Chapter 1

Introduction

1.1 Introduction

Public interest in the environment and its effects on the society have been increased in recent years. These are shown more in stringent developed country regarding environmental pollution. Numerous directives are encompassing, noise, water and air pollution, general waste management and protection of flora and fauna. These directives have compelled environmental agencies to improve existing methods of pollution management. The issues of water pollution and waste water management are of particular significance as water is essential for life. It is widely used by society for industrial and domestic purposes most obviously in manufacturing, sanitation, cooking, drinking and bathing. Also, consideration must be given to marine and river environments in terms of fish and shellfish habitats. Coastal waters are also important, particularly in tourist areas, which are detrimentally affected if polluted. To this end, strict regulations exist which affect how waste water treatment must be undertaken and where effluent can be discharged.

Solute transport through the groundwater has become an important topic of research in the interdisciplinary branches of science and engineering, called hydrogeology. The word hydrogeology is the combination of three words hydro means 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 on earth and other planets are studied. This branch also subdivides into many branches like chemical hydrology, echo hydrology, surface hydrology, hydrogeology, hydro informatics, hydro meteorology 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 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 the water and solute that moves beneath the earth. The water that moves below the earth surface is called groundwater and the area where it moves generally called aquifer.

1.2 Groundwater contamination

Water is one of the primary elements for living things on earth. It is presented in two forms, surface water and groundwater, of which only 2.5% is fresh water. More than two-thirds of this freshwater is covered by the glacier and ice caps. Ninety-seven percent of the freshwater comes from groundwater. 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 essential source of drinking water in both urban and rural areas.

As the primary source of drinking water is the groundwater; groundwater contamination is a serious issue for living things. Contaminated groundwater is very harmful to the environment, human health and widely affect the wildlife. It may not damage humans and animal health immediately but can be dangerous after long term exposure. Groundwater contamination through septic tank waste can have serious effects on human health. There are many micro-organisms and a large number of synthetic chemicals for contaminating groundwater. Drinking water due to the presence of bacteria and viruses may cause hepatitis, cholera, etc. and also it may cause methemoglobinemia or blue baby syndrome for containing a high amount of nitrates. 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 considerable distance in unseen aquifers. It is expensive to get clean groundwater after contamination.

Contaminants after releasing from the environment move within an aquifer similarly as groundwater moves. In an aquifer those substances transport along with groundwater flow of from high concentration area to the low concentration area. Groundwater becomes contaminated from natural sources or various types of human activities. Its quality is affected due to residential, municipal, commercial, industrial and agricultural activities. Groundwater and surface water are interconnected. Since the activities on the land surface e.g., the release of stored industrial wastes, contaminated recharge water, source septic system or due to leakage of underground storage systems, etc., contaminants reach to the groundwater through porous media. This form of environmental degradation occurs when pollutants are directly or indirectly discharged into the water bodies. The natural contamination depends on the 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. Due to the increase of population it is overexploited and thus it is 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 [1, 2, 3, 4, 5, 6, 7].

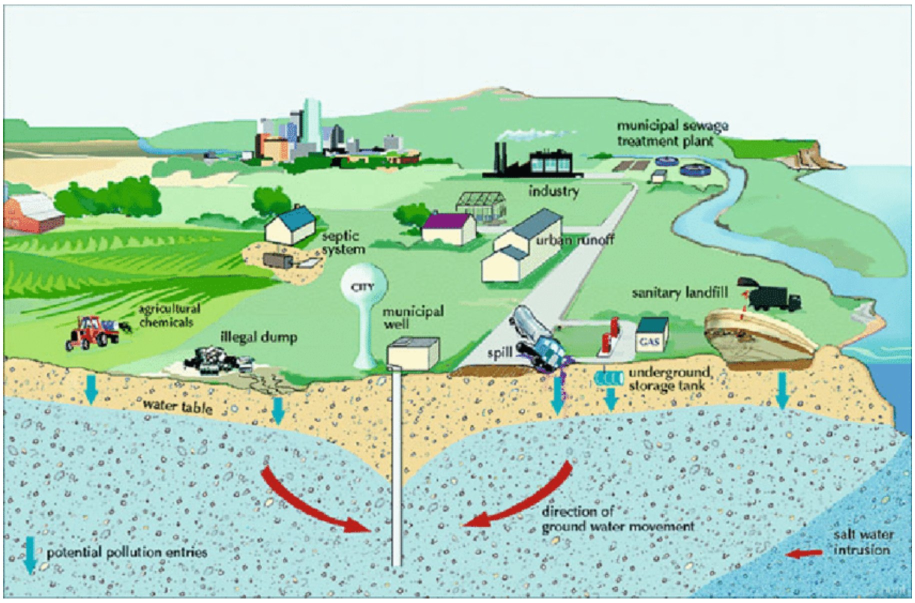

Figure 1.1: Sources of groundwater contamination

Near the coast, a vacuum is created by over pumping an aquifer which can quickly be filled up with salty seawater 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 has large impact on the water in an aquifer compared to point-source.

If groundwater is contaminated overall, then the rehabilitation is deemed to be too difficult and expensive and thus it may become unusable for decades. In that case, searching for the other source of water is the only option though it is quite 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 carry out this, good knowledge about the physical, chemical and biological processes that control the transport of solute in groundwater is necessary at the outset. The attention should be given to describe the problem domain, boundary conditions and model parameters for creating the numerical groundwater models of field problems.

1.3 Reaction-advection-diffusion equation

The most of the structures through which groundwater moves are porous type, thus there is plenty of scope of research in the field of solute transport in artificial [8, 9, 10] or natural porous media. Mathematical modeling of solute transport in groundwater is an important area of research, where many powerful techniques are used to solve the existing problems on contamination. Many engineers and scientists have predicted the movement of the solute in the groundwater system through experiments and theoretical studies.

The pollutant creates a contaminant plume within an aquifer which spreads over a wide range due to dispersion (diffusion) and movement of water. The transportation of the plume called a plume front can analyze through a transport model, called the solute transport model. Solute transport modeling is useful to predict the solute concentration in aquifers, lakes, rivers, and streams too. A large number of mathematical models for solute transport in groundwater were presented by engineers and scientists [1, 11, 12, 13, 14]. Hydrologists and researchers have mainly used groundwater modeling for the analyses of the resource potential and prediction of future impact on the environment under different conditions. Anderson *et al.* [2] described the applied groundwater models, simulation of flow and advective transport in their monograph. Charbeneau [3] explained the groundwater hydraulics and pollutant transport in his book. Kehew [4] demonstrated the applied chemical hydrology. In 2005, Rausch [15] described the modeling of solute transport and also provided analytical solution. All these investigations concern about possible contamination of the subsurface environment and have enhanced the research of solute transport phenomena in porous media.

There are many natural systems those can be modeled such as pollution of groundwater, atmospheric pollution caused by smoke or dust and thermal pollution of river systems by using partial differential equation (PDE). The velocities of the transport medium are computed by solving the equations describing flows in porous media. The flow equations are nonlinear, but advection and diffusion are of primary importance.

