Simulation Foundations, Methods and Applications

S.K. Basu
Naveen Kumar *Editors*

Modelling and Simulation of Diffusive Processes

Methods and Applications

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Preface

This edited book on “Modeling and Simulation of Diffusive Processes: Methods and Applications” contains contributions from authors with a variety of academic backgrounds. It is an outgrowth of the International Conference on Simulation and Modeling of Diffusive Processes and Applications (ICMSDPA12) organized in Banaras Hindu University, India during October 9–12, 2012. There are contributors from outside ICMSDPA12 also to make the book more broad-based. This book addresses some of the issues in simulation modeling and simulation over a number of application areas. There are fifteen chapters in the book.

The first chapter is on diffusive processes and modeling: an introduction by Naveen Kumar and S. K. Basu. It deals briefly with a number of processes which are intimately connected with the diffusion processes, advection–diffusion equation (ADE) in different coordinate systems, mentioning different transformations generally used, different analytical and numerical methods. The effect of fractional order space derivative with skewness parameter on the mass transport has been explained through simulation using ADE for a simplified wound healing problem. Lastly, simulation study about the effect of ionic diffusion on the controlled release of nutrients from a coated spherical fertilizer granule is explained.

The second chapter on diffusion and transport of molecules in living cells by Ruchi Gaur, Lallan Mishra, and Susanta K. Sen Gupta deals with diffusion and different models of it, and relevance of different transport phenomena in living cells.

The third chapter on modeling diffusion and transport of suspended sediment in open channels, using two-phase flow theory by Sanjeev Kumar Jha and Fabián A. Bombardelli deals with a general framework of sediment transport in open channels as a two-phase flow, composed of mass and momentum equations for both phases (water and sediment). The authors discuss two levels of model complexity based on the nature of the terms involved in modeling: the complete two-fluid model (CTFM), and a partial two-fluid model (PTFM).

The fourth chapter on mathematical modeling of peristaltic transport of nanofluids by Dharmendra Tripathi and O. Anwar Bég reviews the challenges and potential of mathematical modeling in biofluid mechanics. The fundamentals of peristaltic transport and nanofluid dynamics have also been described qualitatively. A novel mathematical model has additionally been presented by the authors, to simulate the influence of nanofluid and thermo-diffusive/diffuso-thermal characteristics on peristaltic heat and mass transfer in a two-dimensional axisymmetric channel for simulation of nanofluid peristaltic drug delivery systems.

The fifth chapter on numerical study on isotachophoretic separation of ionic samples in microfluidics by Partho P. Gopmandal and S. Bhattacharyya deals with a high resolution numerical algorithm to analyze two-dimensional isotachophoresis (ITP) of electrolytes of different mobility in a wide micro-channel based on a finite volume method over a staggered grid arrangement along with a higher-order upwind scheme. The model is based on equations for conservation of mass and charge and also electro-neutrality condition.

The sixth chapter on thermal characterization of non-homogeneous media by Helcio R. B. Orlande, Carolina P. Naveira-Cotta, Henrique Massard da Fonseca, Diego Knupp, Renato M. Cotta, and Olivier Fudym presents application of a Markov chain Monte Carlo (MCMC) method, within the Bayesian framework, for the identification of non-homogeneities or inclusions in a medium through the solution of an inverse heat conduction problem. They present two different approaches in conjunction with the MCMC method. A nodal approach which locally linearizes the inverse problem by using temperature measurements for the computation of the sensitivity matrix, and an expansion of unknown spatially-dependent thermophysical properties in terms of eigen functions, which is used in conjunction with the Generalized Integral Transform Technique (GITT).

The seventh chapter on scale dependent porous dispersion resulting from the cumulative effects of velocity fluctuations by Wynand S. Verwoerd deals with semi-analytical stochastic model of the dispersion effects of macroscopic drift velocity fluctuations leading to significant insights like enhancement of intrinsic dispersion by a fluctuation, beyond the value associated with flow at the mean drift velocity. This enhancement manifests as a factor multiplying the spatial variance of the solute plume, so that the effects of a sequence of fluctuations accumulate as a product, implying an exponential rise of dispersion with the distance travelled as a solute plume traverses the fluctuation sequence. This behavior is tempered by an annealing effect downstream of a velocity step, which has a length scale related to plume extension.

The eighth chapter on modeling nitrogen fate and transport at the sediment-water interfaceby M. M. Hantush, and L. Kalin deals with analytical models describing transport and fate phenomena at media interfaces. The first problem discussed is modeling of nitrogen cycling at the sediment-water interface at the bottom of lakes. The second is modeling atmospheric input of oxygen into under-saturated lakes. The third model describes polychlorinated biphenyl redistribution at the sediment-water interface.

The ninth chapter on modeling groundwater flow in unconfined aquifers by S. N. Rai deals with groundwater flow equations to describe two dimensional groundwater flows in inhomogeneous anisotropic unconfined aquifer, inhomogeneous, isotropic unconfined aquifer, in leaky unconfined aquifer, in homogeneous isotropic sloping aquifer in response to intermittently applied time varying recharge and/or pumping from multiple basins of rectangular shapes and wells, respectively along with the initial and boundary conditions and methods of their solutions. The governing flow equations are used for the development of analytical/numerical models to predict water table fluctuations in the flow system under consideration.

The tenth chapter on two-dimensional solute transport from a varying pulse type point source by Premlata Singh, Sanjay Kumar Yadav, and Alexander V. Perig deals with solute transport originating from a source through a heterogeneous horizontal medium assuming temporal dependence of velocity and dispersivity.

The eleventh chapter on the problems of futile cycles in metabolic flux modeling: flux space characterization and practical approaches to its solution by Wynand S. Verwoerd and Longfei Mao deals with metabolic capabilities and behaviours of an organism by development of flux models of genome scale with flux balance analysis (FBA). For elimination of futile cycles in the FBA results, the authors introduce a simple notion to cut off the circulating flux layer while obtaining the same objective value. To comprehensively elucidate the alternate optimal solutions without the interference of futile values, they present flux variability analysis with target flux minimization, a combined pipeline approach based on FBA and flux variability analysis.

The twelfth chapter on contaminant concentration prediction along unsteady groundwater flow by Mritunjay Kumar Singh and Priyanka Kumari deals with the contaminant concentration pattern of one-dimensional advection-dispersion equation along a homogeneous semi-infinite aquifer with pulse type boundary condition for different forms of velocity expressions.

The thirteenth chapter on wavelet-multigrid method for solving modified Reynolds equation modeling synovial fluid flow in a normal human knee joint by S. C. Salimath deals with modified Reynolds equation, incorporating surface roughness and poroelastic nature of articular cartilage enabling bio-medical engineers in selecting suitable design parameters, giving deeper understanding of the lubrication of knee. The results obtained could guide the new material experimentation for knee replacement with mechanical characteristics.

The fourteenth chapter on a basic concept on modeling soil organic carbon by Nimai Senapati, Subhadip Ghosh, Heiko Daniel, and Amitava Rakshit discusses SOC models as important means of improving our understanding of C turnover process as well as underlying C stabilization mechanisms in soil. The SOC models often simulate the dynamics of different macro- and micro-nutrients along with SOC dynamics inadequately. They also often do not account soil pH and do not simulate the whole process of soil aggregation and the dynamics of soil biota explicitly. Inclusion of all these process/factors/parameters in the SOC models could represent the complex real life systems in a better way and might improve the overall model performance.

The fifteenth chapter on crop growth simulation modeling by Avnish Kumar Bhatia deals with crop growth models emphasizing crop physiology, weather parameters, soil parameters, and management practices to simulate growth and yield of crops. Crop simulation models compute growth values on a day to day basis using the relations among values of crop growth and weather parameters. A generic model can be developed using common crop physiological processes. Validating and fine tuning of crop model is an important step before using it for actual prediction tasks. The author opines that future crop models should rely on improving the mechanism of interacting with environment and society.

