CHAPTER 2

LITERATURE REVIEW

In this chapter, different techniques used by various authors to solve mathematical models are explained. This includes several studies, the effect of various parameters, and models used by previous researchers of the area under study.

2.1 REVIEW OF LITERATURE

Mathematical modeling is an effective tool for designing the practical problems experienced in the industry for research. The physical phenomena in sciences and engineering are expressed in the form of mathematical models. Such physical phenomena depend on several parameters, which provide linearity and nonlinearity in equations (Arora et al., 2005). These models differ from one another concerning validity and accuracy ranges (Dhawan and Kapoor, 2011). Sufficient efforts are put on by the researchers to examine the behavior of these phenomena experimentally. For a better understanding of the concept and to identify the gap in the literature, it would be beneficial to study the relevant research work. Some significant studies carried out in this area are listed below:

Lapidus and Amundson (1952) studied the effect of longitudinal diffusion in chromatographic columns and obtained a differential equation for the wash liquor. Brenner (1962) proposed the pulp washing models based on the axial dispersion. In a study, Sherman (1964) described the mathematical model for the overall movement of solute in the bed of non-porous granular material by replacing molecular diffusion coefficient with longitudinal dispersion coefficient. Pellet (1964) introduced a mathematical model combining the effects of particle diffusion and axial dispersion. Pellet (1964) studied the longitudinal dispersion of solute, intra-particle diffusion of solute, and liquid-phase mass transfer for the particles of cylindrical and spherical geometry by using modified step function input. In another study, Grähs (1974) divided the packed bed of cellulose fibers into three different zones namely zone of flowing liquor, stagnant liquor, and certain physical features of the fibers (fiber porosity and fiber radius) were ignored. Later, Perron and Lebeau (1977) neglected the longitudinal dispersion coefficient to study sodium chloride washing and obtained a differential equation for the wash liquor.

Most of the researchers such as Brenner (1962), Potůček (1997), and Liao and Shiau (2000) used the axial dispersion model to describe the washing operation of the pulp fibre bed. These models are based on the continuity, adsorption, desorption, and diffusion-dispersion phenomena. According to Ganaie et al. (2014), for the efficient analysis of a packed bed of porous particles, the following assumptions are worth consideration:

- The packed bed is assumed to be macroscopically uniform.
- The particles are supposed to be of uniform cylindrical size.
- The particle diameter is taken as very small as compared to axial distance.
- The intrafiber diffusion coefficient is not dependent on particle radius and cake thickness.
- The fibre consistency, porosity of the bed, and particle are considered to be interrelated with each other.
- The movement of solute within the lumen of the fiber is explained by Fick's diffusion phenomena.

Further, Arora et al. (2006) explained that majority of the researchers go along with spherical solid particles for the development of the mathematical model used to describe the pulp washing processes because the reason for higher diffusion in spherical particles and a lesser amount of dispersion arises owing to the non-compressible character of the solid particles.

Most of these studies focused on developing discretization in spatial and temporal directions. Such physical phenomena depend on many parameters which provide the nonlinearity in equations. The effect of the process can better be understood from the solutions for these equations, and this is helpful for the industries to make suitable strategies. However, according to Mittal et al. (2013), such derived models are complicated, and obtaining their solution is an extremely complex process as it involves first and second-order partial derivatives in space and time.

2.2 STUDY OF VARIOUS MATHEMATICAL MODELS

There is a plethora of literature available on the mathematical models solved by various authors. However, keeping in view the scope of the present study, the related models are summarized below:

Brenner (1962) solved a well-established model for the diffusion-type equation (dimensionless) describing the mixing between solute and solvent ‘phases’ and axial dispersion coefficient given as:

$$\frac{\partial C}{\partial T}=\frac{1}{Pe}\frac{\partial^2 C}{\partial X^2}-\frac{\partial C}{\partial X}, \tag{2.1}$$

with boundary conditions:

$$\left.\begin{aligned} C=\frac{1}{Pe}\frac{\partial C}{\partial X} \qquad & at \;\; X=0 \\ \frac{\partial C}{\partial X}=0 \qquad & at \;\; X=1 \end{aligned}\right\} \qquad \text{for} \;\; T\geq 0, \tag{2.2}$$

and the initial condition:

$$C(X,0)=1. \tag{2.3}$$

Also, Brenner (1962) discussed the boundary conditions suitable for the displacement process. It was assumed that at the inlet of the pulp bed there is no loss of solute when the displacing fluid is added. The second boundary condition was imposed at the exit level that the concentration of solute passes through a maximum or minimum so that an unacceptable conclusion is avoided. The study described the rapid convergence of solution using Laplace transform. Besides, the main parameter involved in the study is the Peclet number (Pe) which is a dimensionless parameter that signifies the ratio of advection to diffusion and indicates the amount of lignin dispersion in the pulp bed and defined as $Pe=\frac{uL}{D_L}$, which involve interstitial velocity (u), longitudinal dispersion coefficient (D_L), and bed thickness (L). Every differential element of solvent at the introduction of the packed bed is instantly mixed with content of the bed and the same amount of fluid is transferred from the bed when $Pe\to 0$. In this situation, the bed performs as a perfect mixing chamber. When $Pe\to\infty$, the conservation of solute mass converges too slowly, and the displacement process suitably moves to the asymptotic solution.