The transport of solute under the combined effect of advection and diffusion is described by the **advection-diffusion equation** (ADE). If the chemical being transported through soil is reactive, then another form of the chemical equation is found to occur with reaction term called **reaction-advection-diffusion equation** (RADE). 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. In practical application advection-diffusion equation describe heat transfer in a draining film [16], contaminant dispersion in shallow lakes [17], flow in porous media [18], the transport of pollutants in the atmosphere [19], the spread of pollutants in rivers and steams [20], oil reservoir flow [21]. Numerical time-domain-diffusion simulations have been used by Voutilainen *et al.* [22] for studying the diffusion behaviour of tracer molecules in rock matrix with homogeneous and heterogeneous porosities. Sun *et al.* [23] proposed a numerical method whose computational efficiency and simulation accuracy is better compared to a reliable method known as Operator splitting during solving advection-dispersion-reaction equations. Baltean *et al.* [24] developed a macroscopic model for the transport of a passive solute using diffusion and convection in a heterogeneous medium. A general approximation for the solution of the one-dimensional nonlinear diffusion equation had been presented by Parlange *et al.* [25], which was applied to arbitrary soil properties and boundary conditions. Muralidhar and Ramkrishna [26] analysed using generalized hydrodynamics that describes fractal diffusion with a frequency and wave number dependent diffusivity.

The reaction-advection-diffusion equation is one of the most challenging equation, which has been used to predict the movement of a pollutant in water body. The general solute transport model is reaction-advection-diffusion equation given by

$$\frac{\partial u}{\partial t} = \nabla.(D.\nabla u) - V.\nabla u + \lambda f(u), \tag{1.1}$$

where u is the transport dependent variable, D is the diffusivity tensor, V is the advective velocity vector. λ is rate coefficient and $f(u)$ is reaction term.

For the constant parameters of transport with respect to position and time, RADE provides explicit closed form solution by using suitable numerical methods. Solution of the equation yields the concentration of solute (pollutant) 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, rate of chemical reactions, initial concentration of solutes in the aquifer and boundary conditions along with the physical boundaries of the groundwater flow system.

1.3.1 Derivation of reaction-advection-diffusion 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

$$J = -D\frac{\partial u(x,t)}{\partial x}, \tag{1.2}$$

where J is the mass flux of solute per unit area per unit time, $u(x,t)$ is the solute concentration, x is the spatial coordinate measured normal to the section and D is the dispersion coefficient. Here negative sign indicates that the dispersion occurrence in the opposite direction of increasing concentration. This dispersion coefficient is sometime taken as constant, for example, in dilute solutions, while in other cases it depends on concentration, for example, in high polymers.

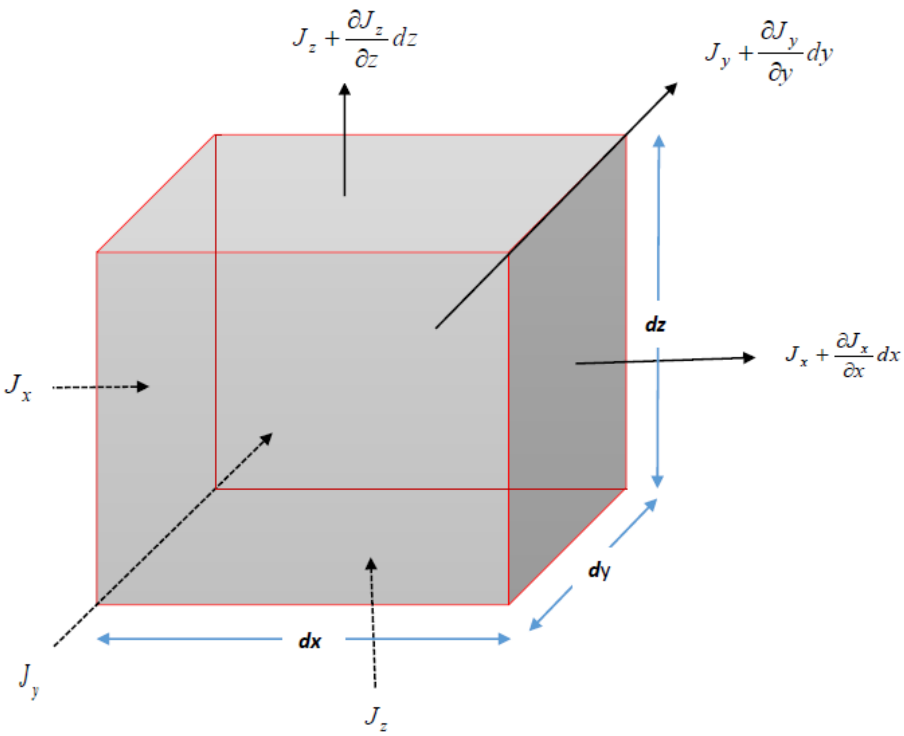

Figure 1.2: Control volume for solute transport through porous media

The fundamental differential equation of dispersion in an isotropic medium is derived from equation (1.2) as follows (the geometry given in Figure 1.2).

Solutes out from the control volume in x-direction, y-direction, and z-direction due to dispersion are $\left(J_x + \frac{\partial J_x}{\partial x}dx\right)dy\,dz$, $\left(J_y + \frac{\partial J_y}{\partial y}dy\right)dz\,dx$, $\left(J_z + \frac{\partial J_z}{\partial z}dz\right)dx\,dy$ respectively

Therefore, net flux in x-direction is $J_x dy\,dz - \left(J_x + \frac{\partial J_x}{\partial x}dx\right)dy\,dz = -\frac{\partial J_x}{\partial x}\,dx\,dy\,dz$.

Similarly, net flux in y-direction and z-direction are $-\frac{\partial J_y}{\partial y}\,dx\,dy\,dz$ and $-\frac{\partial J_z}{\partial z}\,dx\,dy\,dz$ respectively.

Total net flux of the representative elementary volume due to dispersion is

$$-\left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}\right) dx\, dy\, dz. \tag{1.3}$$

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

$$\frac{\partial u}{\partial t} dx\, dy\, dz. \tag{1.4}$$

As per the law of conservation of mass,

$$\frac{\partial u}{\partial t} dx\, dy\, dz = -\left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}\right) dx\, dy\, dz. \tag{1.5}$$

Now, substituting the values of J_x , J_y and J_z in equation (1.2), we get

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial u}{\partial z}\right), \tag{1.6}$$

which is the classical dispersion equation.

