two channels or one or two open or closed cavities. In this case, it is possible to use conventional fluid mechanics and convective heat transfer to describe what happens at every point of the fluid, and solid-filled spaces. But when the distance is large, there are many channels and cavities in the problem solver field of vision, the complications of the flow paths rule out the conventional approach. As engineers focus more and more on designed porous media at decreasing pore scales, the problems tend to fall between the extremes noted above. In this intermediate range, the challenge is not only to describe coarse porous structures, but also to optimize flow elements and to assemble them. The resulting flow structures design the porous media (Nield and Bejan (2006)).

The usual way of deriving the laws governing the macroscopic variables is, to begin with, the standard equations obeyed by the fluid and to obtain the macroscopic equations by averaging over volumes or areas containing many pores. There are two ways to do the averaging spatial and statistical. In the spatial approach, a macroscopic variable is defined as an appropriate mean over a sufficiently large representative elementary volume (r.e.v). This operation yields the value of that variable at the centroid of that volume. In the statistical approach, the averaging is over an ensemble of possible pore structures that are macroscopically equivalent. A difficulty is that usually the statistical information about the ensemble has to be based on a single sample, and this is possible only if statistical homogeneity (stationarity) is assumed. If one is concerned only with deriving relationships between the space-averaged quantities and is not concerned about their fluctuation, then the results obtained by using the two approaches are essentially the same. Thus in this situation, one might as well use the simpler approach, namely the one based on the r.e.v.

1.12 Governing Law

The basic law governing the flow of fluids through porous media is **Darcy’s Law** which was formulated by the French civil engineer Henry Darcy in 1856 on the basis of his experiments on vertical water filtration through sand beds (see Fig. 1.8). From the experiments, he concluded that the flow rate is proportional to the applied pressure difference. It has been derived from the Navier–Stokes equations through homogenization. It is similar to Fourier's law in the field of heat conduction, Ohm's law in the field of electrical networks, or Fick's law in diffusion theory. It is refined by Morris Muskat for single-phase flow and given as

$$Q = \frac{-\kappa A(p_b - p_a)}{\mu L}, \tag{1.4}$$

where Q (m^3/s) is the total discharge, κ (m^2) is the intrinsic permeability of the medium, A (m^2) is the cross-sectional area to flow, $p_b - p_a$ (pascals) is the total pressure drop, μ (Pa·s) is the viscosity, and L (m) is the length over which the pressure drop is taking place. The negative sign is needed because fluid flows from high pressure to low pressure.

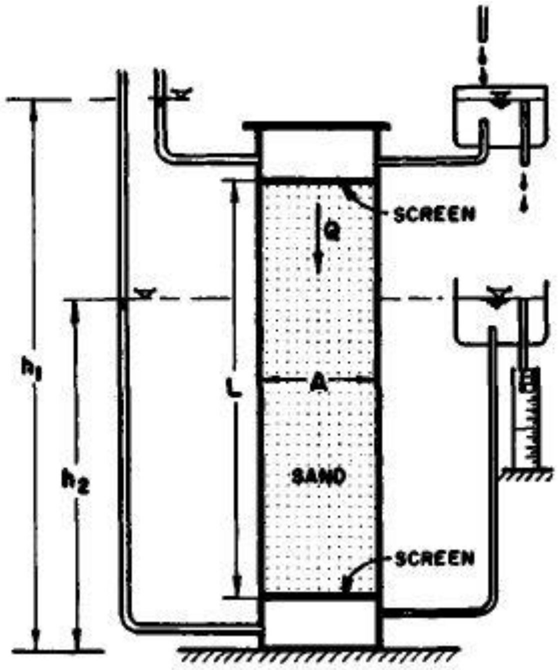

Fig. 1.8 Darcy's experiment (Bear (1972))

Dividing both sides of the equation (1.4) by the area, we get

$$q = -\frac{\kappa}{\mu}\nabla p, \tag{1.5}$$

where q is the flux (m/s) and $\boldsymbol{\nabla} p$ is the pressure gradient vector (Pa/m). The value of flux, which is also known as Darcy flux or Darcy velocity, is not the velocity which the fluid travelling through the pores is experiencing. The fluid velocity (v) related to Darcy flux (q) by the porosity (φ) is

$$v = \frac{q}{\varphi}, \tag{1.6}$$

which means only a fraction of the total formation volume is available for flow.

From Darcy's law, one can conclude that

(i) In the absence of a pressure gradient over a distance, no flow occurs.

(ii) If the pressure gradient is there, the flow will occur from high pressure towards low pressure.

(iii) Due to the high-pressure gradient, the discharge rate is high.

(iv) The discharge rate of fluid will often be different through different formation materials even if the same pressure gradient exists in both cases.

(v) Darcy's law is valid only for laminar flow. Due to that, it can apply for groundwater flow. Any flow with Reynolds number less than one is laminar, and it would be valid to apply Darcy's law. Experimental tests have shown that flow with Reynolds numbers up to 10 may still be Darcian, as in the case of groundwater flow. The Reynolds number for porous media flow is

$$\mathrm{Re} = \frac{\rho v d_{30}}{\mu}, \tag{1.7}$$

where ρ(m/V) is the density of water, v(L/t) is the specific discharge (not the pore velocity), d_{30}(L) is a representative grain diameter for the porous media, and μ is the viscosity of the fluid.

Darcy's law is used to analyze water flow through an aquifer and equivalent to the groundwater flow equation with conservation of mass principle.

1.13 Additional Forms of Darcy's law

1.13.1 Darcy's Law in Petroleum Engineering

To determine the flow through permeable media, the most simple equation of one-dimensional homogeneous rock formation with a single fluid phase and constant fluid viscosity is

$$Q = \frac{\kappa A}{\mu}\left(\frac{\partial p}{\partial x}\right), \tag{1.8}$$

where Q is the flow rate of the formation (V/t), k is the permeability of the formation (typically in milidarcys), A is the cross-sectional area of the formation, μ is the viscosity of the fluid (centipoise), $\partial p/\partial x$ represents the pressure change per unit length of the formation. This equation can also be solved for permeability and is used to measure it, forcing a fluid of known viscosity through a core of a known length and area, and measuring the pressure drop across the length of the core.

Approximately all oil reservoirs have a water zone below the oil leg, but few of them also have a gas cap above the oil leg. A simultaneous flow and immiscible mixing of all fluid phases in the oil zone occur due to the reservoir pressure drops. To improve oil production, operator of the oil field may also inject water (and/or gas). The petroleum industry is, therefore, using a generalized Darcy equation for a multiphase flow that was developed by Morris Muskat, an American petroleum engineer.