Fan et al. (1971) solved the axial dispersion model represented by nonlinear differential equations (dimensionless) associated with chemical reactors is given as:

$$\frac{1}{Pe}\frac{d^2 C}{dX^2}-\frac{dC}{dX}=R\phi(C). \tag{2.4}$$

Fan et al. (1971) used the collocation method having the quality of easy adaptability for a computer program and is based on the selection of the collocation points to solve the model. The technique needed very short computational time and involves fewer stability difficulties. The three categories of collocation methods described in the study as interior, boundary, and mixed. The mixed collocation method was employed in which the trial function is equated to zero at collocation points which are chosen as the roots of a function that is orthogonal to the interior residual. The roots of Tschebysheff interpolation polynomials were preferred to minimize the residuals. Fan et al. (1971) further suggested that the selection of optimal step size of domain depends on certain parameters like *Pe* and accurate results for the solution profiles can be derived with a small step size for small *Pe*.

Raghavan and Ruthven (1983) used the orthogonal collocation method (OCM) to find the solution of the axial dispersion plug-flow model describing the flow pattern of particle diffusion and external fluid.

The particle diffusion model is:

$$D_F\left(\frac{\partial^2 q}{\partial r^2}+\frac{2}{r}\frac{\partial q}{\partial r}\right)-\frac{\partial q}{\partial t}=0, \tag{2.5}$$

The boundary conditions are:

$$\frac{\partial q}{\partial r}=0 \quad \text{at} \quad r=0 \quad \text{and} \quad -D_F\left(\frac{\partial q}{\partial r}\right)=\frac{k_f\omega}{K}\left(q\,|_{r=R}-c\right) \quad \text{at} \quad r=R. \tag{2.6}$$

The model for external fluid is:

$$u\frac{\partial c}{\partial x}+\frac{\partial c}{\partial t}+\left(\frac{1-\varepsilon}{\varepsilon}\right)\left[\frac{3k}{R}\left(c(x,t)-\frac{q\,|\,\rho=R}{K}\right)\right]=D_L\frac{\partial^2 c}{\partial x^2}, \tag{2.7}$$

with boundary conditions:

$$uc-D_L\frac{\partial c}{\partial x}=0 \quad \text{at} \quad x=0 \qquad \text{and} \qquad \frac{\partial c}{\partial x}=0 \quad \text{at} \quad x=L. \tag{2.8}$$

Raghavan and Ruthven (1983) proved that the axial *Pe* has more influence on adsorber performance. When axial *Pe* decreases to about 40, the breakthrough time reduces. Whereas, when *Pe* is greater than 40, the parameter has a minimum effect on the performance. Since *Pe* is inversely proportional to axial dispersion (D_L) therefore, axial dispersion is negligible with the increase in *Pe*. In this case, the breakthrough curve bears the effect only on bed parameters such as length and film resistance. However, it is independent of the distribution ratio and its effect can be significant expected only in the case when the impact of axial dispersion is more influential. Thus, the breakthrough curve reflects only the effect of parameters like *Pe*, mass transfer coefficient, and bed length parameters under the most practically significant conditions. Further, the study revealed that the Biot number (*Bi*) that connects the mass transfer resistance within and on the surface should be less or near to10.

Kim (1989) studied the behavior of the mass balance equation (dimensionless) involving unsteady-state diffusion, reaction, and adsorption in a spherical nature porous particle as detailed below:

$$\frac{\partial C}{\partial t}+\frac{(1-\varepsilon)}{\varepsilon}\frac{\partial Q}{\partial T}=\frac{1}{r^2}\frac{\partial}{\partial r}\left(D\frac{\partial C}{\partial r}\right)-\frac{(1-\varepsilon)}{\varepsilon}kC \quad , \tag{2.9}$$

with boundary conditions:

$$\left.\begin{aligned} C&=0 \qquad at \;\; X=0\\ \frac{\partial C}{\partial X}&=0 \qquad at \;\; X=1\end{aligned}\right\} \quad \text{for } \; T\geq 0\,, \tag{2.10}$$

and the initial condition as in equation (2.3)

The linear adsorption isotherm was assumed in a state of equilibrium i.e., $Q=kC$.

The study compared the concentration profiles of LDF (Linear driving force) formulas with the exact solution and found results in good agreement.

Ma and Guiochon (1991) used orthogonal collocation on a finite element (OCFE) method for the process of integration of a kinetic model and compared the derived results with the finite difference method (FDM). Ma and Guiochon (1991) derived the numerical solution for a nonlinear model (dimensionless) of chromatography given as:

$$\frac{\partial C_i}{\partial T}+\mu\frac{\partial Q_i}{\partial T}=D\frac{\partial^2 C_i}{\partial Z^2}-u\frac{\partial C}{\partial Z} \quad , \tag{2.11}$$

$$\frac{\partial Q_i}{\partial T}=K_i(f(C_1,C_2,.....)-Q_i)\,, \tag{2.12}$$

where C_i, Q_i are the concentration of the i^{th} compound in the mobile and stationary phase, K_i is the mass transfer coefficient in the i^{th} compound, and $f(C_1,C_2,.....)$ is the equation of equilibrium isotherm. The initial and boundary conditions are given as:

$$C(X,0)=1. \tag{2.13}$$

$$\left.\begin{array}{ll} Pe\,C = \dfrac{\partial C}{\partial X} & at \;\; X = 0 \\ \dfrac{\partial C}{\partial X} = 0 & at \;\; X = 1 \end{array}\right\} \text{ for all } \quad T \geq 0, \tag{2.14}$$

The study supported the special advantage of the finite element method (FEM) in terms of computation time, as a shorter time was taken in calculations in comparison with the FDM for transitory phenomena which take place in a 3-D space. The study further held that the FEM uses interpolation for each element whereas a step function to approximate the solution was used with the FDM. The study preferred the OCM because it has the advantage of calculating the solution profiles with high efficiency. Moreover, this method needs less computation time to update the elements and is beneficial for a situation where the re-collocation is taken. This technique helps to achieve more accurate results in calculations for diffusion problems and is beneficial for local estimation and grid refinement. The study also highlighted that selection of diffusion-coefficient plays the main role in the use of computer programs and proves the efficiency of the technique.