Total mass of solute transported per unit cross sectional area due to advection and dispersion in x-direction is

$$J_x = (v_x.u.dy\, dz - D_x \frac{\partial u}{\partial x} dy\, dz)/dy\, dz = v_x u - D_x \frac{\partial u}{\partial x}. \tag{1.7}$$

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

$$J_y = (v_y.u.dz\, dx - D_y \frac{\partial u}{\partial y} dz\, dx)/dz\, dx = v_y u - D_y \frac{\partial u}{\partial y}, \tag{1.8}$$

$$J_z = (v_z.u.dx\,dy - D_z\frac{\partial u}{\partial z}dx\,dy)/dx\,dy = v_z u - D_z\frac{\partial u}{\partial z}. \tag{1.9}$$

Total net flux of the representative elementary volume due to advection is

$$-\left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}\right)dx\,dy\,dz. \tag{1.10}$$

The rate of change of mass is

$$\frac{\partial u}{\partial t}dx\,dy\,dz. \tag{1.11}$$

As per the law of conservation of mass,

$$\frac{\partial u}{\partial t}dx\,dy\,dz = -\left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}\right)dx\,dy\,dz. \tag{1.12}$$

Now, substituting the value of J_x , J_y and J_z in equation (1.2), we get

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D_x\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial u}{\partial z}\right) - \frac{\partial}{\partial x}(v_x u) - \frac{\partial}{\partial y}(v_y u) - \frac{\partial}{\partial z}(v_z u). \tag{1.13}$$

This is the classical advection-dispersion equation for 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, one more term be added in the last equation known as reaction term R and the above equation becomes

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D_x\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial u}{\partial z}\right) - \frac{\partial}{\partial x}(v_x u) - \frac{\partial}{\partial y}(v_y u) - \frac{\partial}{\partial z}(v_z u) + R. \tag{1.14}$$

It can be expressed as follows

$$\frac{\partial u}{\partial t} = \nabla.(D.\nabla u) - V.\nabla u + R,$$

which is known as reaction-advection-diffusion equation.

The important tool for taking into account the memory effect in the porous media is the use of fractional-order derivatives. In contrast to integer-order differential operator, which is the local operator, a fractional-order differential operator is nonlocal 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 of the histories of its previous states. For this realistic property, the usage of fractional-order system is becoming popular to model the behavior of real system in various fields of science and engineering.

1.4 Fractional calculus

The fractional calculus is a generalization of the integer order differentiation and integration to arbitrary order. It plays an important role in describing many physical and chemical phenomena in various branches of science and engineering, which can be modeled into fractional-order differential equations. One of the most important fractional-order differential equations is the fractional-order RADE. Renowned Mathematicians like J. Liouville, B. Riemann, G. W. Leibniz, H. Weyl, N. H. Abel, A. K. Grünwald, A.V. Letnikov and J. Caputo have contributed much towards the development of fractional calculus. Fractional calculus provides an excellent technique for a description of memory and hereditary property of various materials and processes [27]. It is found that fractional derivatives are very effective for the physical problems such as diffusion process, rheology and fluid mechanics, etc. During the last few decades, fractional calculus has received great importance due to its various applications in applied science and engineering which are modeled mathematically by fractional-order partial differential equation (FPDE) [28]. Till date though in the mathematical model there is no acceptable geometrical or physical interpretation, but researchers from different parts of the world are actively engaged to explore it. In the fractional differential equation, fractional space derivatives are used to model anomalous diffusion or dispersion, and it is seen from the literature survey that in some diffusion processes Fick's second law fails to describe the related transport behaviour. The phenomenon which is characterized by the nonlinear growth of the mean square displacement of a diffusion particle over time is called anomalous diffusion.

1.4.1 A brief history

Many authors have cited a particular date as the birthday of so-called "Fractional Calculus." In a letter dated September 30, 1695 L'Hopital wrote to G.W Leibniz and asked him about a specific notation he had used in his publication for the nth-derivative of the linear function $f(x) = x^n$ i.e., $\frac{d^n x^n}{dx^n}$. L'Hospital posed the question to Leibniz, what would the result be if $n = 1/2$. Leibniz's response: "An apparent paradox, from which one-day useful consequences will be drawn." In these words, fractional calculus was born. From this letter, we can say that the integer-order and the fractional-order derivatives were born almost at the same time.

After the letter of 1695, there were many other letters written regarding this subject. In 1697, G.W. Leibniz sent letter to J. Wallis and J. Bernoulli and mentioned the possibility of fractional-order differentiation, that for non-integer value of n is

$$\frac{d^n e^{ax}}{dx^n} = a^n e^{ax}.$$

After Leibniz died, several other authors devoted their time to this subject. In this sequence, Leonard Euler contributed to the generalization of fractional differential calculus. Daniel Bernoulli generalized the notion of factorial $n!$ to non-integer values, which is called Gamma function $\Gamma(\cdot)$.

Between 1810 and 1819, Sylvestre Francois Lacroix, the French mathematician used Euler's derivation for his textbook 'Traite du Calcul Diferentiel et du Calcul Integer' [29]. Lacroix generalized the derivative from integer-order to arbitrary order α of x^β as

$$\frac{d^\alpha x^\beta}{dx^\alpha} = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha+1)} x^{\beta-\alpha}. \tag{1.15}$$

In 1822, Joseph Fourier generalized the notion of differentiation for arbitrary function through his book [30]. Until 1822, there were no attempts to describe physical phenomena of generalized arbitrary derivatives like integer-order derivatives only interest was on to set the basis of fractional differential calculus.

Niels Henrik Abel in 1823, applied the fractional differential calculus in the solution of the tautochrone problem [31]. Later in 1832, Liouville presented two different definitions for fractional derivatives [32]. The first definition is based on a series that means he expanded the function $f(x)$ in the ‘form of series as

$$f(x) = \sum_{n=0}^{\infty} C_n e^{a_n x}, \tag{1.16}$$

whose arbitrary α order derivative is

$$D^{\alpha} f(x) = \sum_{n=0}^{\infty} C_n \, a_n^{\alpha} \, e^{a_n x}, \tag{1.17}$$

which is restricts the series that depends on the order of differentiation to be convergent. According to the second definition of fractional derivative, it was applied to the function of the form $x^{-\alpha}$ with $a > 0$. He considered $I = \int_0^{\infty} u^{a-1} e^{-xu} \, du$. after transformation $xu = t$, it gives

$$x^{-a} = \frac{1}{\Gamma(a)}.I.$$

Applying the derivative operator D^{α} on both sides of the equation and using equation (1.15), we get

$$D^{\alpha} x^{-a} = \frac{(-1)^{\alpha} \Gamma(a+\alpha)}{\Gamma a} x^{-a-\alpha}. \tag{1.18}$$

The disadvantage of second definition is that it is not suitable to a wide class of function.

The main difference between Lacroix and Liouville definitions on fractional derivative is that according to Lacroix definition fractional derivative of constant gives a non zero value, while other one gives zero. This leads to a great discussion in the 19*th* century, regarding whose definition was the correct one.