The editors have attempted, through these chapters from different contributors, to put in one place wide ranging areas where simulation-modeling techniques are being used for better understanding of the underlying processes. The editors feel that this volume would be quite useful for researchers and advance graduate students from multiple disciplines where simulation-modeling is of major interest.

S. K. Basu
Banaras Hindu University Naveen Kumar

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We wish to express our sincere gratitude to the contributors, whose contributions made possible publishing of this edited book. Thanks are also due to those contributors who responded to our requests, but their contributions could not be accommodated because of slack fitting with the title of the book. The reviewers of the chapters deserve cordial and sincere thanks.

We are also thankful to our institution, Banaras Hindu University for providing the ambience for completing the manuscript. The first editor is fortunate to have the complete support of his wife, Nilanjana and son, Subhaditya in this endeavour. The second editor has the complete support of his wife, Shashi and daughter, Paridhi. We appreciate their commendable and sincere cooperation for our work.

Contents

Chapter 1
Diffusive Processes and Modelling: An Introduction

Naveen Kumar and S. K. Basu

1.1 Introduction

Diffusion is a very common natural process occurring everywhere in physical, chemical, biological, geological systems. Considering the centrality of the diffusive process, understanding the effects of diffusion on different systems are of outmost importance. Assessment and management control of the degradation of our environment due to solute mass transport from a variety of sources of pollutants is a growing discipline. Mathematical modelling and computer simulation of these processes is nowadays one of the important approaches in quantitative analysis of different aspects of the discipline. One of the important analytical tools in this regard is the use of the advection–diffusion equation.

When a certain mass of solute is introduced in a medium, experience shows that the solute particles gradually spreads and occupies an increasing portion of the domain. If the medium is advective then this spreading is faster. This mixing and spreading is known as diffusive phenomenon (if there is no flow in the domain) or advective–diffusive phenomenon in the presence of advection. When a blob of ink is dropped in a glass of water, the water becomes coloured eventually; spreading of gas from the leakage point in the direction of wind, these are simple examples of diffusive and advective–diffusive processes, respectively.

Pollution can be classified on the basis of the medium in which it is occurring, such as air pollution, soil pollution, surface water pollution, and groundwater pollution, etc. Its source may be natural or anthropogenic. There are varieties of sources of pollution due to human activities [1–4]. One type of the source of these pollutions is a point source. Stationary point sources include volcanoes, factories, electric power plants, mineral smelters, petroleum refineries, and different small scale

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industries; while mobile point sources include all sorts of transport vehicles moving on road, rail, or in the air. A point source is a specific site in a medium (air, water, or soil) where the discharge of pollutant's solute particles in the form of effluents or particulate matters from such a source, enters the environment, and is transported away from the source due to diffusion and advection.

Groundwater pollution occurs due to infiltration of wastes from garbage disposal sites, septic tanks, mines, discharge from surface water bodies polluted due to industrial and municipal wastes [5–6]. Medium of advective–diffusive transport may be porous (soil field, aquifer, oil reservoir) or open medium (air, surface water bodies). In the real cases, medium is seldom homogeneous. Instead, it is heterogeneous. In the former case, the transport properties (porosity in porous medium), hydraulic conductivity, permeability remain uniform with position. In the latter case, these become position dependent or spatially dependent**.** Similarly, if these do not depend upon direction, the medium is isotropic, otherwise the medium is anisotropic. The source of advective–diffusive transport may be a point source (for example, garbage disposal sites, mines, etc.), or line source (for example, interface of sea water in aquifer), or surface source (for example, along agriculture field with high doses of chemical fertilizers) [7].

A point source may be of continuous type or pulse type. In either case, the point source may be uniform or of varying nature. In the presence of the source of pollution, the input concentration may be uniform or of increasing nature. As soon as the source of pollution is eliminated, the input concentration becomes zero or starts decreasing. Solution of a dispersion problem for a pulse type point source is useful in predicting the rehabilitation time period of a polluted domain once its source is eliminated. Smokes coming out of a chimney, wastes from a drainage system reaching a particular location in rivers, lakes, etc. are examples of uniform pulse-type point sources. As soon as the source is eliminated, the input becomes zero. Infiltration from surface point sources reaches groundwater level or oil reservoirs, degrading their quality (an example of varying pulse-type point source). As soon as the source is eliminated, the input starts decreasing, instead of becoming zero. The pollutant's solute transport from a source along the flow field through a medium of air or soil or water is described by a partial differential equation of parabolic type derived on the principle of conservation of mass, and is known as the advection–diffusion equation, also written as ADE in abbreviated form [8–11].

This chapter discusses various diffusive processes, develops the ADE equation and illustrates the use of this equation with fractional derivatives and skewness parameter for wound healing, and ionic diffusion of nitrogen phosphorus potassium (NPK) release from coated fertilizer granules.

1.2 Diffusive Processes

There are a number of processes which are intimately connected with the diffusion processes. These are Brownian motion, chemotaxis, osmosis, random walk. We briefly describe these processes in this section.

1.2.1 Brownian Motion

In the early 1800s, Robert Brown a botanist, studied pollen samples with a microscope and noted that the pollen grains exhibited movement. The phenomenon recorded by Brown is known as the Brownian motion. In essence, all atoms, ions, and molecules are in constant random motion, even those within a solid. The molecular motion in solids is not very much; the molecules simply vibrate in place. This movement is due to the collision of invisible water molecules with those particles. For example, a sphere of 1 μm in diameter in air is subjected to 10^{16} collisions per second. The distance of the particle from its initial position increases with time, although at any given moment the displacement may be either forward or backward with equal probability. This result was derived by Einstein in 1906. The diffusion coefficient (D) for a spherical particle in a liquid is related to its root mean squared displacement (x_{rms}) from the initial position at time t by $x_{rms} = \sqrt{2Dt}$. Suspended particles undergo Brownian motion and so these particles tend to move from regions of high concentration to ones with low concentration (diffusion) and this makes the concentration of suspended particles uniform over a long time.

1.2.2 Diffusion

Diffusion is the passage of particles from a region of higher concentration to a region of lower concentration. Unless physically blocked, diffusion will always occur. More technically, diffusion can be defined by chemical potential. Chemical potential is the measure of free energy available to do work to move a mole of particles from one location to another. Another way of stating diffusion is molecular movement from regions of higher chemical potential to areas of less chemical potential.

A continuous time stochastic process with (almost surely) continuous sample paths having the Markovian property is called diffusion. The simplest and most fundamental diffusion process is Brownian motion $B(t)$ (which is sometimes called the Wiener process $W(t)$). $B(t)$ is Brownian motion if it is a diffusion process satisfying (i) $B(0) = (0)$, (ii) expected value of variance $B(t) = 0$, variance $B(t) = \sigma^2 \times t$, (iii) $B(t)$ has stationary, independent increments.

1.2.3 Chemotaxis

Chemotaxis is the process where cells, bacteria, and other single-cell or multicellular organisms direct their movements according to certain chemicals in their environment. This is important for bacteria to find food by moving towards the highest concentration of food or to go away from harmful molecules. In multicellular organisms, chemotaxis is crucial for early and subsequent phases of development as well as in normal function. Leukocytes in blood move towards a region of bacterial infection. The movement is up a chemical gradient caused by infection. There are numerous examples in biology for this chemotactic movement. In diffusion, the movement is down a concentration gradient, while in chemotaxis the movement is up a concentration gradient.

1.2.4 Osmosis

Osmosis is the movement of water molecules from a region of higher water potential to a region of lower water potential through a semipermeable membrane. Semipermeable membranes allow the passage of some materials but block the passage of others. Water potential is a measure of chemical potential of water molecules. Pure water under atmospheric pressure has potential zero. When solute is added to water, its potential becomes negative. The direction of water flow is then from greater water potential to less water potential, that is, from pure water side to the side with solutes.