Dawson (1995) presented the upwind-mixed FEM to compute the numerical solution of the advection-diffusion equation given as:

$$(\phi c)_t + \nabla.(uc - D\nabla c) = q\tilde{c} \text{ on } \Omega \times [0,T] \;, \tag{2.15}$$

where Ω denotes the spatial domain in R^2, c is the concentration in flowing medium, $\tilde{c}$ is the concentration at sources, u is fluid velocity and D is diffusion tensor dependent on u. Dawson (1995) presented the solution of the equation using an implicit scheme that forms a non-symmetric system of an equation that is difficult to solve. He suggested that explicit schemes are beneficial for time-dependent problems. Moreover, these schemes can be extended to solve nonlinear advection problems with upwind differences.

While describing the process of porous structure, Kill et al. (1995) explored the mathematical models that are expressed in terms of parabolic PDEs involving temporal and spatial derivatives. The study assumed the particles as of constant size and isothermal in nature. The effective diffusivity in the particles was taken constant and the external mass transfer resistance was neglected. Besides, the rate of the first order was taken in the concentration of the gaseous reactant. The differential equations were transformed into a set of initial value problems using the OCM. The method was found to be an effective solution technique for the problems encountered in heat and mass transfer processes.

Kukreja (1996) discussed the pulp washing process in detail and derived the complete mechanism for mathematical models of different zones of pulp washing. All stages like washing and dewatering zone and the related equations are also explained in detail. The efficiency parameters related to pulp washing like displacement ratio, wash ratio, efficiency and dilution factor are also discussed.

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial z^2} - u \frac{\partial c}{\partial z} - \frac{(1-\varepsilon)}{\varepsilon} \frac{\partial n}{\partial z}, \qquad (2.16)$$

With different boundary and initial conditions.

The model equations are solved using Laplace transform method and results are validated from the data of a rotary vacuum washer. The study has also given the information about important parameters like bed porosity, cake thickness, time of washing, interstitial velocity, mass transfer rate and amount of wash water added on pulp washing.

Zheng and Gu (1996) solved the model equation describing the fixed bed tabular reactor of one-dimensional mass balance equation involving axial dispersion given as:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial z^2} - u \frac{\partial c}{\partial z} - \frac{(1-\varepsilon)}{\varepsilon} R, \qquad (2.17)$$

where R is the consumption rate of the reactant. The study used the Laplace transform method to approximate the analytical solution. The experimental data on glucose was used to examine the effluent concentrations for different flow rates in the study. Further, the study proved that the exact value of concentration was in good agreement with the results for a lower value of Pe and Bi. Also, the effluent concentration can reach the steady-state value faster after the startup period, but the conversion ratio was found to be lower with the increase in Pe and decease in Bi. Further, more accurate results can be derived by increasing the number of partitions for higher values of Pe and Bi.

In a study, Potůček (1997) gave a detailed description of the one-dimensional plug flow models (dimensionless) considering axial dispersion as:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial z^2} - \frac{u}{\varepsilon} \frac{\partial c}{\partial z}. \qquad (2.18)$$

The study used the boundary conditions considered by Brenner (1962) which were suitable for the displacement process and applied the cubic spline method to solve the model. The solution of the axial dispersion model describing the miscible fluid displacement in beds with finite thickness was expressed in terms of exit solute concentration. The study predicted the washing efficiency as a function of Pe. It has an inverse relation to the diffusion coefficient and plays an important role in evaluating the washer performance. The study further explained that the shape of the breakthrough curves indicates the flow rate of displacement washing through the pulp bed and must lie between the ideal limits of perfectly mixed flow and plug flow. Based on experimental results, the study proved that the increase in initial bed lignin concentration decreases the wash yield. Potůček (1997) further noticed that the type of pulp or fibre characteristics were the main variable that affect the dispersion coefficient. Despite this, the average pore size, the difference in geometry, and the pore size distribution that occurs in fibre material were influencing dispersion in the pulp bed.

Liao and Shiau (2000) established that the analytical solution is fitted to the experimental data by considering the practical example of an activated carbon fixed bed adsorber used to remove phenol from wastewater. The study used the axial dispersion model (dimensionless) to estimate the kinetic behavior and proficiency of a fixed bed adsorber given as:

$$R_d \frac{\partial C}{\partial T} = \frac{1}{Pe} \frac{\partial^2 C}{\partial X^2} - \frac{\partial C}{\partial X}, \qquad (2.19)$$

with boundary conditions:

$$\left.\begin{aligned} C &= 0 \qquad && at \quad X = 0 \\ \frac{\partial C}{\partial X} &= 0 \qquad && at \quad X = 1 \end{aligned}\right\} \qquad \text{for} \quad T \geq 0, \qquad (2.20)$$

and the initial condition:

$$C(X,0) = 1, \qquad (2.21)$$

where R_d is the retardation coefficient defined as the removal rate of adsorbed solute on the particle surface. The study used the analytic and numerical technique to solve the above model with linear adsorption isotherm and experimentally examined the validity of this model. Liao and Shiau (2000) proved that a rapid converging solution can be derived using the Laplace transform and used a series expansion technique to solve the model for a small value of *Pe*. The case of perfect mixing and perfect displacement were discussed, and it was suggested that an asymptotic solution is used to examine the conditions when R_d is small and *Pe* is large. The mixing effect was more when the value of *Pe* was low by keeping the value of R_d as constant. In the case when *Pe* was constant and the value R_d was large, the level of breakthrough curves rises more slowly, and a larger breakthrough time was needed in this condition. The large value of *Pe* and constant R_d made the effluent concentration of adsorbate reached the influent concentration rapidly, however, it needed a larger breakthrough time. In the case of small *Pe* and constant value of R_d, the breakthrough curve gave a similar effect.

Szukiewicz (2000) highlighted that the fixed-bed reactors are normally used for heterogeneous catalytic processes in the industry. The study suggested two groups of models: pseudo homogeneous and heterogeneous models. The first type of model considered the same temperature and constituent concentrations in the catalyst particles and fluid bulk. Owing to this assumption, these models were expressed as PDEs for the fluid phase only and are comparatively easy but generally are of low accuracy. The other method for the mathematical model was considered for the adsorption and diffusion process. The later type of model considered fluid and the catalyst pellets described by PDEs were mainly used for reactors and gave accurate results in comparison to the first type. Szukiewicz (2000) presented an approximate model for the diffusion and reaction process with high accuracy which was useful for the process of diffusion-reaction in porous catalysts and process that considers internal diffusion and adsorption given as:

$$\frac{\partial c}{\partial t}=\frac{\partial^2 c}{\partial x^2}+\frac{2}{x}\frac{\partial c}{\partial x}-\phi^2 R_A(c)\,. \qquad (2.22)$$

It was found that more accuracy can be achieved in short time when the Thiele modulus (ϕ), which is the ratio of reaction and diffusion rate, is higher.

While extending his earlier work, Szukiewicz (2001) derived the effect of the Thiele modulus and *Bi* and highlighted that the external mass-transfer resistance decreases when the value of the Thiele modulus increased that affects the chemical reaction. The study observed that the accuracy of calculations is higher influenced by *Bi* and found that accuracy of the approximate model was better when the *Bi* was small, and the Thiele modulus was large. The accuracy of the approximation model was very high for the entire range of Thiele modulus regardless of external mass-transfer resistance and the geometry of the pellet.

Shiraishi (2001) solved the axial dispersion model (dimensionless) which is extensively used for tubular flow reactors and combines the effect of the chemical reaction and reactant flow given as:

$$\frac{1}{Pe}\frac{d^2C}{dX^2}-\frac{dC}{dX}=kC^n\,. \qquad (2.23)$$

The study used the numerical method in which the fundamental differential equation was transformed into S-system (synergistic and saturable system) canonical form and was solved with the shooting method combined with the Taylor's series method. Also, this scheme was used to investigate the accuracy of numerical solutions for the range of parameters such as *Pe*, dimensionless kinetic constant (*k*), and reaction order (*n*). The was also proposed that the method is also beneficial for numerical calculations in the engineering field and gives accurate results up to three significant digits.

Carrara et al. (2003) considered the mathematical model associated with substrate concentration profile involving mass transfer resistance, axial dispersion flow, and an isothermal tubular reactor given by:

$$\frac{1}{Pe}\frac{d^2C}{dz^2}-\frac{dC}{dz}-C_tC(1-\alpha)=0\,, \tag{2.24}$$

where C_t is dimensionless mass transfer coefficient, C is dimensionless substrate concentration in bulk motion, z is dimensionless axial co-ordinate, and α is dimensionless substrate concentration. The study discussed the solution of a mathematical model describing the dispersion flow in the reactor represented by a second order PDE using OCM based on an approximation of the solution using a series. The solution of this equation accurately determined the effect of important factors involved in this process such as back mixing, and diffusional resistance to improve the theoretical values obtained.

Farooq and Karimi (2003) considered the two-dimensional (2D) model involving diffusion in both axial as well as radial directions.

The mass balance equation for the solute in a radial direction is:

$$\frac{D_m}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)=v(r)\frac{\partial c}{\partial x}-D_m\frac{\partial^2 c}{\partial x^2}\,, \tag{2.25}$$

where D_m is molecular diffusivity, c is the concentration of solute in fluid, v is fluid velocity, r is the radius and x is the axial distance. The boundary conditions and initial conditions are the same as considered by Brenner (1962).

The dispersed plug flow model involves axial dispersion as:

$$D_L\frac{\partial^2 c}{\partial x^2}=v\frac{\partial c}{\partial x}+\frac{2k}{R}c\,, \tag{2.26}$$

where D_L is axial dispersion coefficient, v is the average fluid velocity, k is mass transfer coefficient, c and is the mixing cup concentration of solute at the axial plane. The radial diffusion and radial concentration gradient are not considered in the plug flow model, but only axial dispersion is involved.

An iterative technique was used in the study to solve the model equations by reducing them into a one-dimensional dispersed plug flow model and it proved that the solution of the plug flow model is improved consistently. It also determined that the error of this model is increased when there is a decrease in the wall resistance.