Following the timeline, B. Riemann was the next well known mathematician to present a definition for the fractional derivative. The idea of Liouvill's influenced, Riemann with his memoirs in which Liouville wrote the ordinary differential equation $\dfrac{d^n y(x)}{dx^n} = 0$ has the complementary solution

$$y_c = c_0 + c_1 x + c_2 x^2 + \cdots + c_{n-1} x^{n-1}.$$

Thus Riemann tried to find the solution $y(x)$ of $\dfrac{d^n y(x)}{dx^n} = f(x)$, where $f(x) \in C[d, e]$ by setting $y^{(k)}(a) = 0$, $a \in (d, e)$ with $0 \leq k \leq n-1$. The solution obtained is unique and given by

$$y(x) = \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} f(t) dt.$$

By extending this to non-integer order α we have Riemann-Liouville definition of fractional order integral as

$$y(x) = J_x^\alpha f(x) = \frac{1}{\Gamma\alpha} \int_a^x (x-t)^{\alpha-1} f(t) dt; \alpha \geq 0,$$

and the fractional order derivative be

$$aD_x^\alpha f(x) = \frac{d^n}{dx^n} aJ_x^{(n-\alpha)} f(x).$$

Consequently, In 1892, Hadamard [33] had given definition for both fractional order integral and derivative. In 1917, Weyl [34] had formulated similar definition to the Riemann-Liouvill definition, but with different Kernel function $(t-x)^{\alpha-1}$ and different terminals of integration. Grunwald [35] and Post [36] had formulated fractional derivative as the limit of a sum, with the help of classical definition of a derivative. In 1927, Marchaud [37] proposed an equivalent fractional derivative of arbitrary order.

An important role was played by Mittage-Leffler function for the generalization of e^x in fractional calculus which was given in 1903. Erdelyi-Kober fractional integral was presented by Erdeyi [38] and Kober [39], which was generalized the Riemann fractional integral and the Weyl integral. Riesz also formulated fractional integral which was successfully used in potential theory. In 1967, M. Caputo introduced a definition known as the Caputo fractional derivative, which is obtained by computing an ordinary derivative followed by the fractional integral.

There are many other definitions exist in the literature [40]. In 1927, Davis [41] shows the benifits from using fractional calculus for functional equations. In 1938, [42] used the Riemann-Liouville and Weyl integral to develop the fractional version of the integration by parts. In 1967, Love [43] devised explit solutions for two integral equations, and also showed necessary and sufficient conditions for existence and sufficient condition for uniqueness of solution. Later in 1971, he extended the properties of the fractional calculus of real order to complex order [44].

For the first conference the credit is due to B. Ross, who shortly after his PhD dissertation on fractional calculus, organized the first conference on Fractional calculus at the University of New Haven in June 1974, and edited its proceedings. One of the important papers was by Campos [45], where a generalization of both the Weyl and Cauchy integrals had been devised. In 1987, the monograph of S. Sanko, A. Kilbas and O. Marichev were referred as "encyclopedia" of fractional calculus, appeared first in Russian later in English edition in 1993. Nowadays, the series of books, journals and texts devoted to fractional calculus and its applications and this list is expected to grow up yet more, in the forthcoming years. But what is the importance of fractional calculus in physical phenomena until recent days, this was regarded as a secret mathematical theory without application of fractional calculus, but in the last few decades there have been lot of research activities on the applications of fractional calculus to very vicarious scientific fields ranging from the physics of diffusion and advection phenomena to control system to finance and economics. Indeed, at present applications related to fractional calculus one found in the areas viz., fractional control of engineering systems, advancement of calculus of variations, optimal control to fractional dynamic system, fundamental explorations of the mechanical, electrical, and thermal constitutive relations and also in various engineering materials such as viscoelastic polymers, foams, gels, and animal tissues, and their engineering and scientific applications, fundamental understanding of wave and diffusion phenomena, application to plasma physics, bio-engineering systems such as brakes and machine tools, image and signal processing etc.

1.5 Fractional-order reaction-advection- diffusion equation

The fractional-order form of the RADE has not yet been studied much. In this thesis, author has mainly investigated numerical solutions of fractional-order reaction-advection-dispersion equation (FRADE) and analyses the solution profile of the considered problems. The growing interest in FRADE is because of their useful applications in the areas like electro magnetics, robotics and controls, acoustics, viscoelastic damping and electro chemistry and in material science, which have motivated the researchers to take up this exercise. The FRADE is promising for an accurate description of the transportation of solute in complex media such as a porous aquifer. In the real world, FRADE has comprehensive applications in engineering, physics, economics, etc. due to the non-local property of fractional order derivative. Because of this property, FRADE has much more memory effect compared to integer order RADE. FRADEs in time, space, time-space have been extensively applied in describing physical and engineering problems such as anomalous diffusion, medicine, biology, solute transport, random and disordered media, control, signal processing and so on. To describe and understand the dispersion phenomena, time, space, time-space FRADEs have fundamental importance and have received considerable attention in recent years. The researchers and engineers are actively engaged to find the solution of RADE in fractional-order system due to its greater flexibility in models, non-local behavior and ultimate convergence to the integer-order system. Through the literature survey, few methods are found for solving FRADE like variable transformation method, Green function method, the implicit and explicit difference methods and the Adomian decomposition method.

In recent years, there are intensive study on fractional calculus for its major applications in various fields viz., chemical, physical, biological, geological and financial systems. For example, the mathematical model on fractional diffusion describes nondiffusive transport in plasma turbulence [46] and a nonlinear fractional diffusion model for capillary flow through porous media [47]. Fractional calculus gives more accurate models of systems under consideration. Using fractional derivative as a mathematical tool to get the development of more robust mathematical model in particular areas of reservoir engineering, is gaining attention in both industry and academic. A realistic model of a physical phenomenon which is not only dependence on time instant, but also the previous time history can be achieved by using fractional order derivative in the place of integer order. In particular, the microscopic behaviours of mass transportation in porous media are complex and the physical phenomena show strange kinetics which cannot be modeled by classical diffusion equation whereas fractional diffusion equation explains their microscopic dynamics.

Due to the complex structure of fractured porous media, it is considered as a fractal. Thus particles those will be migrated along fractures at pore channels will behave as complex motion and as a result, the force field becomes stochastically distributed fracture. Thus the diffusion equation in the porous media will behave similar to the equation of anomalous diffusion. The fractional diffusion equation was first derived for the media of fractal geometry by Nigmatullin [48, 49, 50] to find better mathematical models for real-world problems. The study on the anomalous diffusion of a contaminants from Fracture into Porous Rock Matrix can be found in [51].

The fractional order transport equations within Liouville equations have been considered [52, 53]. Uchaikin and Sibatov [54] have solved the fractional-order transport equation in disordered semiconductors. Later, Kadem and Baleanu [55] have investigated the solution of the fractional order transport equation. The fractional order transport equations are also reported in [56] based on Levy stable processes. The anomalous transport in fractional order system has been considered in the research articles [57, 58, 59]. The microscopic behaviours of mass transportation in porous media are complex and the physical phenomena show strange kinetics which cannot be modeled by classical diffusion equation whereas fractional diffusion equation explains their microscopic dynamics. The fractional order form of the law of conservation of mass is described in the research article of Wheatcraft and Meerschaert [60] where the need of the fractional conservation of mass equation is described to model the fluid flow. The fractional order form of groundwater flow problem can be seen in [61, 62] in which they have 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.* [63, 64] have explained that the fractional order form of advection-diffusion equation is useful for contaminant flow in heterogeneous porous media and earth surfaces such as natural rivers.