1.13.2 Darcy – Forchheimer Law

To analyze the non-linear behavior of the pressure difference vs. flow data, an additional inertial term is added to Darcy's equation, known as the Forchheimer term.

$$\frac{\partial p}{\partial x} = -\frac{\mu}{\kappa} q - \frac{\rho}{\kappa_1} q^2, \tag{1.9}$$

where the additional term κ_1 is called inertial permeability.

The gas flows into a gas production well, the irregular surface of the fracture walls, and high flow rate in the fractures may be high enough to justify the use of Forchheimer's equation.

1.13.3 Darcy's Law for Gases in Fine Media (Knudsen Diffusion or Klinkenberg Effect)

For gas flow in small characteristic dimensions, giving rise to additional wall friction (Knudsen friction). For a flow in this region, where both viscous and Knudsen friction is present, Knudsen presented an equation, given as

$$N = -\left(\frac{\kappa}{\mu} \frac{p_a + p_b}{2} + D_K^{eff} \right) \frac{1}{R_g T} \frac{p_b - p_a}{L}, \tag{1.10}$$

where N is the molar flux, Rg is the gas constant, T is the temperature, D_K^{eff} is the effective Knudsen diffusivity of the porous media. The model can also be derived from the first-principal-based binary friction model (BFM). The differential equation of transition flow in porous media based on BFM is given as

$$\frac{\partial p}{\partial x} = -R_g T \left(\frac{\kappa\, p}{\mu} + D_K \right)^{-1} N. \tag{1.11}$$

Above equation is valid for capillaries and porous media. This Knudsen effect and Knudsen diffusivity are useful in mechanical, chemical, geological, and petrochemical engineering. Using the definition of molar flux, the above equation can be re-written as

$$\frac{\partial p}{\partial x} = -R_g T \left(\frac{\kappa\, p}{\mu} + D_K \right)^{-1} \frac{p}{R_g T} q. \tag{1.12}$$

1.13.4 Darcy's Law for Short Time Scales

Similar to a modified form of Fourier’s law in Heat transfer, an additional term, i.e., the time derivative of the flux may be added to Darcy's law for very short time scales, which gives valid solutions at very small times, which is defined through the following equation:

$$\tau \frac{\partial q}{\partial t} + q = -\kappa \nabla h, \tag{1.13}$$

where τ is a very small time constant. The main reason for doing this is that the regular groundwater flow equations have singularities at constant head boundaries at very small times which lead to a hyperbolic groundwater flow equation, which is more difficult to solve and is only useful for an infinitesimal time.

1.13.5 Brinkman Form of Darcy's Law

Brinkman introduced an additional term in 1949 to figure out transitional flow between boundaries,

$$\beta \nabla^2 q + q = -\frac{\kappa}{\mu} \nabla p, \tag{1.14}$$

where β is an effective viscosity term. When the grains of the media are porous, this additional term is encountered. Since it is difficult to use, so it is generally neglected.

1.14 Mathematical Modeling

The declination of groundwater has increased research interests in the field of solute transport in natural or artificial porous media (Bear (1972); Vafai (2005)), since most of the structure through which groundwater moves is porous type structure. The areas where some works have already been done are the contamination of water by substances of many kinds and the study of the behavior of compounds into the porous domain.

The pollutant creates a contaminant plume within an aquifer which spreads over a wide area due to dispersion and movement of water. The movement of the plume called a plume front, can be analyzed through a transport model, called the solute transport model. Mathematical modeling of solute transport in groundwater is an important area of research, where a number of powerful techniques are used to solve the existing problems on contamination. Many mathematical models for solute transport in groundwater were presented by a number of engineers and scientists like Fried (1975), Bear and Verruijt (1987) and Javendal et al. (1984), Raj et al. (2002), Kumar et al. (2003), etc. The research article of Rai (2004) contains discussions on the role of mathematical modeling in groundwater resources management. Hydrologists, civil engineers and researchers have especially used groundwater modeling for the analyses of the resource potential and prediction of future impact on the environment under different conditions. Many experiments and theoretical studies are already done to predict the movement and behavior of the solute in the groundwater system. Many engineers and scientists are involved in doing their best to solve these types of serious issues. Anderson and Woessner (1992) described the applied groundwater models, simulation of flow and advective transport in their monograph. In 2000, Charbeneau (2000) explained the groundwater hydraulics and pollutant transport in his book. Kebew (2001) explained the applied chemical hydrology in the year 2001. In 2005, Rausch et al. (2005) described the modeling of solute transport and also provided an analytical solution. Solute transport modeling is helpful to predict the solute concentration in aquifers, rivers, lakes and streams too. All these investigations concern about possible contamination of the subsurface environment and have enhanced the research of solute transport phenomena in porous media.

The general solute transport model is the reaction-advection-dispersion equation (RADE) since it has the combined effects of advection, dispersion and reaction processes due to which solutes are transported down with the stream along the flow also get dispersed and sometimes react with the medium through which it moves. Mathematically it is represented as

$$\frac{\partial c}{\partial t} = \nabla.\left(d\,\nabla c\right) - \nabla.\left(vc\right) + R, \tag{1.15}$$

where c describes the species concentration for mass transfer problem and temperature for heat transfer problem, d is the mass diffusivity for particle motion and thermal diffusivity for heat transfer, v is the average velocity and for flows in porous media v is the superficial velocity, R is the reaction term for the species c.

Here the first term on the right-hand side of the equation (1.15) is accounting for dispersion phenomena, the second term accounting for the advection process and the last one is the reaction kinetics. When the solute does not react with the medium through which it moves and does not show any type of radioactive decay then it is called conservative system otherwise non-conservative for which reaction term has been encountered in above model. If only diffusion process is responsible for the movement of solute, then it is known as diffusion equation and is given as

$$\frac{\partial c}{\partial t} = \nabla.(d.\nabla c). \tag{1.16}$$

If the transport of solute in an aquifer due to the combined effects of advection and dispersion then it is described by advection-dispersion equation (ADE), which is mathematically represented by

$$\frac{\partial c}{\partial t} = \nabla.(d\,\nabla c) - \nabla.(vc). \tag{1.17}$$

ADE is a deterministic equation which is parabolic in nature. If the transport of solute in an aquifer is due to the combined effects of reaction and dispersion, then it is described by reaction-dispersion equation (RDE), which is mathematically represented by

$$\frac{\partial c}{\partial t} = \nabla.(d\,\nabla c) + R. \tag{1.18}$$

For the constant parameters of transport with respect to position and time, ADE is linear and provides explicit closed-form solution. A solution of the equation yields the solute concentration as a function of time and distance from contamination source. The equations are ultimately solved using the data of the groundwater velocity, coefficients of dispersion, the rate of chemical reactions, the initial concentration of solutes in the aquifer and boundary conditions along with the physical boundaries of the groundwater flow system. RADEs have broad applications in different areas such as medical science, mechanical engineering, environmental engineering, petroleum engineering, chemical engineering, heat transfer, soil sciences, as well as in biology.

