

# Chapter 3

## Numerical solution of fractional-order advection-reaction-diffusion equation

### 3.1 Introduction

It is known to us that the process diffusion is a physical process where molecules of a material move from an area of high concentration to an area of low concentration. The word had been derived from the Latin word *diffundere*, which means spread out of a substance from an area of high concentration to an area of low concentration. An important feature of diffusion is that it is dependent on particle random walk. Diffusion usually occurs in a solution in gas or in a liquid. It describes the constant movement of particles in all directions bumping into each other in all kinds of liquids and gases.

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Diffusion is important to living things as it explains how useful materials and waste products can move from high concentration to the low concentration of the cells. We know that the quantity of  $O_2$  is more in lung than in the blood, while there is more  $CO_2$  molecules in the blood than in the lung. So  $O_2$  molecules will tend to move from lung into the blood, whereas  $CO_2$  molecules will tend to move into the lung from blood. In cell biology, the small molecules are simply diffused through the cell membrane, but larger molecules only get through using energy.

The spontaneous movement of particles occurring due to the difference of concentration between substances or molecules between two areas (along the concentration gradient) is relative to the phenomena of diffusion. In biology, diffusion is a type of passive transport which means that it is a net movement of molecules in and out of the cell through the cell membrane. Diffusion does not involve chemical energy unlike the case of active transport. Facilitated diffusion occurs when molecules diffuse via special transport proteins found within the membrane.

Physically the diffusion or advection-diffusion equation becomes useful to investigate the catalytic processes in regular, heterogeneous, or disordered systems [97, 98]. Another example is an irreversible first-order reaction of transported substance so that the rate of removal is proportional to the field variable as given by Crank *et al.* [99]. The above type of anomalous diffusion is a ubiquitous phenomenon in nature and appears in different branches of science and engineering.

Einstein's theory of Brownian motion reveals that the mean square displacement of a particle moving randomly is proportional to time. But after the advancement of fractional calculus, it is seen that the mean square displacement for an anomalous diffusion equation having time fractional derivative grows slowly with time. For the simple fractional order diffusion equation ( $\partial^\alpha u / \partial t^\alpha = \partial^2 u / \partial x^2$ ), the mean square displacement is  $X^2(t) \approx t^\alpha$ , where  $0 < \alpha < 1$  is the anomalous

diffusion exponent. An important characteristic of this evolution equation is that it generates the fractional Brownian motion, a generalization of Brownian motion. If we replace the integer order with fractional order time derivative, it changes the fundamental concept of time and thus the concept of evolution in the foundations of physics. The fractional order derivative has a physical meaning related to the statistics of waiting times according to the Montroll-Weiss theory. The relation was established by R. Hilfer through his two research articles. Through the first one, Hilfer and Anton [100] showed that Montroll-Weiss continuous time random walks with a Mittag-Leffler waiting time density are rigorously equivalent to a fractional master equation. After that through the other article [101] explained that this underlying random walk the model is connected to the fractional time diffusion equation in the usual asymptotic sense of long times and large distances. Thus for simulating diffusive phenomena of a simple model it needs the random walk approach.

Gorenflo *et al.* [102] have given an important result stating that the time fractional diffusion of order  $\alpha$ ,  $0 < \alpha < 1$  generates a class of symmetric densities whose moments of order  $2m$  are proportional to the  $m\alpha$  power of time. We thus obtain a class of Non-Markovian stochastic processes, which exhibits a variance consistent with slow anomalous diffusion. Metzeler *et al.* [57] have shown that anomalous diffusion is based upon Boltzman statistics using fractional order Fokker-Plank equation approach. Many researchers have used fractional equations during description of Levy flights or diverging diffusion. Since ultimate behavior of the fractional order system response converges to the response of the integer-order version of the model, therefore the fractional calculus is known as the extension of classical mathematics. In the last two decades, fractional differential equations have been widely used by the researchers not only in science and engineering but also in economics and finance. It is also a powerful tool in modeling multi scale problems,

characterized by wide time or length scale. The attribute of the fractional order differential operator is its non-local property, which takes into account the fact that the future state not only depends upon the present state but also upon all of the history of its previous states. Nowadays, the fractional order system has gained popularity in the investigation of dynamical system since it allows greater flexibility in the model.