Elementary particles perform complex motion due to the effect of various force fields of various motions and as a result trajectories of the particles reproduce geometrical objects of complex structure. In this case, it will never follow the Gaussian distribution and the traditional Fick's law cannot be used towards modeling of the diffusion equation. For deviation from the traditional Darcy's law, various strategies have been adopted, among those the most realistic approach is the continuous time random walk (CTRW) approach, where the mean squared displacement of the particles is described by the nonlinear power law $\langle x^2(t)\rangle \approx t^{\alpha}, 0 < \alpha \leq 1$. The conventional relation for the standard order diffusion process can be recovered through $\alpha = 1$.

1.6 Mathematical preliminaries

In this section, some notations and definitions are given which are used in the thesis.

1.6.1 Riemann–Liouville operator

Definition: The Riemann–Liouville fractional integral operator of order $\alpha > 0$ of a function $f(x) \in [a, b]$ is defined by [65, 66]

$$J_x^{\alpha} f(x) = \frac{1}{\Gamma\alpha}\int_0^x (x-\xi)^{\alpha-1} f(\xi) d\xi, \alpha > 0, x > 0,$$
$$J_x^0 f(x) = f(x).$$

The Riemann-Liouville fractional derivative operator is denoted by $D_x^{\alpha} f(x)$ and defined by

$$D_x^{\alpha} f(x) = \frac{1}{\Gamma(1-\alpha)}\frac{d}{dt}\int_a^x \frac{f(\xi)}{(x-\xi)^{\alpha}} dx, \alpha \in (0,1). \tag{1.19}$$

In general,

$$D_x^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_0^x \frac{f(\xi)}{(x-\xi)^{\alpha-n+1}} d\xi.$$

Properties of Riemann–Liouville operator

1. $J_x^\alpha J_x^\beta f(x) = J_x^\beta J_x^\alpha f(x)$.

2. $J_x^\alpha J_x^\beta f(x) = J_x^{\alpha+\beta} f(x)$.

3. $J_x^0 f(x) = f(x)$.

4. $J_x^\alpha x^p = \dfrac{\Gamma(p+1)}{\Gamma(\alpha+p+1)} x^{\alpha+p}$.

1.6.2 Caputo fractional derivative

Definition: The definition of the Caputo fractional derivative which is frequently appeared in the porous media literature is defined by [65]

$$D^\alpha f(x) = \begin{cases} \dfrac{1}{\Gamma(n-\alpha)} \int_0^x \frac{f^{(n)}(t)}{(x-t)^{\alpha+1-n}} dt, & \text{if } n-1 < \alpha < n, \\ \dfrac{d^n f(x)}{dx^n}, & \text{if } \alpha = n \in N. \end{cases} \tag{1.20}$$

And $D^\alpha C = 0$, for a constant C.

Therefore, it follows that

$$D^\alpha x^\beta = \begin{cases} 0, & \text{if } \beta \in N_0 \text{ and } \beta < \lceil \alpha \rceil \\ \dfrac{\Gamma(\beta+1)}{\Gamma(\beta+1-\alpha)} x^{\beta-\alpha}, & \text{if } \beta \in N_0 \text{and} \beta \geq \lceil \alpha \rceil \text{ or } \beta \notin N \text{and} \beta > \lfloor \alpha \rfloor, \end{cases} \tag{1.21}$$

where $\lceil \alpha \rceil$ is ceiling function and $\lfloor \alpha \rfloor$ is floor functions are define later.

Properties of Caputo fractional derivative

1. Let $f \in C^n_{-1}, n \in N \cup 0$ then $D^\alpha f(x), 0 \leq \alpha \leq n$ is well defined and $D^\alpha f(x) \in C_{-1}$.

2. If $n-1 \leq \alpha, n \in N$ and $f(t) \in C^n_m, m \geq -1$, then $(J^\alpha_x D^\alpha) f(x) = f(x) - \sum_{k=0}^{n-1} f^k(0+) \dfrac{x^k}{k!}, x \geq 0$.

1.6.3 Laplace transformation

Definition: Let $f(t)$ is a piecewise continuous function on every finite interval on semi-axis $(t \geq 0)$ and there exist some constants M and p such that $|f(x)| < M\, e^{p\,t}$, for all $t \geq 0$, then Laplace transformation $F(s) = L[f(t)]$ exists for all $s > c$ and defined by [67]

$$L[f(t)] = \int_0^\infty f(t)\, e^{-st} dt.$$

1.6.4 Inverse Laplace transformation

Definition: An integral formula for the Inverse Laplace transform, called the Mellin's inverse formula, is defined through the Bromwich integral is given by the line integral:

$$f(t) = L^{-1}[F(s)] = \frac{1}{2\pi i} \lim_{T\to\infty} \int_{\gamma - iT}^{\gamma + iT} F(s)\, e^{st} ds,$$

where the integration is done along the vertical line $Re(s) = \gamma$ in the complex plane such that γ is greater than the real part of all singularities of $F(s)$ and $F(s)$ is bounded on the line.

1.6.5 Floor and Ceiling functions

The Floor of a real number α, denoted by $\lfloor \alpha \rfloor$, is the largest integer that is less than or equal to α. It is expressed express in the following way

$$\lfloor \alpha \rfloor = \max\{n : n \in Z, n \leq \alpha\}.$$

The Ceiling of a real number α, denoted by $\lceil \alpha \rceil$, is the smallest integer that is greater than or equal to α. It is expressed as

$$\lceil \alpha \rceil = \min\{n : n \in Z, n \geq \alpha\}.$$

1.6.6 Kronecker product

Definition: Let two matrices P of order $m \times n$ and Q of order $p \times q$ then the Kronecker product of P and Q is denoted by $P \otimes Q$, which is the $mp \times nq$ matrix having the following block structure [68]

$$P \otimes Q = \begin{pmatrix} p_{11}Q & p_{12}Q & \cdots & p_{1n}Q \\ p_{21}Q & p_{22}Q & \cdots & p_{2n}Q \\ \vdots & \vdots & \vdots & \vdots \\ p_{m1}Q & a_{m2}Q & \cdots & p_{mn}Q \end{pmatrix}. \tag{1.22}$$

where

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ p_{m1} & a_{m2} & \cdots & p_{mn} \end{pmatrix}, \; Q = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & q_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ q_{m1} & q_{m2} & \cdots & q_{mn} \end{pmatrix}.$$

1.6.7 Error function and complementary error function

Error function denoted by $erf(t)$ and defined as

$$erf(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-x^2}\, dx,$$

with $erf(-\infty) = -1$ and $erf(\infty) = 1$.