1.14.1 Dispersion

The first term on the right-hand side of the equation (1.15) denotes the dispersion phenomena due to the spreading of the solute plume. It is composed of both mechanical dispersion and molecular diffusion which cannot be distinguished on the Darcy scale.

1.14.1.1 Mechanical Dispersion

In the case of flow through porous media, the solute containing water is not moving at the same velocity as that of water. As a result, additional mixing occurs along the flow path. This additional mixing is called mechanical dispersion. Or we can say, true velocities at points in the aquifer will differ from this average value, in both magnitude and direction. Local variations in ground-water velocity may not greatly affect the bulk movement of groundwater, but they do control the fate of solute particles. It describes the mixing and spreading of solutes along and transverse to the direction of flow in response to local variations in interstitial fluid velocities. On a microscopic scale it results from (i) the distribution of velocities within an individual pore due to friction effects along the surface of soil grains, (ii) difference in size of pores, (iii) difference in path length for individual solute particles, and (iv) the effect of converging and diverging flow paths (Wexler (1992)). On a macroscopic scale, it results from local variations in hydraulic conductivity, and thus fluid velocity, owing to the heterogeneity of aquifer material. It is described by Fick’s first law. The mixing that occurs in the direction of flow is called longitudinal dispersion and spreading normally to the direction of flow is called transverse dispersion.

1.14.1.2 Molecular Diffusion

The term Diffusion comes from the Latin language which means “to spread out”. Diffusion is a fundamental process result from the random collision of solute molecules and produces a flux of solute particles from areas of higher to lower solute concentration (Bear, 1979). Bear and Bachmat (1967) state that the coefficients of molecular diffusion in an isotropic medium are dependent on the diffusion coefficient of the particular solute in water and tortuosity of the medium. Rates of molecular diffusion are independent of ground-water velocity, and diffusion occurs even in the absence of fluid movement. Typically not as large as mechanical dispersion.

To see this process easily, one can do a simple experiment. A flask may be taken with full of clear water where water at rest, when a drop of ink is added in top of the flask in such a way that no convection current is set up then in starting it can be seen that a clear boundary between the ink and water but as the time passes it is seen that the ink gets faint towards the bottom, i.e., from area of higher to lower concentration and after some time the whole water will have the same colour (see Fig. 1.9). It is due to the spreading of ink molecules throughout the water by the process of diffusion. This spreading of molecules cannot be seen through natural way, but through a microscope, an individual molecule of ink can be seen. From where the movement of the individual molecule due to its kinetic energy and collision with the other molecules of ink and water are observed. Another interesting example is if someone uses the perfume then the nearby person can smell it due to the diffusion process.

Fig. 1.9 Example of the diffusion process

1.14.1.3 Derivation of Dispersion Equation

According to Fick's first law, the dispersion coefficient is the proportionality constant between the molar flux and the concentration gradient and is given by

$$F = -D\frac{\partial C}{\partial x}, \tag{1.19}$$

where F is the mass flux of solute per unit area per unit time, C is the solute concentration, x is the spatial coordinate measured normal to the section and D is the dispersion coefficient. Here a negative sign indicates that the dispersion occurs in the opposite direction of increasing concentration. This dispersion coefficient is sometimes taken as constant for example in dilute solutions, while in other cases it depends on concentration for example in high polymers.

The fundamental differential equation of dispersion in an isotropic medium is derived from equation (1.19) as follows following the geometry is given in Fig. 1.10:

Solutes entering into the control volume in the *x*-direction, *y*-direction, and *z*-direction due to dispersion are given by $F_x dydz$, $F_y dzdx$, and $F_z dxdy$, respectively.

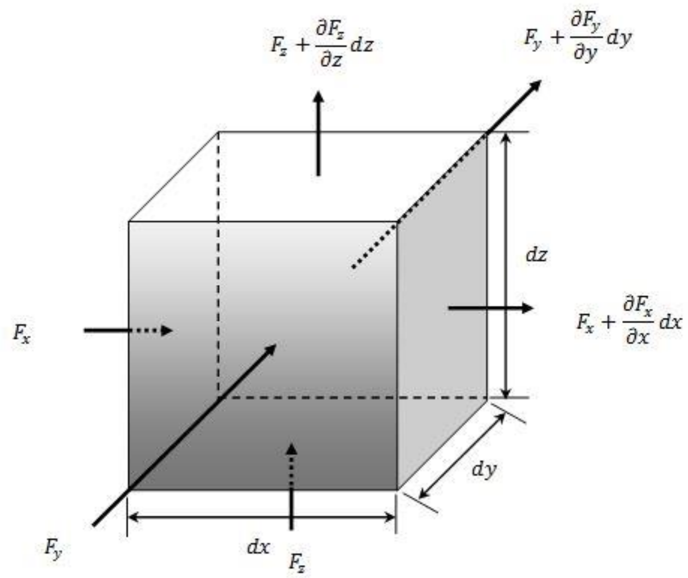

Fig. 1.10 Elementary control volume

Solutes out from the control volume in the *x*-direction, *y*-direction, and *z*-direction due to dispersion are $\left(F_x + \frac{\partial F_x}{\partial x} dx\right) dydz$, $\left(F_y + \frac{\partial F_y}{\partial y} dy\right) dzdx$, and $\left(F_z + \frac{\partial F_z}{\partial z} dz\right) dxdy$, respectively.

Therefore, net flux in the x-direction is $F_x dydz - \left(F_x + \frac{\partial F_x}{\partial x} dx\right) dydz = -\frac{\partial F_x}{\partial x} dxdydz.$

Similarly, net fluxes in the *y*-direction and *z*-direction are given by $-\frac{\partial F_y}{\partial y} dxdydz$, and $-\frac{\partial F_z}{\partial z} dxdydz$, respectively.

The total net flux of the representative elementary volume due to dispersion is

$$-\left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right) dxdydz. \tag{1.20}$$

The rate of change of mass is the representative elementary volume is

$$\frac{\partial C}{\partial t} dxdydz. \tag{1.21}$$

As per the law of conservation of mass,

$$\frac{\partial C}{\partial t}dxdydz = -\left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right)dxdydz. \tag{1.22}$$

Now, substituting the value of F_x, F_y and F_z according to the equation (1.19), we get

$$\frac{\partial C}{\partial t} = \left(\frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right)\right), \tag{1.23}$$

which is the classical dispersion equation.