Biological membranes in many cases are semipermeable allowing passage of some molecules/ions and blocking passage of others. Transport of molecules/ions across the membrane is controlled by many factors such as particle size (smaller-sized molecules/ions have greater chance of crossing the membrane), concentration of molecules/ions (the more the concentration, the greater the chance), temperature (higher temperature gives higher energy to the molecules/ions for crossing the membrane), electrical charge, pressure on the particles.

The osmotic pressure ascribed to the suspended particles is given by $pV = RTz$, where V / z, is sufficiently large, z is gram molecule of a nonelectrolyte dissolved in a volume V at temperature T [12]. Suspended particles undergo irregular movement on account of the molecular movement of the liquid according to molecular–kinetic theory of heat. The solvent exerts pressure on the suspended particles as given by:

$$p = \frac{RT}{V}\frac{n}{N} = \frac{RT}{V}C, \tag{1.1}$$

where n is the number of suspended particles present in volume V, N is the actual number of molecules contained in a gram molecule, and C is the concentration. Let the suspended particles of spherical shape with average radius a be in a liquid with viscosity μ, and D, denotes the coefficient of diffusion of the suspended particles. As a result of diffusion, $-D(\partial C / \partial x)$ particles pass across unit area in unit time, where D satisfies the diffusion equation. In dynamic equilibrium D is given by:

$$D = \frac{RT}{N}\frac{1}{6\pi a \mu}. \tag{1.2}$$

1.2.5 Random Walk

A drunken person comes out of a bar and takes discrete steps of equal lengths on the street in front of the bar. The person may take a step towards left or right randomly with equal probability. Decision for moving left or right is taken independently. The total number of different paths that a drunken person can take, given the condition that the first return be at the $2k^{\text{th}}$ step is:

$$\mathrm{TP} = \frac{2}{k}\binom{2k-2}{k-1}. \tag{1.3}$$

The probability that the drunken man reaches the bar for the first time after $2k^{\text{th}}$ steps is $\mathrm{TP}/2^{2k}$. Given that the drunken man is at the bar at step $2k$, the probability that this is his first return visit is $1/(2k-1)$.

Diffusion processes are intimately related to random walks. Let us consider the random walk on R (a set of real numbers). Let the initial position of a particle be $x_0 = 0$. Tossing a fair coin, if we get heads then we set $x_{i+1} = x_i - 1$, otherwise we set $x_{i+1} = x_i + 1$. This can be seen to be associated with a partial difference equation satisfied by the distributions of positions that the random walk passes at successive time steps:

$$\begin{aligned}\mathrm{Prob}[x_i = k] - \mathrm{Prob}[x_{i-1} = k] = \frac{1}{2}\{&\mathrm{Prob}[x_{i-1} = k-1] \\ &+ \mathrm{Prob}[x_{i-1} = k+1] - 2\times\mathrm{Prob}[x_{i-1} = k]\}.\end{aligned}$$

This is a discrete diffusion process. The heat or diffusion equation

$$\frac{\partial p_t(x)}{\partial t} = \frac{\partial^2 p_t(x)}{2(\partial x)^2} \tag{1.4}$$

causes suitable functions from R to R to evolve as a function of time [13]. The operator $\partial^2/2(\partial x)^2$ is the infinitesimal generator of one-dimensional Brownian motion. If $p_0(x)$ is a density function, the distribution $p_t(x)$ obtained by solving the heat equation is also the probability density of the Brownian motion witnessed at time t, if its position at zero time was chosen according to the density $p_0(x)$. Thus, Brownian motions are related to continuous time diffusions.

1.3 Advection–Diffusion Equation (ADE)

Let us consider a small cubical element of volume *dxdydz* of sides, $PQ = dx$, $PS = dy$, $\mathrm{PA} = dz$, surrounding a position $P(x, y, z)$ in a Cartesian three-dimensional frame of reference as shown in Fig. 1.1 in a moving fluid containing solute. Let the concentration of solute at this position be denoted by $c(x, y, z)$.

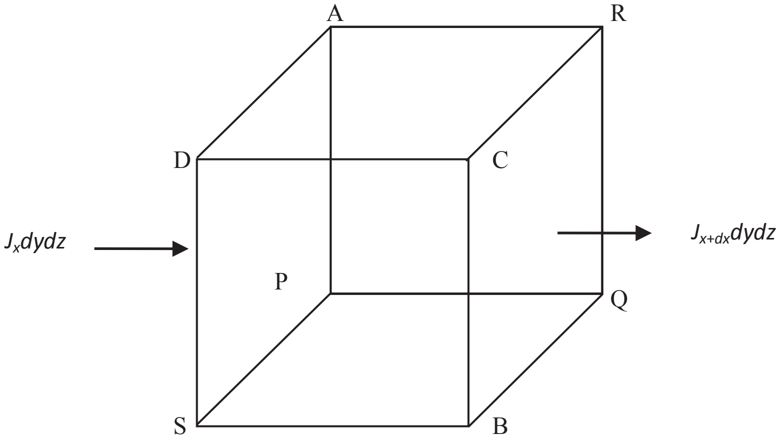

Fig. 1.1 Mass gain inside an elementary volume

Solute mass entering the elemental volume through the face PADS is $J_x dydz, J_x$, is the flux along the x-axis. Solute mass leaving the elemental volume through the face QBCR is $J_{(x+dx)} dydz$. Net gain inside the elemental volume along the x-axis is:

$$dydz(J_x - J_{(x+dx)}) = dydz[J_x - (J_x + dxJ_x{}' + \ldots)] = dxdydz(-\partial J_x / \partial x).$$

In the Taylor series expansion, the infinite series is truncated after the first order derivative term. Similarly, that along the y- and z-axes are $dxdydz(-\partial J_y / \partial y)$, and $dxdydz(-\partial J_z / \partial z)$, respectively. Total gain inside the elemental volume is:

$$-dxdydz\left(\frac{\partial \bar{J}_x}{\partial x} + \frac{\partial \bar{J}_y}{\partial y} + \frac{\partial \bar{J}_z}{\partial z}\right).$$

By Fick's first law of diffusion, the flux J_x is proportional to the concentration gradient, $J_x \propto -(\partial c / \partial x)$, where negative sign occurs because the positive x-axis direction is from higher concentration to lower concentration. Similarly, we have in the other two directions, $J_y \propto -(\partial c / \partial y)$ and $J_z \propto -(\partial c / \partial z)$, respectively. The diffusive current densities $\bar{J}_{diff}(J_x, J_y, J_z)$ and convective current density $\bar{J}_{conv}$ through the elemental volume are given as follows:

$$J_x = -D_x \frac{\partial c}{\partial x};\; J_y = -D_y \frac{\partial c}{\partial y};\; J_z = -D_z \frac{\partial c}{\partial z} \text{ and } \bar{J}_{conv.} = \bar{v}c, \tag{1.5}$$

respectively, where D_x, D_y, D_z are the proportionality constants, known as diffusion or dispersion parameters along the x-, y-, and z-axes, respectively and

$\bar{v}(u, v, w)$ is the flow velocity. Total current density through the elemental volume is given by:

$$\bar{J} = \bar{J}_{diff} + \bar{J}_{conv}. \tag{1.6}$$

According to conservation of mass, net rate of change of solute mass inside the elemental volume is equal to the net gain in the mass inside the volume, that is:

$$dxdydz\frac{\partial C}{\partial t} = -dxdydz\left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}\right) \tag{1.7}$$

$$\text{or}\quad \frac{\partial C}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} = 0. \tag{1.8}$$

Using the appropriate expressions from above, we have:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial c}{\partial z}\right) - \frac{\partial}{\partial x}(uc) - \frac{\partial}{\partial y}(vc) - \frac{\partial}{\partial z}(wc). \tag{1.9}$$