The complementary error function $erfc(t)$ is defined as

$$erfc(t) = 1 - erf(t) = \frac{2}{\sqrt{\pi}} \int_t^\infty e^{-x^2}\, dx.$$

1.7 Numerical methods

1.7.1 Finite difference method

The finite difference method (FDM) is one of the oldest numerical methods which is applied to find the solution of differential equations. In 1768, Hirsch [69] sites Euler as being the first to use FDM. The FDM is a simple approach, based on the properties of Taylor series expansions and of, the subsequent application of the definition of its derivatives [69, 70]. There are several options for the solution of such a scheme, some of which are described in details in the articles [69, 70, 71, 72].

In general with the governing equations for unsteady fluid flow, our mathematical model equations contain partial derivative with respect to both time and space. The finite difference method replaced PDEs with finite difference equations, in terms of spatial and temporal grid co-ordinates. By this replacement, the method converts the PDEs written as a continuum function to an arithmetic representation, which allows the equation to be solved more easily [73]. The finite difference equations link the values of dependent variables at a set of points such that, a grid of points is used to represent the continuous physical domain. The resulting numerical scheme is therefore based upon values defined at predetermined grid points.

This method requires use of a regular grid and to facilitate explanation of the approach, and it will be considered that it is uniform, although this is not essential. The grid must be constructed such that the nodal points are located at the intersection of either curved lines or rectilinear. These lines appear as a set of numerical coordinates, which is illustrated in one-dimension.

1.7.1.1 Construction of the method

Difference approximations may be constructed in various ways, among which Taylor's formula is probably the simplest one to serve our present purposes. First, the region is discretized into finite grids as shown in Figure 1.3. Now consider the space-time region such that space $x \in [0, L]$ is discretized by dividing the length of the intervals into M equal subintervals of length h and then the time t is discretized with time spacing $k > 0$ such that $t_{j+1} = t_j + k$ with $t_0 = 0$. The partial derivatives in the PDEs at each grid point are approximated from the neighbouring values by using Taylor's theorem [74]. Next the values of dependent variables at each and every internal grid point are calculated using the given initial and boundary conditions. FDM requires more grid points to achieve reasonable accuracy.

1.7.1.2 Finite Difference approximation of derivatives

In the finite difference approximation the notations used are h is the spatial step, k is the time step, $x_i = a + ih, i = 0, 1, 2, \cdots, M$ points are the coordinates of the mesh and $M = \frac{(b-a)}{h}, t_j = jk, j = 0, 1, 2, \cdots, N, N = \frac{T}{k}$. The values of the solution $u(x, t)$ at these grid points are given by $u(x_i, t_j) \simeq u_i^j$, where u_i^j are the numerical estimates of the exact value of $u(x, t)$ at the point (x_i, t_j).

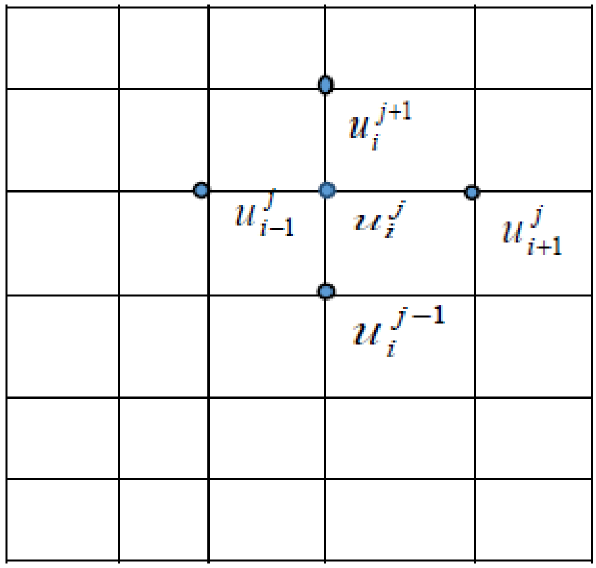

Figure 1.3: A partition of the $(x, t)-$ plane into uniform cells of size $h \times k$.

The forward space and time difference schemes are

$$\frac{\partial u}{\partial x}(x_i, t_j) \simeq \frac{u_{i+1}^j - u_i^j}{h}, \tag{1.23}$$

$$\frac{\partial u}{\partial t}(x_i, t_j) \simeq \frac{u_i^{j+1} - u_i^j}{k}, \tag{1.24}$$

and the backward difference schemes for space and time are given by

$$\frac{\partial u}{\partial x}(x_i, t_j) \simeq \frac{u_i^j - u_{i-1}^j}{h}, \tag{1.25}$$

$$\frac{\partial u}{\partial t}(x_i, t_j) \simeq \frac{u_i^j - u_i^{j-1}}{k}. \tag{1.26}$$

Forward and backward difference approximations are first order accuracy in x and t. Another finite difference approximation of second order accuracy which is central difference scheme given by the relations:

$$\frac{\partial u}{\partial x}(x_i, t_j) \simeq \frac{u_{i+1}^j - u_{i-1}^j}{2h}, \tag{1.27}$$

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_j) \simeq \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2}. \tag{1.28}$$

One can also approximate higher order derivative using finite difference approximation [75].

1.7.2 Bellman method

If $f(t)$ is sufficiently smooth function to permit the approximate method, then substituting $e^{-t} = x$ in

$$F(s) = L[f(t)] = \int_0^\infty f(t)\, e^{-st} dt,$$

we obtain

$$F(s) = \int_0^1 x^{s-1} C(x)\, dx, \tag{1.29}$$

where $C(x) = f(-ln(x))$.

Applying the Gaussian quadrature formula to equation (1.29), we get

$$F(s) = \sum_{i=1}^{N} w_i \, x_i^{s-1} C(x_i), \tag{1.30}$$

where $x_i^{'}\text{s}\,(i = 1, 2, 3, \cdots, N)$ are the roots of the shifted Legendre polynomial $P_N(x) = 0$ and $w_i^{'}\text{s}\,(i = 1, 2, 3, \cdots, N)$ are corresponding weights of the equation

$$F(s) = w_1 x_1^{p-1} C(x_1) + w_2 x_2^{p-1} C(x_2) + w_3 x_3^{p-1} C(x_3) + \cdots + w_N x_N^{p-1} C(x_N).$$

Substituting $p = 1, 2, \cdots, N$ in above equation, we obtain

$$\begin{aligned}
&w_1 C(x_1) + w_2 C(x_2) + w_3 C(x_3) + \cdots + w_N C(x_N) = F(1), \\
&w_1 x_1 C(x_1) + w_2 x_2 C(x_2) + w_3 x_3 C(x_3) + \cdots + w_N x_N C(x_N) = F(2), \\
&\cdots\cdots\cdots\cdots \\
&w_1 x_1^{N-1} C(x_1) + w_2 x_2^{N-1} C(x_2) + w_3 x_3^{N-1} C(x_3) + \cdots + w_N x_N^{N-1} C(x_N) = F(N),
\end{aligned} \tag{1.31}$$

which can be written in the matrix form as follows:

$$\begin{pmatrix} w_1 & w_2 & \cdots & w_{N-1} & w_N \\ w_1 x_1 & w_2 x_2 & \cdots & w_{N-1} x_{N-1} & w_N x_N \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ w_1 x_1^{N-1} & w_2 x_2^{N-1} & \cdots & w_{N-1} x_{N-1}^{N-1} & w_N x_N^{N-1} \end{pmatrix} \begin{pmatrix} C(x_1) \\ C(x_2) \\ \vdots \\ C(x_N) \end{pmatrix} = \begin{pmatrix} F(1) \\ F(2) \\ \vdots \\ F(N) \end{pmatrix}. \tag{1.32}$$

The discrete values of $C(x_i)$ are calculated from equation (1.32) and finally the function $f(t)$ can be calculated by using interpolation.