1.14.2 Advection

Advective transport describes the bulk movement of solute particles along the mean direction of fluid flow at a rate equal to the average interstitial fluid velocity. In a saturated medium, this velocity can be calculated from Darcy's law as

$$v = -\frac{k}{\eta}\frac{dh}{dx}, \tag{1.24}$$

where v is the average fluid velocity, k is the permeability of the porous medium, η is the effect1ive porosity and dh/dx is the gradient of the pressure head.

1.14.2.1 Derivation of Advection Equation

The amount of solute transported by the advection process is a function of the quantity of fluid flowing and the concentration of solute in the fluid. Therefore, the mass flux due to advection in *x*-direction, *y*-direction, and *z*-direction are $F_x = v_x C$, $F_y = v_y C$, and $F_z = v_z C$, respectively.

The total net flux of the representative elementary volume due to advection is

$$-\left(\frac{\partial F_x}{\partial x}+\frac{\partial F_y}{\partial y}+\frac{\partial F_z}{\partial z}\right)dxdydz. \tag{1.25}$$

The rate of change of mass is the representative elementary volume is

$$\frac{\partial C}{\partial t}dxdydz. \tag{1.26}$$

As per the law of conservation of mass,

$$\frac{\partial C}{\partial t}dxdydz=-\left(\frac{\partial F_x}{\partial x}+\frac{\partial F_y}{\partial y}+\frac{\partial F_z}{\partial z}\right)dxdydz. \tag{1.27}$$

Now, substituting the value of $F_x, F_y,$ and F_z, we get

$$\frac{\partial C}{\partial t}=-\left(\frac{\partial}{\partial x}(v_xC)+\frac{\partial}{\partial y}(v_yC)+\frac{\partial}{\partial z}(v_zC)\right), \tag{1.28}$$

which is the classical advection equation. For the homogeneous aquifer, *v* is constant then the above equation can be written as

$$\frac{\partial C}{\partial t}=-\left(v_x\frac{\partial C}{\partial x}+v_y\frac{\partial C}{\partial y}+v_z\frac{\partial C}{\partial z}\right). \tag{1.29}$$

1.14.3 Derivation of Reaction-Advection-Dispersion Equation

The total mass of solute transported per unit cross-sectional area due to advection and dispersion in the *x*-direction is

$$F_x=\left(v_xCdydz-D_xdydz\right)/\,dydz=v_xC-D_x. \tag{1.30}$$

Similarly, the total mass of solute transported per unit cross-sectional area due to advection and dispersion in the *y*-direction is

$$F_y=\left(v_yCdzdx-D_ydzdx\right)/\,dzdx=v_yC-D_y. \tag{1.31}$$

Similarly, the total mass of solute transported per unit cross-sectional area due to advection and dispersion in the *z*-direction is

$$F_z = \left(v_z C dxdy - D_z dxdy\right)/\, dxdy = v_z C - D_z . \tag{1.32}$$

The total net flux of the representative elementary volume due to advection is

$$-\left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right) dxdydz. \tag{1.33}$$

The rate of change of mass is the representative elementary volume given by

$$\frac{\partial C}{\partial t} dxdydz. \tag{1.34}$$

As per the law of conservation of mass,

$$\frac{\partial C}{\partial t} dxdydz = -\left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right) dxdydz. \tag{1.35}$$

Now, putting the value of F_x, F_y, and F_z in the equation (1.35), we get

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial x}\left(v_x C\right) - \frac{\partial}{\partial y}\left(v_y C\right) - \frac{\partial}{\partial z}\left(v_z C\right). \tag{1.36}$$

This is the classical advection-dispersion equation for the conservative solute in porous media. The conservative solute means that the solute does not interact with the porous medium or it does not undergo biological or radioactive decay. For a non-conservative solute, one more term be added in the last equation known as the reaction term and the above equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial x}\left(v_x C\right) - \frac{\partial}{\partial y}\left(v_y C\right) - \frac{\partial}{\partial z}\left(v_z C\right) + R, \tag{1.37}$$

where R denotes the reaction term and this equation is known as reaction-advection-dispersion equation.

1.15 Volume Averaging Method

Multiphase systems dominate nearly every area of science and technology, and the method of volume averaging provides a rigorous foundation for the analysis of these systems. The development is based on classical continuum physics, and it provides both the spatially smoothed equations and a method of predicting the effective transport coefficients that appear in those equations. The method of volume averaging is rigorously used to model the solute transport in porous media. Stephen Whitaker and his co-workers have done great work in this field, the details of which can be found in the monograph by Whitaker (1999) entitled "The Method of Volume averaging". The other numerical methods to correlate the macroscopic transport coefficients to the microstructure using the closure formulations can be found in Plumb and Whitaker (1988a,b); Quintard and Whitaker (1967, 1994a,b,c, 2000); Wood et al. (2003) . The solute transport problems in homogeneous porous media using the single-equation and two-equation approaches have been given by Caillabet et al. (2001); Quintard and Whitaker (1993); Quintard et al. (1997), Quintard et al. (2001).

1.16 Special Functions

In this section, some definitions of special functions are given which are normally used in fractional calculus as well as in the subsequent chapters during numerical computation.

1.16.1 Gamma Function

The Euler's Gamma function is the generalization of *n!* by $\Gamma(n+1)$ which allows *n* to take non-integer value as well as complex value (Kilbas et al. (2006)). It is given as

$$\Gamma(z) = \int_0^{\infty} e^{-x} x^{z-1} dx. \tag{1.38}$$

Gamma function follows the following reduction formula

$$\Gamma(z+1) = z\Gamma(z). \tag{1.39}$$

1.16.2 Mittag-Leffler Function

In 1903, Mittag-Leffler defined a function $E_{\alpha}(z)$ which is the generalization of the exponential function and one parameter function. It is known as a Mittag-Leffler function of the first kind and is given by

$$E_{\alpha}(z) = \sum_{p=0}^{\infty} \frac{z^p}{\Gamma(\alpha p+1)}, \alpha > 0. \tag{1.40}$$

The Mittag-Leffler function of the second-kind $E_{\alpha,\beta}(z)$ (Kilbas et al. (2006)) which is a two parameters function is given by

$$E_{\alpha,\beta}(z) = \sum_{p=0}^{\infty} \frac{z^p}{(\alpha p+\beta)}, \alpha > 0, \beta > 0. \tag{1.41}$$

For $\beta = 1$,

$$E_{\alpha}(z) = E_{\alpha,1}(z). \tag{1.42}$$

1.16.3 Celling Function

In 1962, this function was introduced by Kenneth E. Iverson in his book titled "A Programming Language". The celling function of real number *x* maps *x* to the least positive integer greater than or equal to x and is denoted by

$$\lceil x \rceil = \min \{ n \in \mathrm{Z} \mid n \geq x \}, \tag{1.43}$$

where Z denotes the set of integers.