Renou et al. (2003) explained that the mathematical formulation of isothermal tubular reactors using mass balances form a system of PDEs used to describe the convection-dispersion-reaction equations. The derived dispersion model in the form of a well-known second-order parabolic equations that deals with non-ideal reactors as:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z} - r(c), \qquad (2.27)$$

where *c (z, t)* is the concentration in the reactor, *D* represents the dispersion coefficient, *v* represents the superficial velocity and *r* represents the reaction kinetics.

The study proposed the sequencing method to prove the superiority and accuracy of the method over traditional methods. It highlighted some advantages of this method such as simplicity and real-time applicability and discussed that in many problems like instability and oscillation, solution arise due to small dispersion coefficient with inappropriate use of the Danckwerts' boundary conditions. Besides, it emphasized that the major factors such as convection and dispersion influence the accuracy of the solution. It also highlighted the applicability of the method for the numerical simulation of the model as a useful tool for an industrial application.

Dehghan (2004) presented the comparison of different numerical techniques for solving the one-dimensional PDE used to describe the quantities such as heat, mass, energy, and vorticity involved in the advection-diffusion equation given as:

$$\frac{\partial c}{\partial t} = \alpha \frac{\partial^2 c}{\partial z^2} - \beta\frac{\partial c}{\partial z} \quad \text{for } 0 < z < 1 \quad \text{and} \quad 0 < t \le T, \qquad (2.28)$$

where α and β are positive constants measuring the diffusion and advection practices respectively.

The implicit BTCS-type finite-difference technique in which the centered-difference scheme was applied for the advection and diffusion term involving spatial derivative and backward-difference scheme was applied for the terms involving time derivative. Dehghan (2004) also described the disadvantage of this scheme owing to the consumption of more CPU time for the procedure and explained that the upwind implicit formula used to approximate PDE is accurate for the first order and justified the use of the Crank-Nicolson scheme for spatial derivatives by proving the second order accuracy. The study highlighted that the time required using explicit FDM is about 3 times smaller in comparison to implicit finite difference schemes.

Coimbra et al. (2004) used the technique of moving finite element method (MFEM) for discretizing the continuous bending spatial grids of the time dependent PDE involved in phenomena related to moving fronts, shocks, and pulses.

The study deals with two one-dimensional problems from mathematical biology describing the flow across a nerve membrane and problems related to the chemical engineering process connecting with convection, diffusion, and reaction. It considered the diffusion–convection–reaction model as:

$$\frac{\partial C}{\partial T} = \frac{\partial^2 C}{\partial X^2} - \lambda \frac{\partial C}{\partial X} - \phi^2 C, \tag{2.29}$$

where C is normalized concentration, X is normalized space variable, t is time variable normalized by diffusion time constant, λ is intra-particle Peclet number and ϕ is Thiele modulus. Coimbra et al. (2004) also derived the results for different values of Pe and ϕ and mentioned the time consumed in this work. The numerical results revealed the capacity of the method to derive the solution with accuracy for time-dependent problems even in the case of a few nodes for the space grid. Further, the method was expanded to simulate the 2D model of a fixed bed reactor associated with heat transfer in both radial and axial dispersions.

Arora et al. (2005) considered the diffusion-reaction problem with different boundary conditions and explained in detail the OCFE method and its convergence criteria with relative error in their work. While solving the linear model proposed by Brenner (1962), it was discussed that the axial dispersion coefficient became higher than the convection for a small value of Pe because the differential element solute added into the bed immediately mixes up with the bed. The study reported that the solution profile follows a Gaussian curve. When the value of Pe increases, elements needed in the spatial domain are greater than 20, however, only 5–7 elements were required when Pe is small. It also highlighted that the large value of Pe makes the outcome of convective transport small. Due to this, a stiffer system of equations was noticed and found that the target of sufficient accuracy of the numerical solutions can be achieved by adding more elements. It was also explained that the relative error was reduced by adding more elements in the domain and supported that although the number of equations was increased with more collocation points and consumption of excess time to achieve the target, however, the same got balanced when the magnitude of relative error was reduced.

Karahan (2006) proposed a numerical scheme to solve the one-dimensional advection-diffusion equation (ADE) describing the transport and diffusion process as:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - u\frac{\partial c}{\partial z} \quad \text{for} \quad 0 < z < L \quad \text{and} \quad 0 < t \le T. \tag{2.30}$$

The study proposed FDM using implicit spreadsheet simulation (ADEISS) for change in spatial and temporal weighted parameters. It obtained the solution using the backward time-centered space (BTCS), upwind scheme, and Crank–Nicolson schemes. Karahan (2006) reported that finite difference is a well-established numerical technique applied to approximate the flow and transport modeling. It was also discussed that the problems associated with environmental pollution for groundwater, rivers, coasts, and the atmosphere can be handled with the mathematical model of diffusion–dispersion that describes the diffusion and transport process.

In a study, Arora et al. (2006) solved another pulp washing model involving the parameters such as *Bi* and *Pe* given as:

$$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial X^2} - \frac{\partial C}{\partial X} - \frac{\mu Bi}{Pe}C, \tag{2.31}$$

with boundary conditions:

$$\left.\begin{aligned} C &= 0 \qquad && at \;\; X = 0 \\ \frac{\partial C}{\partial X} &= 0 \qquad && at \;\; X = 1 \end{aligned}\right\} \quad \text{for} \;\; T \ge 0, \tag{2.32}$$

and the initial condition:

$$C(X,0) = 1. \tag{2.33}$$

The study divided the domain into 25 elements and took three interior collocation points to discretize the model equation. It was noticed that the relative error was nearer to zero for $Pe < 20$ and $Bi < 5$ and achieved stability of numerical results for $Pe > 60$. The model associated with the diffusion-reaction problem given by Liao and Shiau (2000) involving R_d with the OCFE was solved and it was observed that absolute percentage error was less tinct values of Pe and $R_d = 1.25$. For $Pe = 40$ and different values of R_d, the error was less than 1% using OCFE as compared to OCM.