Equation 1.9 is known as the ADE in general form in three dimensions. The coefficients $D_x, D_y,$ and $D_z,$ may be the function of position, time as well as concentration. If it is not so, then these components are called dispersion coefficients. In case any one of the six coefficients is function of independent variables, the partial differential equation (Eq. 1.9) remains linear. In case any one of the coefficients depends upon the dependent variable, $c,$ the partial differential equation is nonlinear. If the velocity depends upon time at a particular position, it is said to be unsteady or temporally dependent. If it varies with position at a particular time, the velocity is said to be nonuniform or spatially dependent. If the medium is porous, velocity vector $\bar{v}$ in the ADE satisfies Darcy's law. If the medium is not porous, it satisfies the laminar conditions of flow. In case all the coefficients in Eq. 1.9 are constants, the ADE becomes:

$$\frac{\partial c}{\partial t} = D_x\frac{\partial^2 c}{\partial x^2} + D_y\frac{\partial^2 c}{\partial y^2} + D_z\frac{\partial^2 c}{\partial z^2} - u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z}. \tag{1.10}$$

The advection–diffusion Eq. 1.9 in one dimension along the x-axis, in general form, may be written as:

$$\frac{\partial c}{\partial t} + \frac{1-n_e}{n_e}\frac{\partial S}{\partial t} = \frac{\partial}{\partial x}\left(D_0 f_1(x,t)\frac{\partial c}{\partial x} - u_0 f_2(x,t)c\right) - \mu_1 c + \mu_2, \tag{1.11}$$

where c is the solute concentration at a position x at time $t,$ in liquid/air phase of the medium, S is the adsorbed concentration on the solid matrix of the porous medium, D_0 represents the solute diffusivity parameter, u_0 is the velocity of the medium transporting the solute particles, n_e is the porosity of the medium. The first and second terms on the left hand side represent the rate of change in concentration in the elementary volume of the liquid and solid phases, respectively, and the terms on the right hand side represent transport due to diffusion, that due to advection, decay in concentration of first order, and growth in concentration in liquid phase of zero order, respectively. The two concentrations c and S may be related by an isotherm:

$$S = k_1 c^p + k_2,\ p = 1, \text{ represents a linear isotherm.} \tag{1.12}$$

The partial differential equation (1.11) is of parabolic type [14]. To solve it analytically or numerically three conditions are required. The partial derivative with respect to the time variable is of first order, so we need only one condition in the time domain, which is defined at only one point of the time domain. Hence, it is called an initial condition. It may be of homogeneous or nonhomogeneous types. The condition is defined usually at $t = 0$. If it is of homogeneous type, it means the domain is initially solute free; otherwise the domain is not solute free. The partial differential Eq. 1.11 has second-order derivative in space variable, so two conditions in the $x-$ domain are needed to get the particular solution. Both the conditions are usually defined at two different points, hence are termed as the boundary conditions. The first condition is usually introduced at the origin, $x = 0$ of the domain. This condition is called *input condition*. It is of first type (solution type) and of inhomogeneous nature in case the input is of uniform nature. The input condition may be of continuous nature or of pulse type. It is of the third type (mixed type) in case the input is of varying nature. In the uniform pulse-type input, the input concentration at the origin of the domain is considered uniform up to certain time period, beyond which it is assumed zero. It may also happen that the source of the input remains uniform up to certain time and after its elimination forever, the input concentration becomes zero. Such situations occur in the case of pollution sources in air and surface water bodies. The smoke coming out of a chimney may be uniform up to certain time, but as soon as the source of the smoke stops working, the input becomes zero. It may also happen that the input increases in a certain time domain due to a variety of reasons and once the source is eliminated, the input starts decreasing instead of becoming zero at once. This type of input source may occur in groundwater reservoirs, whose source of pollution is on the earth's surface and the pollutants infiltrate through the soil to reach the groundwater. This situation may be described by varying pulse-type input. The second boundary condition is introduced at the other end of the domain. It may be of the first, second (flux type), or of the third type.

The term 'free-boundary value problem' is commonly used when the boundary is stationary. Moving boundaries, on the other hand, are associated with time-dependent problems and the position of the boundary has to be determined as a function of time and space. Moving boundary problems are often called Stefan problems, with reference to the early work of J. Stefan who, around 1890, was interested in the melting of the polar ice cap [15]. Alloy solidification problems differ from the classical Stefan problems in that the melting temperature is not known in advance;

it depends on the composition of the alloy. Typically, an alloy is considered to comprise a pure substance containing small concentrations of one or more impurities. The solidification of an alloy calls for a simultaneous study of the processes of the heat flow and the diffusion of impurities.

1.3.1 Transformation Equations

To solve the ADE with constant coefficients, some transformations are used. Moving coordinate transformation equations

$$X = x - ut, \quad T = t \tag{1.13}$$

reduce the one-dimensional advection–diffusion equation

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x} \tag{1.14}$$

into the diffusion equation

$$\frac{\partial K}{\partial T} = D_x \frac{\partial^2 K}{\partial X^2}. \tag{1.15}$$

where $K(X,T)$ is the new dependent variable in the new space and time variables. The same diffusion equation in the same independent variables may also be obtained by applying another transformation

$$c(x,t) = K(x,t)\exp\left(\frac{ux}{2D} - \frac{u^2 t}{4D}\right), \tag{1.16}$$

on the ADE (Eq. 1.14). A transformation $X = x - \lambda t$ (similar to that given in Eq. 1.13) reduces the ADE (Eq. 1.14) into an ordinary differential equation [16]

$$D_x \frac{d^2 c}{dX^2} - (u - \lambda)\frac{dc}{dX} = 0. \tag{1.17}$$

A transformation known as similarity transformation

$$X = \frac{x}{\sqrt{t}} \tag{1.18}$$

reduces the diffusion equation (Eq. 1.15) into an ordinary differential equation

$$D_x \frac{d^2 K}{dX^2} + X\frac{dK}{dX} = 0 \tag{1.19}$$

for $D_x = D_y$, the two-dimensional diffusion equation in Cartesian system of coordinates

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) \tag{1.20}$$

reduces into the radially symmetric polar system

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r}\right) \tag{1.21}$$

by using the transformation $x^2 + y^2 = r^2$. Similarly, a transformation $x^2 + y^2 + z^2 = r^2$ reduces the three-dimensional diffusion equation

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right) \tag{1.22}$$

into radially symmetric diffusion equation in spherical system of coordinates

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}\right) \tag{1.23}$$

A new independent variable X is introduced, using an operator:

$$\frac{\partial}{\partial X} = f_1(x,t)\frac{\partial}{\partial x} - f_2(x,t). \tag{1.24}$$

Operating it on a dependent variable ϕ, we get a linear first order partial differential equation as:

$$f_1(x,t)\frac{\partial \phi}{\partial x} - \frac{\partial \phi}{\partial X} = f_2(x,t)\phi. \tag{1.25}$$

It is equivalent to a system of three ordinary differential equations:

$$\frac{dx}{f_1(x,t)} = \frac{dX}{-1} = \frac{d\phi}{f_2(x,t)}. \tag{1.26}$$

One solution of it is:

$$X = -\int \frac{dx}{f_1(x,t)} \quad \text{or} \quad \frac{dX}{dx} = -\frac{1}{f_1(x,t)}. \tag{1.27}$$

Introduction of this transformation with a suitable form of $f_1(x,t)$ helps to reduce the variable coefficients of ADE (Eq. 1.3) into constant coefficients; hence enables us to use the Laplace integral transformation technique (LITT), which is the simplest and most useful among the analytical methods being used. The transformation may be modified according to the need, for example, negative sign may be omitted [17–18].

In another diffusive process, known as chemotaxis in which the mass movement is from lower concentration towards higher concentration, the flux components in Eq. 1.5 will be positive, and may be referred to as chemotactic flux. Hence, the mass conservation Eq. 1.15, in the presence of both diffusion and chemotaxis, may be derived as:

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} - \rho_x \frac{\partial^2 c}{\partial x^2}, \tag{1.28}$$

where the dependent variable c and the coefficient ρ_x may be termed as the cell density and chemotactic coefficient, respectively.