1.16.4 Generalized Hypergeometric Function

A generalized hypergeometric function ${}_pF_q(a_1,...,a_p;b_1,...,b_q;x)$ can be defined by convergent generalized hypergeometric series, in which ratio of successive coefficients indexed by n is a rational function of n for example

$$\frac{c_{k+1}}{c_k}=\frac{P(k)}{Q(k)}=\frac{(k+a_1)(k+a_2)...(k+a_p)}{(k+b_1)(k+b_2)...(k+b_q)(k+1)}x. \tag{1.44}$$

The function ${}_2F_1(a,b;c;x)$ is the first hypergeometric function to be studied and known as the hypergeometric function.

1.16.5 Hypergeometric Function

It is a special type of function which is represented by the hypergeometric series. It is a solution of a second-order linear ordinary differential equation with regular singular points at the origin. It is defined for $|z|<1$ as

$${}_2F_1(a,b;c;z)=\sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{(c)_n}\frac{z^n}{n!}, \tag{1.45}$$

where $(\wp)_n$ is the Pochhammer symbol defined by

$$(\wp)_n=\begin{cases}1 & n=0\\ \wp(\wp+1)...(\wp+n-1) & n>0\end{cases}. \tag{1.46}$$

It is undefined if c equals a non-positive integer and the series terminates if either a or b is a non-positive integer.

1.17 Fractional Calculus

Fractional calculus is as old as integer order calculus in which the order of differentiation and integration can be any real or complex number instead of only integer order. The birth year of fractional calculus is considered as 300 years back at the end of 17th-century with the letter exchange between G. de L'Hospital and G. W. Leibniz. In 1695, G. W. Leibniz wrote a letter to L'Hospital in which he raised the following question: "Can the meaning of derivatives with integer order be generalized to derivatives with non-integer orders?" L'Hospital was interested about that question and replied by another question to Leibniz: "What if the order will be ½"? In a reply dated September 30, 1695, the exact birth date of fractional calculus, Leibniz wrote: "It will lead to a paradox, from which one-day useful consequences will be drawn". The question raised by L'Hospital has been the topic of research for more than 300 years. From 1695 to till date more than 300 years are gone in which a lot of works have been done in that field by 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.

Furthermore, it leads to a new branch of mathematics, namely fractional calculus (Miller and Ross (1993)), in which only fractional order differentiation and integration are considered in starting. But nowadays, arbitrary real and complex numbers can be considered as an order of differentiation and integration (Kilbas (2006)).

From the end of 17th-century to 18th-century, no work has been found in this field in literature. 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 19th-century, S. F. Lacroix defined the derivative of arbitrary order in 1819 using Gamma function as

$$\frac{d^{1/2}}{dx^{1/2}}\left(x^m\right)=\frac{\Gamma(m+1)}{\Gamma(m+1/2)}x^{m-1/2}. \tag{1.47}$$

In 1822, Joseph Fourier expressed the function *f(x)* in integral form as

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)dt\int_{-\infty}^{\infty}\cos\alpha(x-t)d\alpha. \quad (1.48)$$

Using the last expression, he found

$$\frac{d^{\mu}}{dx^{\mu}} f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)dt\int_{-\infty}^{\infty}\alpha^{\mu}\cos\left(\alpha(x-t)+\frac{\mu\pi}{2}\right)d\alpha. \quad (1.49)$$

Fourier stated that the number μ that appears in the above would be regarded as any quantity whatsoever, positive or negative.

In the monograph of B. Ross (1975) titled "Fractional Calculus and Its Applications", it is mentioned that, in 1823, Niels Henrik Abel used the fractional derivative during the solution of an integral equation arising infamous Tautochrone problem. In 1832, J. Liouville was first to give the definition of a fractional derivative and he defined the fractional derivative of the special class of functions which can be expanded in the series form. In 1844, G. Boole developed the symbolic method for solving linear differential equations with constant coefficient using fractional calculus. In 1847, Bernhard Riemann was the first who proposed the definition of fractional integration as

$$D^{-\mu} f(x) = \frac{1}{\Gamma(\mu)}\int_{c}^{x}(x-t)^{\mu-1} f(t)dt + \Psi(x), \quad (1.50)$$

where $\Psi(x)$ is the Riemann's complementary function.

In 1869, Riemann-Liouville definition of fractional derivative appeared in the work of Sonin (1869) using Cauchy integral formula. In 1893, the fractional derivative was used in electromagnetic theory by Oliver Heaviside and he developed the generalized operator in his work. In 1917, H. Weyl and G.H. Hardy studied some properties of fractional differentiation and integration. But the work in the field of fractional calculus accelerated in the second half of the 20th-century. In June 1974, B. Ross organized the first conference on fractional calculus and its application at the University of New Haven after his Ph.D. dissertation on fractional calculus and after that lot of research articles have been published in this field. The second conference on this field organized in 1984, where some open questions were raised by eminent mathematicians. After the book “An Introduction to the Fractional Calculus and Fractional Differential Equations” by K. S. Miller and B. Ross (1993) and the book “Fractional Differential Equations” by Igor Podlubny (1999), this field seeks the attention of a lot of researchers from a different background. These books with the books “Application of Fractional Calculus in Physics” by Hilfer (2000), “The Analysis of Fractional Differential Equation” by Diethelm (2004), “Theory and Application of Fractional Differential Equation” by Kilbas et al. (2006) are tremendously popularised the fractional calculus in different fields of science and engineering like Electromagnetics, Robotics and Controls, Acoustics, Viscoelasticity, Electrochemistry, Biology, Signal and Image Processing, Fluid Dynamics etc. It is noticed that many physical phenomena are greatly described by the theory of fractional calculus. The integer order differential operator is a local operator whereas fractional order differential operator is a non-local operator in the sense that it takes into account the fact that the future state not only depends upon the present state but also upon all the history of its previous states. Therefore, it leads to model many natural phenomena containing long memory for example atmospheric diffusion of pollution, cellular diffusion process, network traffic, dynamics of a viscoelastic material, electronics etc. All these systems have non-local dynamics which cannot be modeled correctly with classical calculus theory. So, fractional calculus plays an important role during the modeling of these systems. Also, a fractional derivative of a function depends on the values of the function over the entire interval due to which it is suitable for modeling of the systems with long-range interactions both in space and time. Fractional differential equation greatly describes the anomalous phenomena in nature and in a complex system such as transport in porous media and provides an excellent instrument for the description of memory and inherent properties of various materials and processes.