Arora et al. (2006) solved the second model and considered the heat equation (dimensionless) as:

$$\frac{\partial C}{\partial T} = \frac{\partial^2 C}{\partial X^2}, \tag{2.34}$$

with boundary conditions as:

$$\left.\begin{aligned} \frac{\partial C}{\partial X} &= 0 \qquad at \;\; X = 0 \\ C &= 0 \qquad at \;\; X = 1 \end{aligned}\right\} \quad \text{for } \; T \geq 0. \tag{2.35}$$

The collocation points were chosen as the zeros of both Legendre and Chebyshev polynomials and found the least relative error with Legendre polynomials. Therefore, it was strongly recommended that the Legendre zeros should be employed as the collocation points instead of Chebyshev zeros. Thereafter, the model of a diffusion-reaction problem (dimensionless) was considered as:

$$\left(1 + \frac{\mu^*}{(1+KC)^2}\right)\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z}, \tag{2.36}$$

where $\mu^* = Ac_0\mu$, $K = Bc_0$

The boundary conditions and initial condition was same as used by Brenner (1962).

It used Langmuir adsorption isotherm for the problem and observed the results of solution profiles for different values μ^*, K , Pe expressed as breakthrough curves which smoothly converge to zero even, when Pe takes large values.

The model of the non-linear diffusion-reaction problem(dimensionless) was given as:

$$\frac{\partial C}{\partial T} + \mu\frac{\partial Q}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z}, \tag{2.37}$$

$$\frac{\partial Q}{\partial T} = P^*(c_0 C(1-Q) - kQ), \tag{2.38}$$

where $P^* = k_1\frac{L}{u}$, $K = \frac{k_1}{k_2}$,

with boundary and initial conditions same as those used by Brenner (1962), the problem involved the mass transfer coefficient and described the performance of miscible fluids during washing and sorption operations. Further, it was reported that the solution profile smoothly approached to steady state situation when the time was increased. The data for simulation purposes was taken from Grähs (1974). The results of OCM and OCFE for $Pe = 71$ and $P^{*} = 0.01983$ were compared and smooth convergence of solution profile to zero was observed.

Tervola (2006) discussed practical applications of the advection-dispersion model used for one-stage cake washing in the fields of pulp fibre, clays, lime mud, and many more as:

$$\frac{\partial C}{\partial T} = \frac{1}{4Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z}, \tag{2.39}$$

with boundary and initial conditions as used by Brenner (1962).

The research used a modified asymptotic formula and Fourier series method based on the Laplace transform to solve this model problem. It explored the solution of the multistage countercurrent pulp washing model to investigate the results of wash effluent movement. It was described that the segregated wash effluent circulation was an attractive option to recover the solute in the process of cake washing and was frequently applied in the pulping chemical industry. The results revealed that a bigger portion of solute was removed, when the *Pe* was high and very small *Pe* was not a case suitable for efficient cake washing. Further, the fraction of solute residing in the cake was reduced with an increase in the *Pe*. Likewise, when wash ratio was nearer to one, the highest portion of effluent solute was detached from the cake. The area for wash liquor became narrow when the *Pe* was high, which made the recovery of the solute better. Because in this case, the entering wash liquid entirely mixed up with the entire content and detached from the element with the same amount of the wash liquor.

Singh et al. (2008) considered the differential equation describing the model of filter cake washing based on longitudinal mixing phenomena by overlooking the accumulation capacity of fibers as given by Brenner (1962).

The problem used to describe the longitudinal dispersion in porous media given as:

$$u\frac{\partial c}{\partial x} + \frac{\partial c}{\partial t} + \left(\frac{1-\varepsilon}{\varepsilon}\right)\frac{\partial n}{\partial t} = D_L\frac{\partial^2 c}{\partial x^2}, \tag{2.40}$$

The adsorption isotherm taken at a finite rate as given below:

$$\frac{\partial n}{\partial t} = k_1 c - k_2 n. \tag{2.41}$$

The model was solved using “pdepe” solver with MATLAB and proved the efficiency of the method by comparing the results with the earlier work of Brenner (1962), Grähs (1974), and Kumar et al. (2010). The study achieved good accuracy of numerical results for the pulp washing model considering the particle diffusion and axial dispersion with negligible error.