1.3.2 Dispersion Theories

There are three theories which relate the dispersivity and velocity parameters occurring as the two coefficients in the one-dimensional ADE (Eq. 1.11), mostly applicable in porous medium. These are as follows:

i. Ebach and White [19], Bear [8] in their one-dimensional analysis suggested that D is proportional to u.

ii. Taylor [20] in his one-dimensional analysis obtained D proportional to u^2. Scheidegger [21] summarized his analysis on the two possible relationships between D and u according to the role played by molecular diffusion: (a) $D \approx \alpha u^2$, where α, a constant of the porous medium alone (dynamic dispersivity), is derived by a dynamic procedure applicable if there is enough time in each flow channel for appreciable mixing to take place by molecular transverse diffusion; (b) $D \approx \beta u$, where β, another constant of the porous medium (geometric dispersivity), is derived by a geometric procedure applicable where there is no appreciable molecular transverse diffusion from one streamline into another. Thus, in all the models in which the combined effect of a velocity distribution across a channel and transverse molecular diffusion are considered [20], the coefficient of dispersion is proportional to u^2. Disregarding molecular diffusion for the situation where only mean motion in a channel is considered and mixing occurs at junctions connecting different channels, one obtains $D \approx u$. Later, Freeze and Cherry [22] modified these dispersion theories and considered dispersion parameter proportional to the velocity raised to a power n, where n ranges between 1 and 2.

iii. According to Matheron and de-Marsily [23], some large subsurface formations exhibit variable dispersivity properties described by a variable D as a function of position or time variables, while the flow domain remains uniform. Such variations may be caused, for example, by multiple length scales in these formations. Such formations are often modelled by a scale-dependent dispersion coefficient in the diffusive flux term in the transport equation. This theory was fully supported in the later works [23–26].

1.3.3 Why Modelling?

The idea of simulating real system or process on a computer rapidly spread among researchers since 1960s. It is accepted as one of the powerful tools for understanding processes and systems for predicting functional or operative conditions. The standard approach is numerically solving a mathematical model that governs a chosen process or system. Generally, the analytical solution is not known or difficult to reach for such situations. Solving mathematical models strongly depends on the used computational techniques and resources.

Shannon defined model as a representation of an object, a system, or an idea in some form other than that of the entity itself. We generally distinguish between two types of models: physical such as scale models, prototype plants, etc., and mathematical models such as partial differential equations (PDE), queuing models, etc. Simulation of a system is the operation of a model, which is a representation of that system. The model is amenable to manipulation which would be impossible, too expensive, or too impractical to perform on the system which it portrays. The operation of the model can be studied, and, from this, properties concerning the behaviour of the actual system can be inferred. Simulation is imitation of the operation of a real-world process or system over time. It generates an artificial history of a system; based on the observation of that artificial history, inferences concerning the operating characteristics of the real system can be drawn. A simulation can be only as good as the simulation model is. A simulation model makes a set of assumptions concerning the operation of the system and is expressed as mathematical, logical, or symbolic expressions between the entities (objects of interest) of the system. From the simulation, data are collected as if a real system was being observed. There are many applications such as designing and analysing manufacturing systems, determining ordering policies for an inventory system, designing communications systems and message protocols, drug design, analysing financial systems, and many more.

1.3.4 Review of Modelling Efforts in Diffusive Processes

Pollutants originating from a variety of natural and anthropogenic sources (volcano, industries, factories, refineries, sewage system, garbage disposal sites, mines, etc.) are major causes of degradation of the environment, air, surface water, soil and groundwater. Mathematical modellers use the ADE to describe the concentration levels at different positions and time, away from its source, through its analytical and numerical solutions. It is possible to solve this equation analytically only in some particular cases. In a more general situation, numerical techniques are required. A number of analytical methods are reviewed in [27]. Most of the analytical solutions for advective–diffusive transport problems in ideal conditions with growth and decay terms, subject to various initial and boundary conditions in semi-infinite or finite media have been compiled in [28–30].

The mechanisms of solute transport and reaction have been studied for many years, and a wide variety of numerical techniques have been developed and successfully applied in many settings. Most of these studies are based on the application of the advection–dispersion–reaction equation (ADRE). Many researchers, recognizing the importance of appropriately treating the hyperbolic part of the ADRE, have utilized various types of characteristic-based solution techniques that do not suffer from nonphysical behaviour such as oscillations at the sharp fronts [31–34]. The two-dimensional multispecies reactive transport in saturated and unsaturated porous media was simulated using Eulerian–Lagrangian localized adjoint methods (ELLAM) [35]. Its applicability and efficiency were assessed by comparing the results with those obtained using a numerical model based on the combination of discontinuous Galerkin and multipoint flux approximation methods.

Following the theories in [20–22] relating D and u in one-dimensional ADE, the number of mass transport studies has increased considerably. Many such models concern homogeneous media, but in reality the ability of the mass to permeate though the medium of air, soil or groundwater varies with position, which is referred to as heterogeneity. Early efforts to describe heterogeneity were achieved by making use of stratification and defining porosity–distance relationship [36–40]. In the former situation, the larger number of layers makes it difficult to get the desired analytical solution. In the latter situation, a numerical method is the only option to deal with the dispersion problems with most of the porosity–distance relationships. Later scale-dependent dispersion has been attributed to heterogeneity. According to the theory [41], some large subsurface heterogeneous formations exhibit variable dispersivity as a function of position or time variable. Based on such observations, analytical solutions to solute transport problems in a semi-infinite medium were obtained [42–45], where the dispersion parameter depends on distance and increases up a limited value. In the third problem, first order reaction coefficient was considered space dependent in the one-dimensional transport of solute through soil. Later an integral expression for a similar problem without using the modified Bessel functions was proposed [45]. Other authors have used simplified one- and two-dimensional models that incorporate variable coefficients to some extent [46–49].

A numerical ADE model with a hyperbolic asymptotic distance-dependent function (HAD) for the dispersion coefficient was proposed and used [50–51]. In a latter study, HAD is adopted and incorporated into the general ADE for describing scale-dependent solute transport in porous media. The problem is solved analytically by applying extended power series method coupled with Laplace transform. The quadrupole method was implemented in order to simulate the effects of heterogeneities on one-dimensional ADE of a passive solute in porous media [52]. Exact solutions of the linear advection–diffusion transport equation with constant and variable coefficients with different forms for both, transient and steady-state regimes was presented by Guerrero and colleagues [27] by using the generalized integral transform technique (GITT). In approximate solutions [53–54], a time-dependent dispersion coefficient was used. Usually, solute transport models assume a constant dispersion coefficient that is calibrated separately for each different downstream sample location, resulting in different dispersion coefficients for the same flow problem. In an attempt to overcome this, the dispersion coefficient as a function of the mean travel distance was used successfully [55]. Another approach is to model dispersivity as a time-dependent function. Based on the numerical results [56], dispersivity has been suggested to have a time-dependent behaviour which reaches asymptotic values after a long time. Analytical solution for time-varying dispersion coefficients have been presented in one dimension [57–58], in two dimensions [59–60], and in three dimensions [61–62]. Presently, the fractional advection–diffusion equation (FADE) is being used to model anomalous transport [63–66].

The importance of ADE is not confined to hydrology and soil sciences only. It has equal importance in other fields as well, some of which are mentioned below:

i. Petroleum engineering: Displacement of oil with gas; petroleum and natural gas production [67].
ii. Chemical engineering: Flow in packed columns involving chemical reactions or separation of chemical components; pore diffusion of gases, chromatography, ion-exchange [68–69].
iii. Modelling of flood waves: Modelling of flood waves in free-flowing rivers, which are more commonly bulk waves. Ferrick [70] classified these waves into (a) diffusion wave and (b) kinetic wave. A diffusion wave is governed by ADE (Eq. 1.11), where dependent variable, c may be replaced by a suitable variable y representing depth of flow; $u =$ wave celerity; $D =$ diffusion coefficient. In case, $(\partial^2 y / \partial x^2) \approx 0$ but $(\partial y / \partial x) > 1$ but, Eq. 1.11 reduces to kinetic wave governed by the kinetic equation [71]. It is to be noted that presence of $(\partial y / \partial x)$ is responsible of inducing diffusion, thus leading to attenuation of a flood wave.
iv. Wound Healing: In case of dermal wound, the variables in ADE (Eq. 1.11) will be: $c =$ cell density, or chemical concentration at position x, and time t, $u =$ convection due to formation of extra cellular matrix (ECM). Readers can find mathematical models using ADE for wound healing in [72–73].