1.7.3 Shifted Legendre collocation method

1.7.3.1 Shifted Legendre polynomial

The Legendre Polynomials $p_n(x),\ n = 0, 1, 2, 3, \cdots$ are the eigenfunctions of the Strum-Liouville problem

$$\frac{d}{dx}[(1-x^2)y^{'}] - 2x\frac{dy}{dx} + n(n+1)y = 0, \qquad x \in [-1, 1], \tag{1.33}$$

with $P_n(1) = 1$.

The Legendre polynomials satisfy the recursion relations

$$P_{n+1}(x) = \frac{2n+1}{n+1}xP_n(x) - \frac{n}{n+1}P_{n-1}(x); \qquad n = 1, 2, 3, \cdots, \tag{1.34}$$

where $P_0(x) = 1$ and $P_1(x) = x$.

Here $P_n(x)$ is defined by the interval $[-1, 1]$. Let us defined the so-called shifted Legendre polynomial $P_n^l(z)$ on the interval $[0, l,]$ by introducing the change of a variable with $x = \dfrac{2z-l}{l}$, which gives rise to

$$P_{n+1}^l(z) = \frac{2n+1}{n+1}\frac{(2z-l)}{l}P_n^l(z) - \frac{n}{n+1}P_{n-1}^l(z); \qquad n = 1, 2, 3, \cdots, \tag{1.35}$$

where $P_0^l(z) = 1$ and $P_1^l(z) = \dfrac{(2z-l)}{l}$.

1.7.3.2 Properties of shifted Legendre polynomials

The analytical form of the shifted Legendre polynomials $P_n^l(x)$ is given by

$$P_n^l(x) = \sum_{k=0}^{n}(-1)^{n+k}\frac{(n+k)!\,x^k}{(n-k)!\,(k!\,)^2(l)^k}. \tag{1.36}$$

The orthogonality condition of the shifted Legendre polynomial [76] is

$$\int_0^l P_m^l(x)P_n^l(x)dx = \begin{cases} \dfrac{l}{2n+1}, & \text{if } m = n, \\ 0, & \text{if } m \neq n. \end{cases} \tag{1.37}$$

1.7.3.3 Shifted Legendre function approximation

Any piecewise continuous function $u(x)$ for $x \in [0, l]$ can be expressed in terms of shifted Legendre polynomials by using the orthogonality condition of shifted Legendre polynomials as

$$u(x) = \sum_{n=0}^{\infty} c_n P_n^l(x), \tag{1.38}$$

where $c_n = \dfrac{(2n+1)}{l} \int_0^l u(x)P_n^l(x)dx$.

In practice, only the first $(m+1)-$ terms of shifted Legendre polynomials are considered. So we have

$$u(x) \approx u_m(x) = \sum_{n=0}^{m} c_n P_n^l(x) = C^T \phi_{m,l}(x), \tag{1.39}$$

where $C^T = [c_0, c_1, c_2, \cdots, c_m]^T$ is the shifted Legendre coefficient vector and $\phi_{m,l}(x) = [P_0^l(x), P_1^l(x), P_2^l(x), \cdots, P_m^l(x)]^T$ is the shifted Legendre vector.

Similarly, a function $u(x,t)$ defined in $0 \leq x \leq l$ and $0 \leq t \leq \tau$ can expressed in terms of shifted Legendre polynomials as

$$u(x,t) \approx u_{n,m}(x,t) = \sum_{i=0}^{n} \sum_{j=0}^{m} a_{i,j} P_i^{\tau}(t) P_j^l(x) = (\phi_{n,\tau}(t))^T . A . \phi_{m,l}(x), \tag{1.40}$$

where A is the unknown matrix of order $(n+1) \times (m+1)$ and a_{ij} can be obtained by the relation.

$$a_{i,j} = \frac{(2i+1)}{\tau}\frac{(2j+1)}{l}\int_0^l \int_0^\tau u(x,t)P_i^\tau(t)P_j^l(x)dxdt,$$

Let $u(x,y,t) \in C([0,l]\times[0,l]\times[0,\tau])$ is approximated by shifted Legendre polynomials $P_{ijk}(x,y,t)$ as

$$\begin{aligned} u(x,y,t) \approx u_{m,m,n}(x,y,t) &= \sum_{i=0}^{m}\sum_{j=0}^{m}\sum_{k=0}^{n} u_{ijk}P_{ijk}(x,y,t) \\ &= (\phi_{n,\tau}(t))^T.U.(\phi_{m,l}(x)\otimes\phi_{m,l}(y)), \end{aligned} \tag{1.41}$$

where U is the unknown matrix of order $(n+1)\times(m+1)^2$, $P_{ijk}(x,y,t) = P_i^l(x)P_j^l(y)P_k^\tau(t)$ and u_{ijk} can be obtained by the relation.

$$u_{ijk} = \frac{(2i+1)}{l}\frac{(2j+1)}{l}\frac{(2k+1)}{\tau}\int_0^l\int_0^l\int_0^\tau u(x,y,t)P_i^l(x)P_j^l(y)P_k^\tau(t)dxdydt. \tag{1.42}$$

The Kronecker product of $\phi_{m,l}(x)$ and $\phi_{m,l}(y)$ is the function vector $(\phi_{m,l}(x)\otimes\phi_{m,l}(y))$ of order $(m+1)^2\times 1$ defined as

$$\begin{aligned} (\phi_{m,l}(x)\otimes\phi_{m,l}(y)) = (\phi_{11}(x,y),\cdots,\phi_{1(m+1)}(x,y),\phi_{21}(x,y),\cdots,& \\ \phi_{2(m+1)}(x,y),\cdots,\phi_{(m+1)(m+1)}(x,y))^T,& \end{aligned} \tag{1.43}$$

where $\phi_{(i+1)(j+1)}(x,y) = P_i(x),P_j(y)$ and $i,j = 0,1,2,\cdots,m$.