In last few decades, many researchers applied the fractional calculus in different areas of science and engineering. In biology and bio-engineering, fractional calculus plays an important role to design artificial biological equipment, describing the complexity of cells and tissues and also encoding the multi-scale pattern of muscle fibers and nerve fibers. The book “Fractional Calculus in Bioengineering” by R. Magin (2006) shows the various applications of fractional calculus in the field of bioengineering. In the field of viscoelasticity, the application of fractional calculus can be seen in the research articles of G.W. Scoot Blair (1947), A. N. Gerasimov (1948), A. Gemant (1950), R. L. Bagley and P. J. Torvik (1984) and many others. The recent book of F. Mainardi (2010) describes the role of fractional calculus in the field of viscoelasticity in more details. In the field of control theory, the work by A. Oustaloup (1983) has a great contribution. In the field of electrical engineering, fractional calculus gave more flexibility for circuits modeling which can be found in the work of A. Le Mehaute and G. Crepy (1983). With the application of fractional calculus, T. Hartley et al. (1995) gave the Hartley-Chua circuit of the system whose order less than three that exhibits chaos behavior. In modeling of nonlinear electrical circuits, Ivo Petras (2010) applied the fractional calculus and presented a fractional order memristor-based Chua's equation where he showed that the system with total order less than three, i.e., less than the number of differential equations exhibits chaos. In the field of transport phenomena, the time fractional order diffusion-wave equation is one of the models that greatly describes the anomalous phenomena such as diffusion through disordered media like porous media, amorphous through fractals, percolation clusters etc. It represents the fractional diffusion equation if the order of time fractional derivative lies between 0 to 1 and fractional wave equation if the order of time fractional lies between 1 and 2. R. W. Schneider and W. Wyss (1986) converted the diffusion-wave equation into the integro-differential equation and derived the corresponding Green functions in the form of Fox function. Y. Fujita (1990) gave the existence and uniqueness of the solution of the space-time fractional diffusion equation. F. Mainardi (1996) obtained the analytical solution for the fractional diffusion-wave equation in one space dimension. To see the more work in the field of fractional calculus we can see the research works of Caputo (1967), Caputo and Mainardi (1971), Heaviside (1971), Oldham and Spanier (1974), Mainardi (1996, 1997), Gorenflo and Mainradi (2000), Carpinteri et al. (2004), Debnath (2003, 2004), Machado et al. (2011) and many others.

1.18 Some Important Definitions of Fractional Derivative and Integral

In Fractional calculus, time to time many definitions of fractional derivative and integration are given by many renowned researchers out of them Riemann-Liouville and Caputo fractional definitions are mostly used nowadays compared to other definitions.

1.18.1 Reimann-Liouville Integral

Let $f(x)$ be a locally integrable function then the Reimann-Liouville integral of fractional order $\mu \geq 0$ is defined by

$$I^{\mu} f(x) = \begin{cases} f(x), & \mu = 0, \\ \dfrac{1}{\Gamma\mu} \displaystyle\int_a^x (x-t)^{\mu} f(t)\, dt, & \mu > 0, \end{cases} \tag{1.51}$$

where $x > a$, $a, x, \mu \in \Re$ *and* $\Gamma(\mu)$ is gamma function.

1.18.2 Some Properties of Reimann-Liouville Integral Operator

(i) $\dfrac{d}{dx}(I^{\mu+1} f(x)) = I^{\mu} f(x),$

(ii) $I^{\mu}(I^{\eta} f(x)) = I^{\mu+\eta} f(x),$

(iii) $I^{\mu} x^{\eta} = \dfrac{\Gamma(\eta+1)}{\Gamma(\eta+1+\mu)} x^{\eta+\mu}.$

1.18.3 Caputo Fractional Derivative

It is introduced by M. Caputo in the year 1967 as

$$D^{\mu} f(x) = \begin{cases} \dfrac{1}{\Gamma(n-\mu)} \displaystyle\int_a^x \dfrac{f^{(n)}(t)}{(x-t)^{\mu+1-n}} dt, & n-1 < \mu < n, \\ \dfrac{d^n}{dx^n} f(x), & \mu = n \in N, \end{cases} \tag{1.52}$$

where $\mu > 0, x > a$ and $a, x, \mu \in R, n \in \mathrm{N}$. It is a fractional derivative of order μ.

1.18.4 Some Properties of Caputo Fractional Derivative

(i) Linearity**:** It follows the linearity property as integer order differentiation as

$$D^{\mu}(a_1 f(x) + a_2 g(x)) = a_1 D^{\mu} f(x) + a_2 D^{\mu} g(x),$$

where a_1 and a_2 are constants.

(ii) $D^{\mu}a = 0,$ where *a* is a constant.

(iii) $$D^{\mu}x^{m} = \begin{cases} 0, & \text{for } m \in N_0 \text{ and } m < \lceil \mu \rceil \\ \dfrac{\Gamma(m+1)}{\Gamma(m+1-\mu)}x^{(m-\mu)}, & \text{for } m \in N_0 \text{ and } m \geq \lceil \mu \rceil, \end{cases}$$

where the function $\lceil \mu \rceil$ is used to denote the ceiling function, i.e., the smallest integer greater than or equal to μ . Also $N_0 = \{0,1,2,...\}$.

(iv) $$I^{\mu}D^{\mu}f(x) = f(x) - \sum_{i=0}^{m-1} f^{(i)}(0^{+})\frac{x^{i}}{\Gamma(i+1)}.$$

1.19 Spectral Methods

In literature, lot of methods viz., finite difference method, finite element method, finite volume method, integral equation method, implicit method, explicit method, multigrid method, spectral method, meshfree method etc. are encountered to solve the linear/non-linear standard as well as fractional order partial differential equations (PDEs) numerically. Among those spectral methods have a sharp edge over all the methods due to its exponential rate of convergence, easy to implement, and have excellent accuracy during the solution of integral and differential equations in the finite or infinite domain. Spectral methods were developed in a long series of papers by Steven Orszag starting in 1969. In this method the solution of the problem is given as a sum of some basis functions like orthogonal functions (Legendre polynomial, Jacobi polynomial, Chebyshev polynomial etc.) and then to choose the coefficients; in such a way that the error between the exact solution and approximate solution will be minimized. Spectral methods and finite element methods are closely related and built on the same ideas. The main difference between them is that the basis functions used in spectral methods are non-zero over the whole domain, while the basis functions used in finite element methods are nonzero only on small sub-domains. Spectral methods are computationally less expensive than finite element methods. In other words, spectral methods take on a global approach while finite element methods use a local approach. Partially for this reason, spectral methods have excellent error properties, with the so-called "exponential convergence" being the fastest possible when the solution is smooth. The implementation of the spectral method is normally accomplished either with collocation (Guo et al. (2012); Bhrawy (2014, 2016)) or a Galerkin (Shields et al. (2017); Chung et al. (2017); Rad and Parand (2017); Doha et al. (2011)) or a Tau approach (Bhrawy et al. (2016); Saadatmandi and Dehgan (2011)). Operational matrix approach with these spectral methods reduces the numerical calculation and save much time. For this reason, the operational matrices for differentiation and integration are found. The operational matrices for different orthogonal polynomials can be found in the literature (Bhrawy (2015, 2016); Saadatmandi and Dehgan (2010, 2011); Bhrawy et al. (2016); Doha et al. (2011, 2012); Saadatmandi et al. (2012)). Out of these spectral methods, spectral collocation method is widely used to solve standard as well as fractional order PDEs because of its easy applicability and high accuracy. In spectral collocation method, collocation points play a significant role because the convergence of the method depends on it. This method is also useful to provide the highly accurate solutions for nonlinear partial differential equations (NPDEs) even using a small number of grids.