1.4 Adevection-Diffusion with Fractional Derivatives

In order to simulate the memory formalism [74], the partial differential equation of fractional order space derivatives may be more useful. Skewness in diffusion may also be considered through a suitable parameter. For example, in wound-healing process, the density of cells and the chemical concentration at the centre and at a position close to the centre of the wound are decided by those at the preceding adjacent position towards the wound margin. Also, a cell may take a skewed path instead of curvilinear path, and it may be captured through a distinct parameter. Following the work in [75–80], we may use fractional order derivative in place of integer order derivative as:

$$\frac{\partial}{\partial x} \approx \left\{ \frac{1+\beta}{2} \frac{\partial^{\alpha-1}}{\partial (x)^{\alpha-1}} - \frac{1-\beta}{2} \frac{\partial^{\alpha-1}}{\partial (-x)^{\alpha-1}} \right\}$$

$$\text{So} \quad \frac{\partial^2}{\partial x^2} \approx \left\{ \frac{1+\beta}{2} \frac{\partial^{\alpha}}{\partial (x)^{\alpha}} - \frac{1-\beta}{2} \frac{\partial}{\partial (-x)} \frac{\partial^{\alpha-1}}{\partial (-x)^{\alpha-1}} \frac{d(-x)}{d(x)} \right\} \tag{1.29}$$

$$\text{or} \quad \frac{\partial^2}{\partial x^2} \approx \left\{ \frac{1+\beta}{2} \frac{\partial^{\alpha}}{\partial (x)^{\alpha}} + \frac{1-\beta}{2} \frac{\partial^{\alpha}}{\partial (-x)^{\alpha}} \right\}, \tag{1.30}$$

where α is the fractional order of the derivative, and β is the skewness parameter. For the *n*th integer order, α is in the range $n-1 \leq \alpha \leq n$. For $\alpha = 2$ and $\beta = 0$ (no skewness), approximation sign (≈) may be replaced by equality sign. As α decreases from 2, the Leὺy probability distribution (LPD) deviates from the Gaussian distribution and the tail of the Leὺy distribution becomes heavier. If β is less than zero, the dispersion is skewed backward representing a slowly evolving contaminant plume followed by a heavy tail. For β greater than zero, the dispersion is skewed forward describing a fast evolving contaminant plume followed by a light tail. Many other works on space-fractional partial differential equations refer to the same equation with minor changes. The finite difference approximations of the fractional order derivatives [81–82] are:

$$\frac{\partial^{\alpha} y}{\partial (+x)^{\alpha}} = \frac{1}{h^{\alpha}} \sum_{k=0}^{i+1} g_k y_{i-k+1}, \quad \frac{\partial^{\alpha} y}{\partial (-x)^{\alpha}} = \frac{1}{h^{\alpha}} \sum_{k=0}^{K-i+1} g_k y_{i+k-1} \tag{1.31}$$

where $g_k = \dfrac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)}$, Γ is the gamma function, and h is the uniform size of the intervals into which the spatial axis is divided.

The classical advection–diffusion equation is mathematically identical to the diffusion equation with drift, and furthermore, the same random walk model underlies both. The mean jump size determines the velocity *v* of the advective drift. This connection between random walk and diffusion is due to Einstein. When the variance of the particle jumps is infinite, the resulting plume follows a stable concentration curve, the solution to an ADE with space derivatives having fractional order. This plume has skewness and a power law leading edge. Random waiting times do not affect the eventual shape of the plume as long as the waiting times have finite mean. When the mean waiting time is infinite, the time derivative has fractional order in the ADE.

1.4.1 Application of Fractional Order Derivative in Wound Healing

We demonstrate the effect of fractional order space derivative and skewness parameter on the dependent variable of the ADE. For this, we consider the problem of epidermal wound healing. The epidermal wound area is assumed to be circular. The healing takes place due to convective and diffusive cell migration. The source is at the boundary of the circular wound region. The growth factors (chemicals) infuse inside the wound region, as a result of which one annular domain, ECM scaffolding, takes place adjacent to the wound boundary. The convection is due to movement of the ECM front towards the centre. As the wound is supposed to be confined to epidermis, the role of blood vessels, oxygen, chemotaxis, etc. is not taken into account. The production term in the convective diffusive equation is assumed to be a function of chemical concentration, while that in the diffusive equation is supposed to be a function of cell density. The loss terms in both the equations are supposed to depend upon the respective dependent variables. The partial differential equations for the diffusion of chemicals (concentration c) and the cells (density n) in polar coordinate system and in nondimensional form are

$$\frac{\partial c}{\partial T} = D\frac{\partial^2 c}{\partial R^2} + \frac{D}{R}\frac{\partial c}{\partial R} + \lambda_c f_c(c) f_1(n) - \mu_n f_2(c),\ 1 > R > 0, \tag{1.32}$$

and

$$\frac{\partial n}{\partial T} = \frac{\partial^2 n}{\partial R^2} - Pe\frac{n}{R} - \left(Pe - \frac{1}{R}\right)\frac{\partial n}{\partial R} + \lambda_n f_n(n) f_3(c) - \mu_n f_4(n),\ 1 > R > 0. \tag{1.33}$$

The nondimensional variables used in above equations are (the asterisks are omitted in the PDEs):

$$n^* = n / n_0,\ c^* = c / c_0,\ R = r / a,\ T = D_{n0} t / a^2,\ Pe = a u_0 / D_{n0},\ D = D_{c0} / D_{n0},$$
$$\lambda_n^* = \lambda_n a^2 / D_{n0},\ \lambda_c^* = \lambda_c a^2 / D_{n0},\ \mu_n^* = \mu_n a^2 / D_{n0},\ \mu_c^* = \mu_c a^2 / D_{n0},$$

where n_0 is the cell density at the unwounded state, c_0 is the chemical concentration at a position adjacent to the wound boundary just after the inflammatory phase (which is at t_0), D_{c0} and D_{n0} are the uniform diffusion parameters of chemicals and the cells, λ and μ with appropriately suffixed, are scalars controlling the production and the loss of cell density and growth factor, respectively, r is the radial direction from the centre ($r = 0$) towards the boundary ($r = a$) of the circular wound of radius a. Cell density and chemical concentration inside the wound region are zero just after the occurrence of wound $(t = 0)$. At the boundary, cell density is the same as if there was no wound. As soon as the wound has occurred, chemicals start infusing inside the region, its level being the maximum adjacent to the boundary by the end of the inflammatory phase. With the progress in the healing process, chemical concentration level lowers down at the boundary and at the interior positions. The input chemical concentration is formulated in this way. At the other end (at the centre), the gradients in both the concentrations will be zero. During the time $0 < t < t_0$, chemical concentration level at the boundary attains a value higher than c_0. This chemical concentration (growth factors) is instrumental in the formation of ECM front near the boundary and its movement towards the centre of the wound area. Thus, the initial and boundary conditions for both the partial differential equations may be written as:

$$n(R,0) = 0; \quad c(R,0) = 0; \quad 1 > R \geq 0, \tag{1.34}$$

$$n(1,T) = 1; \quad c(1,T) = \exp(1 - T / T_0); \quad T > 0, \tag{1.35}$$

$$\frac{\partial n}{\partial R} = 0; \quad \frac{\partial c}{\partial R} = 0, \text{ at } R = 0; \quad T \geq 0, \tag{1.36}$$

where T_0 is the nondimensional form of t_0. We assume that $f_c(c)$ in Eq. 1.32 increases as $c \to c_0$, and also $f_n(n)$ in Eq. 1.33 increases as $n \to n_0$. The functions in production and loss terms of both the Eqs. 1.32 and 1.33 are assumed to be of increasing nature. An exponential function is a general form to represent the changes; as it may be reduced to linear, quadratic, or other higher degree expressions under different approximations as required in modelling of many natural processes. Since the nondimensional dependent variables (n, c) in our model are always in the range 0–1, this limits the rapid growth of exponential functions. We consider:

$$f_n(n) = \frac{1}{n - n_0}, \quad f_1(n) = \exp(\sqrt{n}), \quad f_2(c) = \sqrt{c},$$

$$\text{and} \qquad f_c(c) = \frac{1}{c - c_0}, \quad f_3(c) = \exp(\sqrt{c}), \quad f_4(n) = \sqrt{n}.$$