Before penetrating from mathematics of fractional calculus to the physical systems, one should have to keep in mind two things, firstly to analyze the importance and physical influence of the memory effects on time and secondly to give proper interpretation of general meaning of non integer operator. The main advantage of the fractional calculus is that it provides an excellent instrument for the description of memory effect of various materials and processes. Fractional derivatives and integrals are useful to explore the characteristic features of anomalous diffusion, transport and fractal walks through setting up of fractional kinetic equations, which are very much useful in the context of anomalous sub-diffusion [58]. The fractional diffusion equation, which demonstrates the occurrence of anomalous sub-diffusion, had already been given an intensive effort to find the accurate solution in straight forward manner [103]. The fractional diffusion equation is useful to describe reactions in the dispersive transport media [104]. Anomalous diffusion processes occur in many physical systems for various reasons including disorder in terms of energy or space or both [105]. Fractional reaction-diffusion equations or continuous time random walk models are also introduced for the description of propagating fronts and two species reactions in sub-diffusive transport media [106]. Chen *et al.* [107] have proposed an implicit difference approximation scheme (IDAS) for solving fractional diffusion equation. Schot *et al.* [108] have given an approximate solution of the diffusion equation in terms of Fox H-function. Zahran [109] has given a closed form

solution in terms of Fox H-function of the generalized fractional reaction-diffusion equation. Many research on fractional order diffusion equations have already been done in [110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124].

Analytic inversion of the Laplace transform is defined as contour integration in the complex plane employing the Cauchy's residue theorem by taking the Bromwich contour. For complicated  $F(s) = L[f(t)]$ , it is too difficult to perform even using symbolic softwares like MATLAB or MATHEMATICA. Therefore it is needed to study some alternative methods [125, 126, 127, 128, 129, 130, 131] to tackle the problem. Bellman *et al.* [131] proposed a numerical method known as to calculate the inverse Laplace transformation. The other popular methods are the Numerical integral method and the Fast Fourier Transform (FFT). The comparison of applicability and accuracy among these methods and the Bellman method was studied by Ueda [132]. In the Bellman method only a few values are sufficient for the inverting process. Therefore this method is useful to the problems that require long CPU time to calculate the values in the Laplace transformed domain. In both the Numerical integral method and FFT method, few parameters are required. In the first one much CPU time is required to invert the problem whereas in the second one it is carried out in less time through proper choices of suitable parameters. In the Bellman method the inverse Laplace transform is evaluated at the roots of the shifted Legendre polynomial with the help of Gaussian quadrature formula taking the corresponding weight function and finally the function  $f(t)$  can be calculated using interpolation.

In this chapter the author has made an endeavour to solve a non- conservative fractional order diffusion equation with boundary conditions through converting it in the frequency domain using Laplace transform technique. To get the solution in time domain, the Inverse Laplace transform is done using Bellman method. The

results obtained using the method for different particular cases clearly exhibit that the method is reliable and easy to implement to get the solution in the time domain.

## 3.2 Solution of the mathematical model

Let us consider the fractional order advection-diffusion equation with reaction term as

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2} - V \frac{\partial u(x, t)}{\partial x} - \lambda u(x, t), \quad 0 < \alpha < 1, \quad (3.1)$$

with  $u(x, 0) = 0$ ,  $u(0, t) = u_0$  and  $u(x, t)$  is finite.

Taking the Laplace transformation on both sides we get

$$\frac{\partial^2 \bar{u}(x, s)}{\partial x^2} - V \frac{\partial \bar{u}(x, s)}{\partial x} - (s^\alpha + \lambda) \bar{u}(x, s) = 0, \quad (3.2)$$

where

$$\bar{u}(x, s) = \int_0^\infty u(x, t) \exp^{-st} dt.$$

The solution of the equation (3.2) can be written as

$$\bar{u}(x, s) = c_1(s) e^{\frac{V|x|}{2}} e^{-\sqrt{s^\alpha + \lambda + \frac{V^2}{4}} \cdot |x|}.$$

Now,

$$\bar{u}(0, s) = c_1(s) = \int_0^\infty u_0 e^{-st} dt = \frac{u_0}{s}.$$

Therefore,

$$\bar{u}(x, s) = \frac{u_0}{s} e^{\frac{Vx}{2}} e^{-\sqrt{(s^\alpha + \lambda_1)} \cdot |x|}, \quad (3.3)$$

where  $\lambda_1 = \lambda + V^2/4$ .