1.7.3.4 Generalized shifted Legendre operational matrix

The derivative of the vector can be expressed by Canuto *et al.* [77] as

$$\frac{d\phi_{m,l}(x)}{dx} = D^{(1)}\phi_{m,l}(x), \tag{1.44}$$

$$\frac{d^k\phi_{m,l}(x)}{dx^k} = (D^{(1)})^k\phi_{m,l}(x), \qquad k = 1, 2, 3, \cdots, n, \tag{1.45}$$

where $D^{(1)}$ is the $(m+1)\times(m+1)$ operational matrix defined by

$$D^{(1)} = (d_{i,j}) = \begin{cases} 4m-2, & \text{for } m = n-i, \begin{cases} i = 1, 3, \cdots, k, \text{when k is odd number}, \\ i = 1, 3, \cdots, (k-1), \text{k is even number}, \end{cases} \\ 0, & \text{otherwise .} \end{cases} \tag{1.46}$$

Saadatmandi and Dehghan [28] have generalized the operational matrix of derivative of shifted Legendre polynomials to the fractional-order derivative in the Caputo sense, which is denoted by $D^{(\alpha)}$ and defined by $D^{\alpha}\phi_{m,l}(x) = D^{(\alpha)}\phi_{m,l}(x)$, where

$$D^{(\alpha)} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \\ \sum_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} \kappa_{\lceil\alpha\rceil,0,k} & \sum_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} \kappa_{\lceil\alpha\rceil,1,k} & \cdots & \sum_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} \kappa_{\lceil\alpha\rceil,m,k} \\ \sum_{k=\lceil\alpha\rceil}^{i} \kappa_{i,0,k} & \sum_{k=\lceil\alpha\rceil}^{i} \kappa_{i,1,k} & \ddots & \sum_{k=\lceil\alpha\rceil}^{i} \kappa_{i,m,k} \\ \vdots & \vdots & \cdots & \vdots \\ \sum_{k=\lceil\alpha\rceil}^{m} \kappa_{m,0,k} & \sum_{k=\lceil\alpha\rceil}^{m} \kappa_{m,1,k} & \ddots & \sum_{k=\lceil\alpha\rceil}^{m} \kappa_{m,m,k} \end{pmatrix}, \tag{1.47}$$

with

$$\kappa_{i,j,k} = \frac{2j+1}{h^{k+1}} \sum_{i=0}^{j} \frac{(-1)^{i+j+k+l}(i+k)!\,(l+j)!}{(i-k)!\,k!\,\Gamma(k-\alpha+1)(j-l)!\,(l!\,)^2(k+l-\alpha+1)}.$$

It is to be noted that in $D^{(\alpha)}$, the first $\lfloor \alpha \rfloor$ rows are all zeros.

For instance, if $\alpha = 0.8, m = 7$, we have

$$D^{(0.8)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1.81521 & 0.495057 & -0.206274 & 0.123764 & -0.0856829 & 0.0641854 & -0.0505703 & 0.0412722 \\ -0.495057 & 4.08422 & 1.06084 & -0.466496 & 0.292585 & -0.209447 & 0.160962 & -0.129386 \\ 1.60893 & -0.565779 & 5.9026 & 1.64087 & -0.752105 & 0.485751 & -0.355496 & 0.27798 \\ -0.618821 & 3.61772 & -0.456273 & 7.51576 & 2.22412 & -1.05229 & 0.694344 & -0.516407 \\ 1.52325 & -0.858364 & 5.23618 & -0.290666 & 9.00084 & 2.80684 & -1.36175 & 0.9136 \\ -0.683006 & 3.40827 & -0.877839 & 6.67292 & -0.0969687 & 10.3949 & 3.38749 & -1.67747 \\ 1.47268 & -1.01933 & 4.93125 & -0.824048 & 7.99458 & 0.1137 & 11.7196 & 3.96537 \end{pmatrix}. \tag{1.48}$$

The fractional-order derivative D^{α} of the function $x^{2.2}$ is to verify the corresponding operational matrix $D^{(\alpha)}$. The fractional- order derivative of the function $f(x) = x^{2.2}$ in Caputo sense is calculated as

$$D^{\alpha} f(x) = \frac{\Gamma(3.2)}{\Gamma(3.2-\alpha)} x^{2.2-\alpha}. \tag{1.49}$$

When $m = 7$ the comparison of the results for fractional-order derivative $\alpha = 0.8$ is shown in Figure 1.4.

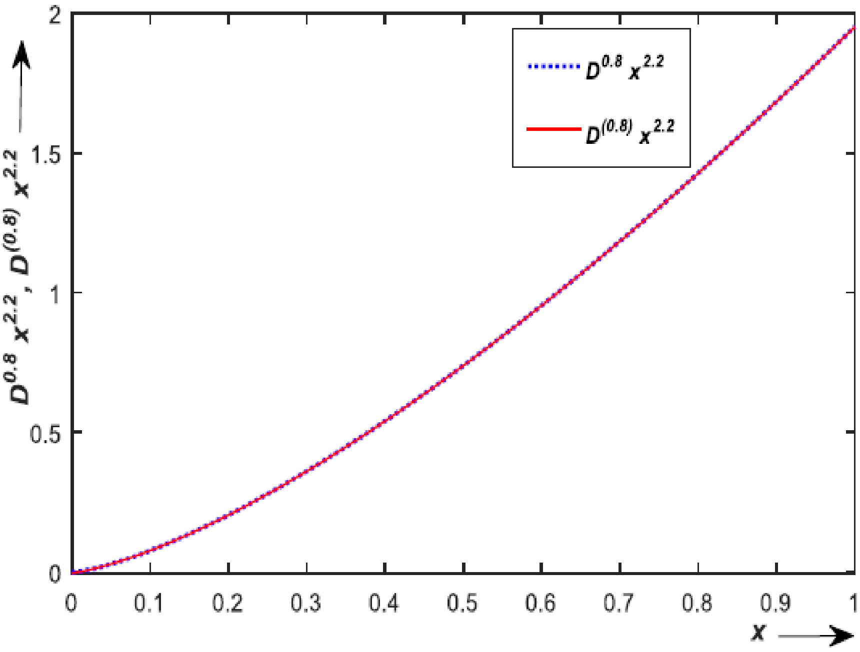

Figure 1.4: Comparison between Caputo fractional derivative and shifted Legendre operational matrix.

In the case of two-dimensional space function, $(\phi_{m,l}(x) \otimes \phi_{m,l}(y))$ be the function vector, which is defined in equation (1.43), then the fractional partial derivative of order $\beta > 0$ with respect to x and y are given by using the properties of the Kronecker product [78] as

$$D_x^{\beta}(\phi_{m,l}(x) \otimes \phi_{m,l}(y)) \approx (D^{(\beta)} \otimes I)(\phi_{m,l}(x) \otimes \phi_{m,l}(y)), \tag{1.50}$$

$$D_y^{\beta}(\phi_{m,l}(x) \otimes \phi_{m,l}(y)) \approx (I \otimes D^{(\beta)})(\phi_{m,l}(x) \otimes \phi_{m,l}(y)), \tag{1.51}$$

where $D^{(\beta)}$ and I are an operational matrix of derivative $\beta > 0$ and identity matrix of order $(m+1) \times (m+1)$ respectively.

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