To demonstrate the effects of fractional order derivative (α) and skewness (β) on the dependent variable, we performed computational experiments to study the two effects on the cell migration from the wound boundary towards its centre in the domain ($a \geq r \geq 0$). The integer order space derivatives in Eqs. 1.32 and 1.33 are replaced by fractional order derivatives as in Eqs. 1.29 and 1.30. Their approximations are used from Eq. 1.31. The input values are chosen as: wound radius $a = 1.0$ cm, cell density at unwounded state $n_0 = 1.0$, chemical concentration at the end of inflammatory phase $c_0 = 1.0$, convective velocity $u_0 = 0.00001$ cm/day, proliferation period $t^* = 21$ days, inflammatory period, $t_0 = 3.5$ days, all the λs, and μs, are assigned a uniform value $0.001(\text{day})^{-1}$, as this is our baseline model, the uniform step sizes along the $R-$ and $T-$ axes are chosen as $h = 0.1$, $\Delta T = 0.0001$ respectively, satisfying the stability criterion. The diffusion coefficient values for the cell and the chemical concentration are taken from some of the works cited above. Biologically plausible values of D_{n0} are in the range 3.5×10^{-11} to $6.9 \times 10^{-9}\,\text{cm}^2/\text{sec}$ [83], depending upon the type of the cell. Higher value of $D_{n0} = 5 \times 10^{-7}\,\text{cm}^2/\text{sec}$

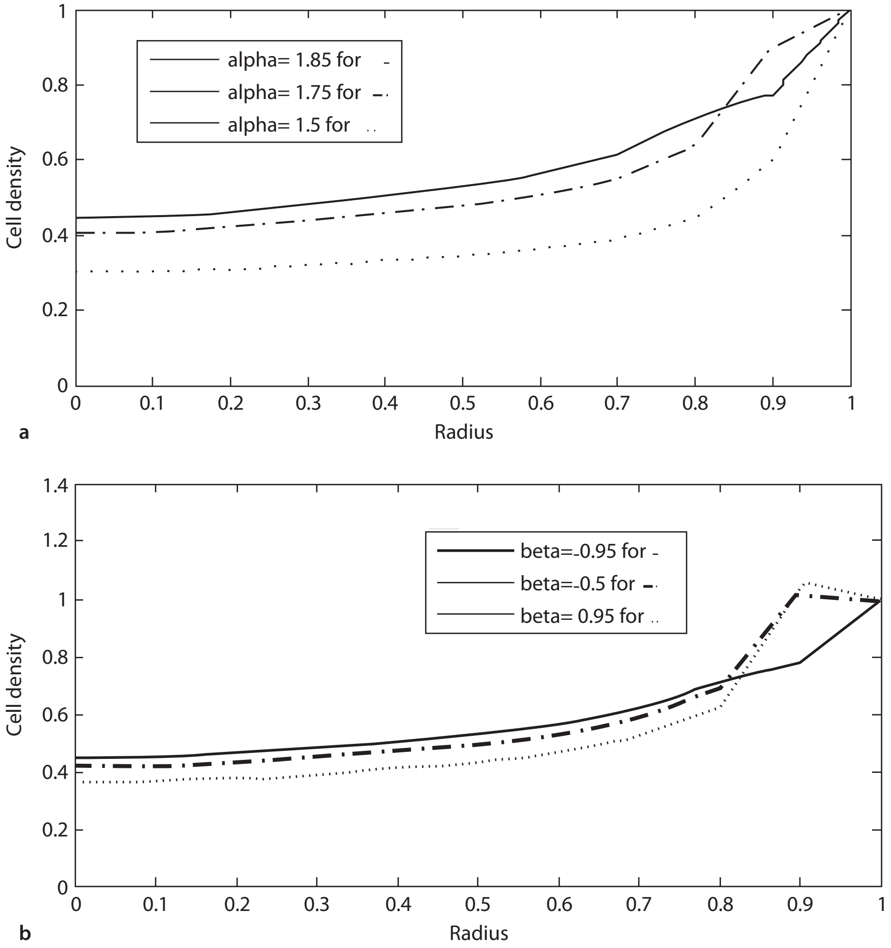

Fig. 1.2 **a** Effect of fractional order of space derivatives on cell migration. **b** Effect of skewness parameter on cell migration

has been considered elsewhere [84]. The value of diffusion coefficient for chemical concentration (growth factors) is suggested to be higher than that of the cells. We have used $D_{n0} = 0.0005\text{cm}^2/\text{day} \approx 0.0005/100000 \approx 5.0\times 10^{-9}\text{cm}^2/\text{sec}$, and 0.0005 cm^2/day. The effect of the fractional order α is studied for $\alpha = 1.85$, 1.75, and 1.5 and is shown in Fig. 1.2. As the order of the space derivative approaches 2 (LPD is closer to the Gaussian distribution), wound at a particular position is healed in a better way. This trend is not observed in the vicinity of the wound boundary (where cell density is 1.0). This is because we have considered an ideal situation by assuming cell diffusion and convective parameters uniform. In the real situation, both will depend upon chemical concentration; in a recent work (to be communicated soon) we have not found this reversal. The effect of skewness on the cell density is studied by performing the simulations for $\beta = -0.95, -0.5, +0.95$, and is shown in Fig. 1.3. It may be observed that the cell density has higher values in the backward skewness domain $(-1 \leq \beta \leq 0)$ compared with those in the forward skewness domain $(0 \leq \beta \leq 1)$. This effect of β is indistinguishable close to the wound boundary, whereas it is pronounced towards the centre of the wound region. The reversal in this trend near the wound boundary is due to the same reason stated above.

1.5 Ionic Diffusion

We illustrate ionic diffusion with the example of NPK release from coated fertilizer granules. Let us consider a spherical coated fertilizer granule which contains three types of nutrients, one is a nonelectrolyte, other is a weak electrolyte, and the third is a strong electrolyte, the diffusion pattern of all of these three substances are different. The unsteady diffusion equations in a spherical domain for the two species, ions and molecules of a weak electrolyte may be written as [85]:

$$\frac{\partial C_1}{\partial t} = D_1\left(\frac{\partial^2 C_1}{\partial r^2} + \frac{2}{r}\frac{\partial C_1}{\partial r}\right) - 2k, \tag{1.37}$$

and $$\frac{\partial C_2}{\partial t} = D_2\left(\frac{\partial^2 C_2}{\partial r^2} + \frac{2}{r}\frac{\partial C_2}{\partial r}\right) + k, \tag{1.38}$$

respectively, where k is the rate of formation of the molecules (the dimmers), C_1 and C_2 are the concentrations; D_1 and D_2 are the diffusion coefficients of the ions and the molecules, respectively. The diffusing coefficient of the ions is expressed in terms of diffusion coefficients of both the ions as:

$$D_1 = \frac{|z_c| + |z_a|}{\dfrac{|z_a|}{D_c} + \dfrac{|z_c|}{D_a}}. \tag{1.39}$$