Finally by applying inverse Laplace transformation, we get

$$u(x, t) = L^{-1} \left[ \frac{u_0}{s} e^{\frac{Vx}{2}} e^{-\sqrt{(s^\alpha + \lambda_1)} \cdot |x|} \right]$$

$$u(x, t) = u_0 \cdot e^{\frac{Vx}{2}} L^{-1} \left[ \frac{e^{-\sqrt{(s^\alpha + \lambda_1)} \cdot |x|}}{s} \right] \quad (3.4)$$

The  $2k - th$  moment of  $\bar{u}(x, s)$  is given by

$$M_{2k}(s) = 2 \int_0^\infty x^{2k} \bar{u}(x, s) dx = \frac{2u_0}{s} \int_0^\infty x^{2k} e^{-\left(\sqrt{(s^\alpha + \lambda_1)} - \frac{V}{2}\right)x} dx$$

$$= \frac{2u_0}{s} \cdot \frac{\Gamma(2k + 1)}{\left(\sqrt{s^\alpha + \lambda_1} - \frac{V}{2}\right)^{(2k+1)}} \quad (3.5)$$

Now considering

$$\left(\sqrt{s^\alpha + \lambda_1} - \frac{V}{2}\right)^{2k+1} = \left(\sqrt{s^\alpha + \lambda_1}\right)^{2k+1} \left(1 - \frac{V}{2\sqrt{s^\alpha + \lambda_1}}\right)^{2k+1}$$

$$\approx \left(s^\alpha + \lambda_1\right)^{\frac{(2k+1)}{2}} \approx s^{(2k+1)\frac{\alpha}{2}}.$$

Therefore,

$$M_{2k}(s) \approx \frac{2u_0\Gamma(2k+1)}{s^{\frac{\alpha}{2}}}. \quad (3.6)$$

Hence the 2k-th moments in the time domain are obtained as

$$M_{2k}(t) \approx \frac{2u_0\Gamma(2k+1)}{\Gamma((2k+1)\alpha/2+1)} t^{(2k+1)\alpha/2}. \quad (3.7)$$

Thus

$$\langle X^2(t) \rangle \approx t^{3\alpha/2}, \quad (3.8)$$

which clearly shows that the fractional order advection-reaction-diffusion equation represents an evolutionary process.

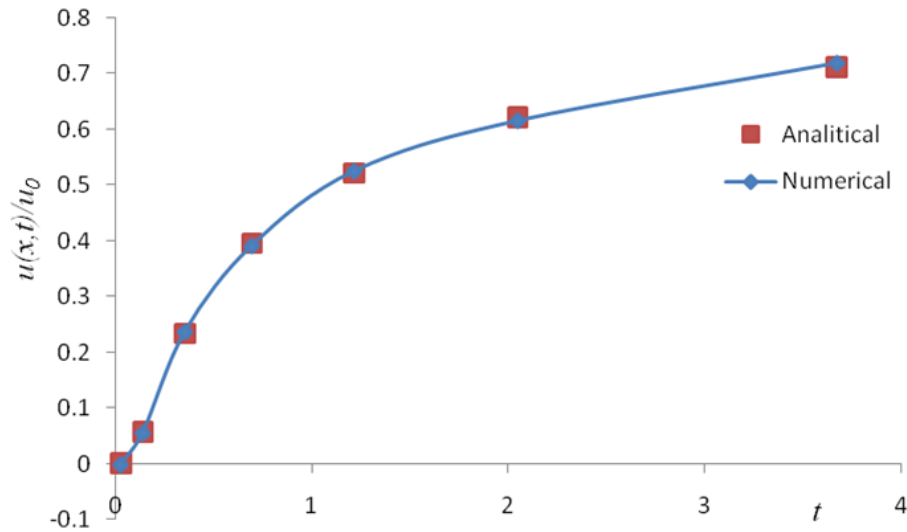
### 3.3 Results and discussion

The numerical values of the normalized field variable  $u(x,t)/u_0$  for various time and for different values of  $\alpha = 0.7, 0.8, 0.9, 1.0$  when  $u_0 = 1, x = 1$  and  $V = 0.6$  are calculated for both conservative and non-conservative systems using Bellman method. During numerical computation the variation of probability density function  $u(x,t)$  is compared with the existing analytical result for standard order diffusion equation i.e.,