1.20 Orthogonal Polynomials

The orthogonal polynomials are the most important polynomials which are frequently used in numerical analysis.

1.20.1 Chebyshev Polynomials of the First-Kind

The Chebyshev polynomial $T_n(x)$ of the first-kind of a degree n in x defined on the interval [-1, 1] is given by

$$T_n(x) = \cos(n\cos^{-1} x), \tag{1.53}$$

where $x = \cos\theta$ and $\theta \in [0, \pi]$ (Mason (1993); Mason and Handscomb (2003)). The polynomials $T_n(x)$ are orthogonal on [-1, 1] with respect to the inner products

$$\langle \mathrm{T_n}(x), T_m(x) \rangle = \int_{-1}^{1} \frac{T_n(x) T_m(x)}{\sqrt{1-x^2}} dx = \begin{cases} 0, & n \neq m, \\ \pi, & n = m = 0, \\ \pi/2 & n = m, \end{cases} \tag{1.54}$$

where $\frac{1}{\sqrt{1-x^2}}$ is weight function. $T_n(x)$ may be generated by using the recurrence relations

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x), \quad n = 2,3,........; \tag{1.55}$$

with $T_0(x) = 1,\ T_1(x) = x.$

1.20.2 Chebyshev Polynomials of the Second-Kind

The Chebyshev polynomial $U_n(x)$ of the second-kind of degree n in x defined on the interval [-1, 1] as

$$U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta}, \tag{1.56}$$

where $x = \cos\theta$ and $\theta \in [0, \pi]$ (Mason (1993), Mason and Handscomb (2003)). The polynomials $U_n(x)$ are orthogonal on [-1, 1] with respect to the inner products as

$$\langle \mathrm{U_n}(x), U_m(x) \rangle = \int_{-1}^{1} \sqrt{1-x^2}\, U_n(x) U_m(x)\, dx = \begin{cases} 0, & n \neq m, \\ \pi/2 & n = m, \end{cases} \tag{1.57}$$

where $\sqrt{1-x^2}$ is weight function. $U_n(x)$ may be generated by using the recurrence relations

$$U_n(x) = 2xU_{n-1}(x) - U_{n-2}(x), \qquad n = 2,3,........; \tag{1.58}$$

with $U_0(x) = 1, \quad U_1(x) = 2x.$

The explicit form of the second-kind Chebyshev polynomials $U_n(x)$ of degree n is given by

$$U_n(x) = \sum_{p=0}^{\lceil n/2 \rceil} (-1)^p \binom{n-p}{p} (2x)^{n-2p}, \qquad n > 0. \tag{1.59}$$

Using Gamma function, the above equation can be re-written as

$$U_n(x) = \sum_{p=0}^{[n/2]} (-1)^p 2^{n-2p} \frac{\Gamma(n-p+1)}{\Gamma(p+1)\Gamma(n-2p+1)} x^{n-2p}, \ n > 0, \tag{1.60}$$

where $[n/2]$ denotes an integral part of *n/2*.

1.20.3 Legendre Polynomials

The classical Legendre polynomials are defined on $[-1,1]$ and given by the following recurrence relation

$$L_{p+1}(z) = \frac{2p+1}{p+1} zL_p(z) - \frac{p}{p+1} L_{p-1}(z), \qquad p = 1,2,\ldots, \tag{1.61}$$

with $L_0(z) = 1$ and $L_1(z) = z$.

1.20.4 Jacobi Polynomials

The classical Jacobi polynomials are represented by $P_i^{(\alpha,\beta)}$ over the interval $[-1,1]$ where $\alpha > -1, \beta > -1$, and i denotes the degree of the polynomial and can be defined by hypergeometric function as

$$P_i^{(\alpha,\beta)}(z) = \frac{(\alpha+1)_i}{\Gamma(i+1)}\, {}_2F_1\left(-i, 1+\alpha+\beta+i; \alpha+1; \left(\frac{1-z}{2}\right)\right), \tag{1.62}$$

or

$$P_i^{(\alpha,\beta)}(z) = \frac{\Gamma(\alpha+i+1)}{\Gamma(i+1)\Gamma(\alpha+\beta+i+1)} \sum_{j=0}^{i} \binom{i}{j} \frac{\Gamma(\alpha+\beta+i+j+1)}{\Gamma(\alpha+j+1)} \left(\frac{z-1}{2}\right)^j. \tag{1.63}$$

It can be generated from the following recurrence relation

$$P_{i+1}^{(\alpha,\beta)}(z) = (a_i z - b_i) P_i^{(\alpha,\beta)}(z) - c_i P_{i-1}^{(\alpha,\beta)}(z), \quad i \geq 1, \tag{1.64}$$

with $P_0^{(\alpha,\beta)}(z) = 1,\; P_1^{(\alpha,\beta)}(z) = \frac{1}{2}(\alpha+\beta+2)z + \frac{1}{2}(\alpha-\beta),$

where $a_i = \dfrac{(2i+\alpha+\beta+1)(2i+\alpha+\beta+2)}{2(i+1)(i+\alpha+\beta+1)}$, $b_i = \dfrac{(2i+\alpha+\beta+1)(\beta^2-\alpha^2)}{2(i+1)(i+\alpha+\beta+1)(2i+\alpha+\beta)}$,

$$c_i = \frac{(2i+\alpha+\beta+2)(i+\alpha)(i+\beta)}{(i+1)(i+\alpha+\beta+1)(2i+\alpha+\beta)}.$$