In the case of a non 1-1 electrolyte, where $|z_c|$ and $|z_a|$ are the ionic charges; D_c and D_a are the diffusion coefficients, of the cation and anion, respectively. In the case of a 1-1 electrolyte, where $|z_c| = |z_a|$, we have:

$$D_1 = \frac{2}{\dfrac{1}{D_c} + \dfrac{1}{D_a}}. \tag{1.40}$$

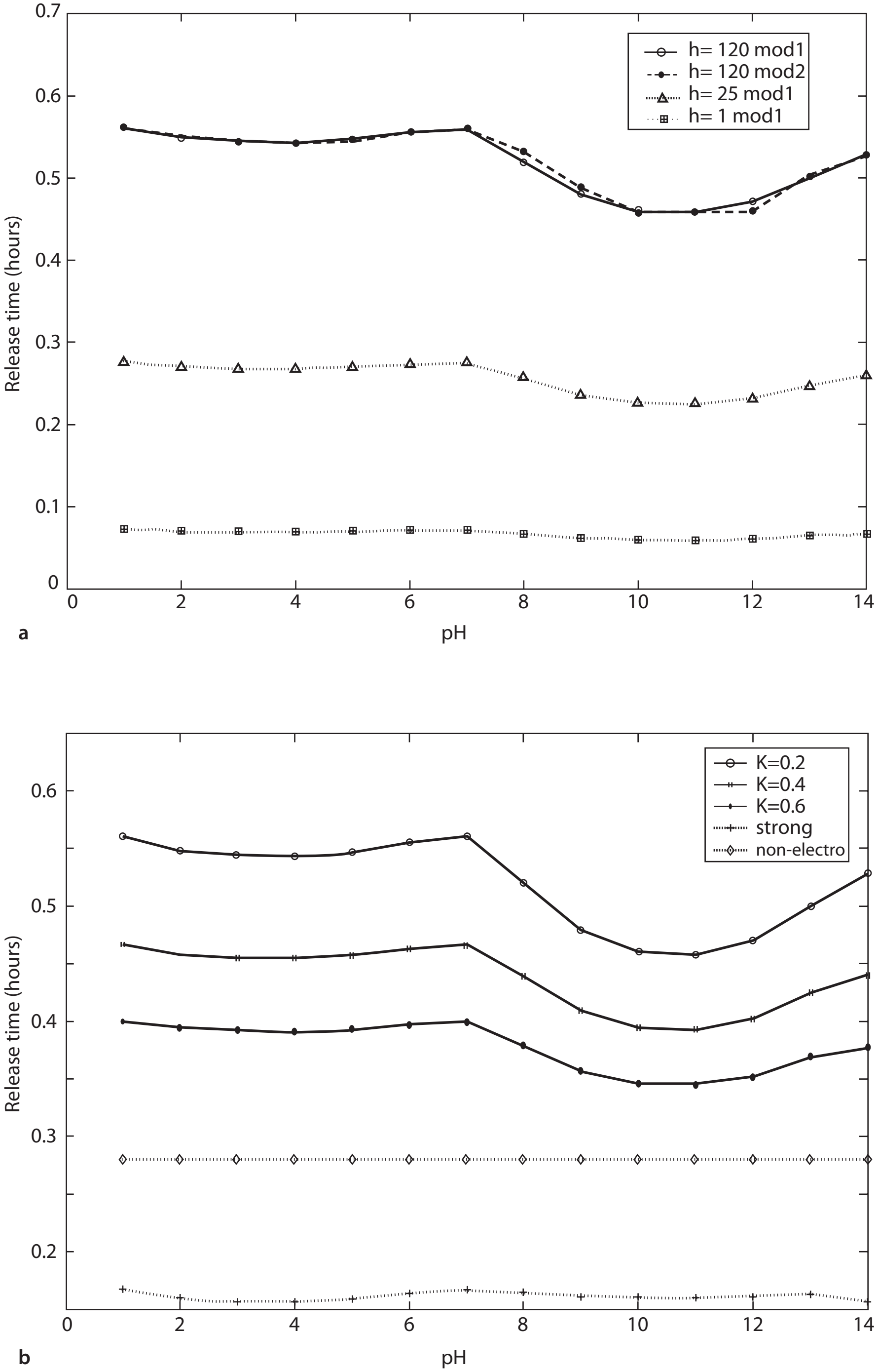

Fig. 1.3 **a** Effect of surface contact area on release time with pH. **b** Effect of association constant of electrolyte nutrient on release time with pH

In an isodesmic model [85]

$$C_2 = KC_1^2, \tag{1.41}$$

where K is an association constant for the diffusing species, which is independent of the size of the aggregate. The total concentration, C_w for weak electrolyte may be written [85] as:

$$C_w = C_1 + 2C_2. \tag{1.42}$$

Using these equations the diffusion equation in terms of one dependent variable, C_1 may be written as:

$$(1+4KC_1)\frac{\partial C_1}{\partial t} = (D_1 + 4KD_2C_1)\left(\frac{\partial^2 C_1}{\partial r^2} + \frac{2}{r}\frac{\partial C_1}{\partial r}\right) + 4KD_2\left(\frac{\partial C_1}{\partial r}\right)^2. \tag{1.43}$$

This is a nonlinear partial differential equation. It suggests strong dependence of the apparent diffusion coefficient of the diffusing substance on the ionic or molecular concentration due to significant interactions among the diffusing species. The linear diffusion equation for a nonelectrolytic substance for diffusion parameter, i.e. $D(C) = D$, in spherical coordinate system may be written as:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right). \tag{1.44}$$

A strong 1-1 electrolyte ionizes completely producing equal number of cations and anions. Although the concentrations of cations and anions C_c and C_a, respectively, may vary through the solution, the concentrations and the concentration gradients of these species are equal everywhere because of electro-neutrality, that is:

$$C_c = C_a \quad \text{and} \quad \nabla C_c = \nabla C_a. \tag{1.45}$$

In the case of strong non 1-1 electrolyte, constraints on the concentration and flux at zero current are:

$$z_c C_c + z_a C_a = 0 \quad \text{and} \quad z_c \nabla C_c + z_a \nabla C_a = 0. \tag{1.46}$$

In the case of 1-1 electrolyte, $z_c = -z_a$. The total concentration of strong electrolyte, C_s is

$$C_s = C_c / |z_a| = C_a / |z_c|. \tag{1.47}$$

The diffusion equation of a strong electrolyte is

$$\frac{\partial C_s}{\partial t} = D_s\left(\frac{\partial^2 C_s}{\partial r^2} + \frac{2}{r}\frac{\partial C_s}{\partial r}\right), \tag{1.48}$$

where the diffusion coefficient, D_s has either of the two expressions of Eq. 1.39 or Eq. 1.40, depending on whether the electrolyte is a non 1-1 or a 1-1 electrolyte. The diffusion equation for a nonelectrolyte is the same as Eq. 1.44 with appropriate meaning of the variables.

Diffusion coefficients of cation and anion depend upon the pH of the soil water. As a result, release time of an electrolytic nutrient depends upon pH. The authors have studied the effects of different parameters such as radius of the granule, its surface area in contact with the soil determined by h, association constant (K), pH on the release time in their recent work [86]. The two figures from this work are being given here as Figs. 1.3a and 1.3b for the readers understanding about the ionic diffusion. In Fig. 1.3a. $h = 1$ represents the basal form of granule application (the granule is totally below the soil surface); hence, the release time is the minimum, while $h = 120$ corresponds to the almost point contact of the granule with the soil.

1.6 Summary

Diffusion is not confined to a particular discipline. Its various forms in different disciplines are explained. The derivation of advection–diffusion equation describing the mass transport through a medium is given. Its forms in different coordinate systems are also given. Different transformations being used by various workers in a variety of disciplines are mentioned. How the heterogeneity of the medium and unsteadiness of advection are addressed by the two parameters of the ADE for reactive and nonreactive solute mass, using the different dispersion theories with different analytical and numerical methods are explained. Most importantly, the effect of fractional order space derivative with skewness on the mass transport, have been explained through the wound healing problem. Lastly, the effect of ionic diffusion on the controlled release of nutrients from a coated spherical fertilizer granule is given.

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