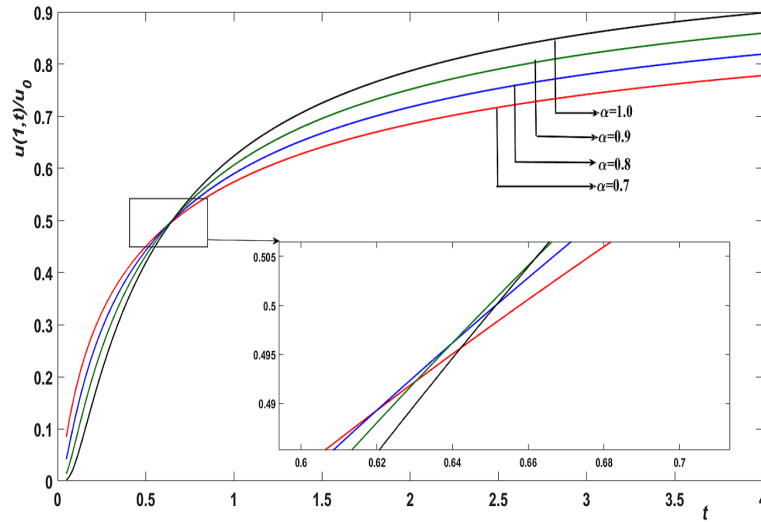
$$u(x,t) = u_0 \operatorname{erfc}\left(\frac{x}{2\sqrt{t}}\right),$$



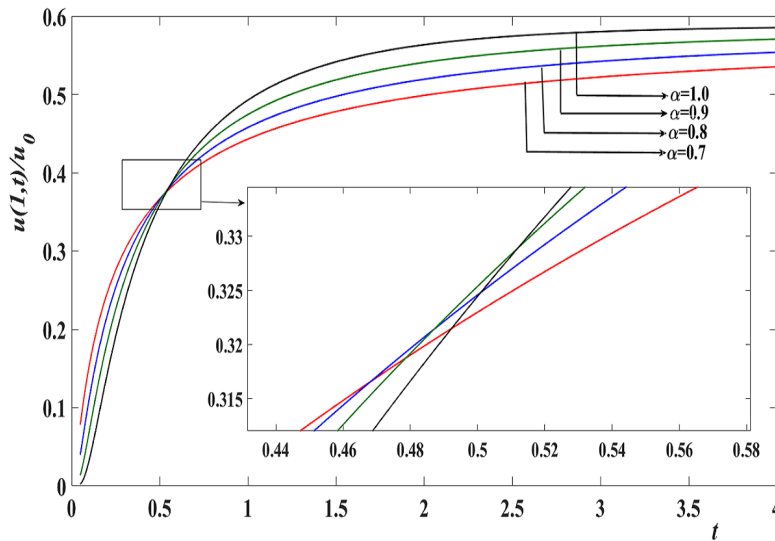
for  $V = 0$  and  $\lambda = 0$  at  $\alpha = 1$  which is depicted through Figure 3.1. The numerical results which are depicted through the figure in absence of advection and reaction terms in standard order conservative system clearly exhibit that the method is effective and reliable. This has motivated me to apply our concerned method to find the numerical solution of our considered model for non-conservative case ( $\lambda \neq 0$ ) for different particular cases. It is seen from Figures 3.2-3.3 that for both conservative and non-conservative systems  $u(x, t)$  increase with the increase of time for fractional order as well as standard order cases. It is also found that for both the cases the values of  $u(x, t)$  initially decrease as  $\alpha$  increases and after a while the results become opposite. The important part of the study is the effect of damping  $u(x, t)$  due to the presence reaction term for non-conservative case as compared to the conservative case.



**Figure 3.1:** Comparison of variation of  $u(x, t)/u_0$  vs.  $t$  with analytical result for  $u_0 = x = 1$  and  $V = \lambda = 0$  at  $\alpha = 1$ .



**Figure 3.2:** Plots of  $u(x,t)/u_0$  vs.  $t$  at  $\alpha = 0.7, 0.8, 0.9, 1.0$ ,  $V = 0.6$  for conservation case ( $\lambda = 0$ ).



**Figure 3.3:** Plots of  $u(x,t)/u_0$  vs.  $t$  at  $\alpha = 0.7, 0.8, 0.9, 1.0$ ,  $V = 0.6$  for non-conservation case ( $\lambda = 0.6$ ).

### 3.4 Conclusion

The author has achieved three important goals through this scientific contribution. The first one is the solution of the fractional order reaction diffusion equation using Laplace transformation method and also using it to exhibit the stochastic nature of the model through calculations of moments. The second one is a comparison of the result with an existing result for conservative case to validate the efficiency of the Bellman method. The advantages of using the method over the other existing numerical methods are only a few numbers of values are required to get the complete solution and also much less time is required to solve the problem. The third one is the showcasing of the damping nature of the solution through graphical presentations for non-conservative case due to effect of reaction term.

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