Arora and Potuček (2012) explained the mechanism of mass transfer rate between fibers and fluid with the 2D model equations. The study revealed that the existing solute in the pores of fibers was drawn-out when the external fluid was introduced into the porous structured bed. Fick’s law was used to describe the transfer of solute inside the fiber pores. Film resistance mass transfer coefficient (k_f) controls the mass transfer from the stationary layer between the external fluid and fiber. This state was described by the model equation in the particle phase given as:

$$\frac{\partial q}{\partial t}+\frac{(1-\beta)}{\beta}\frac{\partial n}{\partial t}=\frac{k_f}{KR}(c-q)\,. \qquad (2.42)$$

The Langmuir adsorption isotherm is used to explain the first type of mechanism rate associated with displacement washing of pulp fibre bed for fluid flow as:

$$\frac{\partial n}{\partial t}=\frac{qk_1}{C_0}\left(N_0-n\right)-k_2 n\,. \qquad (2.43)$$

The mathematical model for bulk fluid is a phase in which the impurities adsorbed within fiber pores and on fiber surface are washed away by the introduction of external fluid. The impurities get detached from the surface of the fiber and mix with external fluid by dispersion which was expressed by D_L (axial dispersion coefficient) and was independent of L (axial distance) described as:

$$u\frac{\partial c}{\partial x}+\frac{\partial c}{\partial t}+2\left(\frac{1-\varepsilon}{\varepsilon}\right)\frac{k_f}{KR}(c-q)=D_L\frac{\partial^2 c}{\partial x^2}\,, \qquad (2.44)$$

with boundary condition

$$uc-D_L\frac{\partial c}{\partial x}=0 \quad \text{at} \quad x=0 \quad \text{and} \quad \frac{\partial c}{\partial x}=0 \quad \text{at} \quad x=L\,. \qquad (2.45)$$

The model equations were solved with OCFE and the applicability of the method was checked by comparing the predicted values with the experimental values. The parameters like *Bi* and *Pe* depend upon axial dispersion coefficient and interstitial wash liquid velocity. However, the interstitial velocity varies with the change in bed porosity and was described by Darcy's law. It was regulated with the help of bed consistency along with a specific volume of fibers. The study verified the theoretical behavior for concentration profiles at the exit solute level for different values of *Pe* and *Bi* =10. It was noticed that the solution profile takes more time to reach the steady state condition for *Pe* = 10 in comparison to *Pe* = 30. Yet, for *Pe* > 30 less significant influence on solution profiles was observed. Further, the study considered the cake thickness comparatively small, therefore, the solute takes more time to leach from fiber surface and this contributes to small *Pe*. A significant effect on solution profile was observed for *Pe* < 30 and *Bi* <10.

Kumar et al. (2009) considered the transport equations involving mass transfer and diffusion based on material balance equations. These transport equations along with the various boundary conditions and the adsorption isotherms were used to express the equilibrium between the solute concentration in the liquor and on the fibers. These equations collectively described the mathematical models of pulp washing involving particle diffusion and axial dispersion such as:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x} - \left(\frac{1-\varepsilon}{\varepsilon}\right)\frac{\partial n}{\partial t}, \qquad (2.46)$$

where D_L is the dispersion coefficient, *u* is the speed of liquor in cake pores, ε is the bed porosity, *t* is time, *x* is the cake thickness, *c* is solute concentrations in liquor and *n* is solute concentrations in fibre.

These transport equations along with the two boundary conditions are the same as those used by Brenner (1962) and Grähs (1974). The adsorption isotherms used to express the equilibrium between the solute concentration on the fibers and in the liquor are given as:

$$\frac{\partial n}{\partial t} = k_1 c - k_2 n, \qquad (2.47)$$

where k_1 and k_2 are mass transfer coefficients.

The system of equations was solved using the “pdepe” solver with MATLAB code and proved that the technique was more appropriate and took less time than the previous techniques. These pulp washing models were used to explain the washing performance in respect of different input parameters like mass transfer coefficient, longitudinal dispersion coefficient, interstitial velocity, and total porosity of the cake. These input parameters were joined to derive the dimensionless parameters such as *Pe* and D_L. The variation in the longitudinal dispersion coefficient and interstitial velocity was observed when the length of the bed was assumed constant.

Sari et al. (2010) proposed the FDM up to the tenth order in space with a combination of the Runge-Kutta method in time to solve the one-dimensional advection-diffusion equation and solved two examples with different values of velocity (u) and diffusion coefficient (D) given as:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x} \quad \text{for } a < x < b \text{ and } 0 < t \leq T. \tag{2.48}$$

The study described the high-order differences using Taylor's series expansion. The numerical computations corroborate accurate results as compared to the work of previous researchers.

Kumar et al. (2010) presented the work on the mathematical model that emphasizes the four stages of the counter-current washing system. The work was based on some assumptions such that pulp fibers packed bed considered to have symmetrical cylindrical fibers of homogeneous structure. The instant behavior of such type of system is described by an equation that involves the variables and their partial derivatives. Two models with different boundary conditions are explored using a "pdepe" solver with MATLAB and experimental data of Grähs (1974) by Kumar et al. (2009) with nonlinear adsorption isotherm as $n = \frac{ABc}{1+Bc}$ for Pe=71.26. It was concluded that boundary conditions have not much significant effect on the washing results.

Dhawan and Kapoor (2011) explored that the advection-dominated transport problems are generally fragmented into a diffusion equation and advection equation given as:

$$\frac{\partial c}{\partial t} + \alpha\frac{\partial c}{\partial x} = k\frac{\partial^2 c}{\partial x^2}, \tag{2.49}$$

where t is the temporal variable, x is the spatial variable, and $k, \alpha > 0$ measures diffusion and advection process respectively.

The equation depends on the advection coefficient and diffusion coefficient. This turns into parabolic when diffusion dominates or hyperbolic in the process when advection dominates. The results of the transport equation were validated by comparing the present algorithm with analytical solutions in unsteady non-uniform flow. The ADE was numerically solved using the B-spline finite element technique and explained that the method is capable enough to produce highly accurate results as compared to the other polynomial approximations.