It forms a class of orthogonal polynomials with respect to the weight function $w^{(\alpha,\beta)}(z) = (1-z)^\alpha (1-z)^\beta$ over the interval $[-1,1]$, i.e.,

$$\int_{-1}^{1} P_i^{(\alpha,\beta)}(z)\, P_j^{(\alpha,\beta)}(z)\, w^{(\alpha,\beta)}(z)\, dz = \delta_{ij} \chi_j^{(\alpha,\beta)}, \tag{1.65}$$

where δ_{ij} is the Kronecker function and

$$\chi_j^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}\Gamma(j+\alpha+1)\Gamma(j+\beta+1)}{(2j+\alpha+\beta+1)\Gamma(j+1)\Gamma(j+\alpha+\beta+1)}. \tag{1.66}$$

Some properties of the Jacobi polynomials

(i) $P_i^{(\alpha,\beta)}(-z) = (-1)^i P_i^{(\beta,\alpha)}(z),$

(ii) $P_i^{(\alpha,\beta)}(1) = \binom{i+\alpha}{i},$

(iii) $P_i^{(\alpha,\beta)}(-1) = (-1)^i \binom{i+\beta}{i},$

(iv) $\frac{d^m}{dx^m} P_i^{(\alpha,\beta)}(z) = \frac{\Gamma(\alpha+\beta+i+1+m)}{2^m \Gamma(\alpha+\beta+i+1)} P_{i-m}^{(\alpha+m,\beta+m)}(z).$

1.21 Shifted Orthogonal Polynomials

The classical orthogonal polynomials discussed above are defined in the interval $[-1,1]$ and to define these polynomials in any arbitrary interval like $[a,b],$ we make this arbitrary interval $[a,b]$ corresponding to the interval $[-1,1]$ with the help of the transformation as

$$\frac{2x-(a+b)}{b-a}, \tag{1.67}$$

where $x \in [a,b].$ These newly defined polynomials are called shifted orthogonal polynomials.

1.22 Linear/Non-linear Partial Differential Equation

A differential equation is said to be a PDE in which unknowns are the function of two or more independent variables. If the domain of the problems contains the space and time variables both as independent variables, then the PDE defined in this domain is known as evolution equation whereas if the domain contains only space variable as an independent variable, then the PDE define in this domain is known as equilibrium or steady-state equation.

A PDE is said to be linear if the unknowns and its derivatives involved in the equation are linear as well as the coefficients present in the equation depend on independent variables only not to unknown. In another way, if the PDE satisfies the law of superposition and law of homogeneity, then it called linear otherwise non-linear.

1.22.1 Law of Superposition

It states that for different inputs *x* and *y* in the domain of the function *f*,

$$f(x+y)=f(x)+f(y). \tag{1.68}$$

1.22.2 Law of Homogeneity

It states that for a given input *x* in the domain of the function *f* and any real number *k*,

$$f(kx)=kf(x). \tag{1.69}$$

1.23 Fractional Differential Equations

Fractional differential equations are the generalization of differential equations with the use of fractional calculus. Those are considered as superset as it contains integer order differential equations and has more potential to describe the natural phenomena accurately which cannot be done with integer order differential equations. In literature, a number of books and research articles are present where different definitions and applications of fractional differential equations are given. In the book "An Introduction to the Fractional Calculus and Fractional Differential equations" by Miller and Ross (1993), the fractional differential equation is defined as

$$\left\lfloor D^{r_m}+b_1D^{r_{m-1}}+b_2D^{r_{m-2}}+\ldots+b_mD^{r_0}\right\rfloor y(t)=0, \tag{1.70}$$

where $r_m, r_{m-1}, r_{m-2}, \ldots, r_0$ be the sequence of strictly decreasing non-negative integers and $b_1, b_2, b_3, \ldots, b_m$ are the constants. But due to the complexity of this equation some conditions are imposed as let r_i be the rational number and if q is the least common multiple of all the denominators of non-zero r_i, we can re-write equation (1.70) as

$$\left[D^{nv} + a_1 D^{(n-1)v} + a_2 D^{(n-2)v} + ... + a_m D^0 \right] y(t) = 0, \text{ where } t \geq 0 \text{ and } v = 1/q. \tag{1.71}$$

This equation is known as fractional order linear differential equation with constant coefficients of orders (n, q). For $q = 1$, the equation will be converted into a standard order differential equation. In the monograph of Kilbas et al. (2006), they have excellently explained the applications of fractional order differential equations and up-to-date development of fractional differential and fractional integro-differential equations.

1.24 Applications of Fractional Differential Equations

Nowadays, no field of science and engineering are available where the fractional differential equation is not applicable. In present time these can be seen in the fields like Anomalous Transport, Solid Mechanics, Bioengineering, Continuum and Statistical Mechanics, Electric Transmission, Ultrasonic Wave Propagation in Human Cancellous bone, Fluid Dynamic, Economics, Non-linear Oscillation of Earthquakes, Colored Noise, Speech Signals, Cardiac Tissue Electrode Interface, Viscoelasticity, Material Science, Electromagnetic Theory, Control Theory and Dynamical system, Optics and Signal Processing, Astrophysics, Geology, Bio-Science, Probability and Statistics, Chemical physics, Solute Transport in porous type structure and so on (Kilbas et al. (2006); Dalir and Bashour (2010); Baillie (1996); He (1998, 1999); Magin (2004); Mainardi (1997); Mandelbrot (1967); Metzler and Klafter (2004)). In all these areas, microscopic behaviors are very complex and the physical phenomena show strange kinetics which cannot be modeled by the classical differential equation for that fractional differential explain their macroscopic dynamics. The fractional order form of the law of conservation of mass is described in the research article of Wheatcraft and

Meerschaert (2008) in which they explained that the fractional conservation of mass equation is needed to model fluid flow when the control volume is not large enough compared to the scale of heterogeneity and when the flux within the control volume is non-linear. The fractional order form of groundwater flow problem can be seen in the work of Atangana et al. (2013, 2014) in which they generalized the classical Darcy law by taking the water flow as a function of a non-integer derivative of the piezometric head. Benson et al. (2000a, 2000b, 2001) have explained that the fractional order form of advection-dispersion equation is useful for contaminant flow in heterogeneous porous media. Atangana and Kilicman (2014) extended it to variable order fractional advection-dispersion equation which shows that the extended form is more reliable to explain the movement of solute in the deformable aquifer. To explain the anomalous diffusion in complex media time-space fractional diffusion models have been considered by Metzler and Klafter (2000), Mainardi et al. (2001), Das (2009 a, 2009b), Das and Kumar (2011), Das et al. (2011), Vishal and Das (2012), Vishal et al. (2013), where time derivative term is corresponding to long-time heavy tail decay and the spatial derivative for diffusion nonlocality. A simple extension of this model to variable order can be found in the research articles of Gorenflo and Mainardi (2003) and Atangana et al. (2014).