Roininen and Alopaeus (2011) explored the fixed bed adsorber which is expressed in the form of a dimensionless model equation given by Liao and Shiau (2000) using the moment method to solve the flow systems involving reaction and axial dispersion with Danckwerts boundary conditions.

The cubic polynomials are used in this technique and the results are obtained with MATLAB ode15s solver. The velocity is considered as constant, but *Pe* and *Da* (Damköhler number) contribute a major role in the numerical approximation of concentration profiles. The study revealed that better approximations can be derived by dividing the domain into more elements and the error decreases more speedily when higher order polynomials or when variables are increased. An increase in *Pe* shows fluctuations that lead to the situation of negative concentrations. Besides, the R_d affects the shape of the breakthrough curve only for the comparatively low *Pe*. It was found that less computational time is used by the OCFE method in comparison with the moment or Galerkin method because the least number of operations are needed for a time step.

Ahmed (2012) explored the ADE widely applicable in industrial practice given as:

$$\frac{\partial c}{\partial t}+\alpha\frac{\partial c}{\partial x}=\beta\frac{\partial^2 c}{\partial x^2}, \tag{2.50}$$

The high value of *Pe* causes oscillations or more damping in numerical results. It was also noticed that error in numerical results is large with an increase in space size and can be minimized by reducing space size and step size of time.

Dhawan et al. (2012) explained the transport phenomena, which is a natural process, that takes place in the fluids along with the combination of advection and diffusion is given by:

$$\frac{\partial c}{\partial t}+\varepsilon\frac{\partial c}{\partial x}=\rho\frac{\partial^2 c}{\partial x^2} \quad \text{for} \quad 0\le x\le L,\ t>0. \tag{2.51}$$

The technique of B-spline functions along with FEM was used to solve this model and a major reduction in the computational cost was observed, while solving the problem. The performance of the scheme is tested for different numerical examples by comparing the accuracy and derived satisfactory results.

Gupta and Kukreja (2012) explored the cubic spline collocation method (CSCM) to solve two linear model equations used by Arora et al. (2006) and one nonlinear problem describing the diffusion–dispersion and adsorption-desorption phenomenon in porous media. The relative error was noticed to be decreasing with this method as compared to OCM and fluctuations was observed with OCM at the initial stage. Gupta and Kukreja (2012) proved that the accuracy of the results can be achieved with an increase in the number of elements for *Pe* in the range of 10 to 40 and results were stable after the division of the domain into 150 elements, when the value of *Pe* is 200. At least second-order uniform convergence was achieved and relative errors and L_2 norm decreased with an increase in mesh points. For the axial dispersion model, the numerical results were compared with OCM and OCFE in terms of elapsed time. It was noticed that solute takes a lesser mean residence time, when comes out from the bed, for *Bi* = 7.5 and *Pe* = 60 in comparison with *Bi* = 1.5 and *Pe* = 10 due to small axial dispersion. As well as the ratio L/D_L was increased, the *Pe* and *Bi* becomes large. This yields the piston-like effect on wash water to remove the solute from bulk fluid due to the cause of less diffusion–dispersion.

This study also considered a nonlinear, non-homogeneous, parabolic equation that describes the behavior of miscible fluids during sorption and washing operations given as:

$$D_L \frac{\partial^2 c}{\partial z^2} = U \frac{\partial c}{\partial z} + \frac{\partial c}{\partial t} + C_F \left(\frac{1-\varepsilon}{\varepsilon} \right) \frac{\partial n}{\partial t}, \tag{2.52}$$

where the solute concentration of the fibre and liquor are linked via Langmuir adsorption isotherm:

$$n = \frac{A_0 c}{1 + B_0 c}. \tag{2.53}$$

The model was solved with CSCM, and the data of Grähs (1974) was used for simulation. It was also proved that washing efficiency increased due to less back mixing, for small D_L. The diffusion of solute from particle pores is reduced when the interstitial velocity was increased due to an increase in axial dispersion and cake thickness. This improved the washing efficiency subject to certain consistency limits.

Ganaie et al. (2013) considered the mass balance equation describing the packed bed containing the symmetrical porous particles (homogeneous in nature) from which wash water moves represented by an axial dispersion model as:

$$u \frac{\partial c}{\partial z} + \frac{\partial c}{\partial t} + \left(\frac{1-\varepsilon}{\varepsilon} \right) \frac{\partial q}{\partial t} = D_L \frac{\partial^2 c}{\partial z^2}, \tag{2.54}$$

with the same boundary and initial condition as taken by Singh et al. (2008) and adsorption isotherm as:

$$q = kc. \tag{2.55}$$

The mixed collocation method with collocation points of shifted Chebyshev polynomials was used to solve the model. The results for *Pe*=0, 32, and 80 in terms of relative error were compared and perfect agreement between the analytic and numerical results was noticed. The error was decreased with an increase in collocation points but after 15 interior collocation points the concentration profiles started overlapping and not much significant change was observed. The concentration profile has a faster rate of convergence and was more peaked for *Pe*= 200.

Mittal et al. (2013) considered diffusion–dispersion, adsorption-desorption phenomena of the porous structured pulp bed for the linear model explored by Arora et al. (2005) and nonlinear model equation used by Gupta and Kukreja (2012) and solved these models with CHCM. The collocation points as the roots of shifted Chebyshev polynomials were taken. The numerical results derived using CHCM were very close to the analytic solution than previous results of OCM and OCFE. The rate of convergence of CHCM was found quadratic with the choice of Chebyshev roots. The concentration of solute at exit level was found to be dependent on *Pe* which is the ratio of axial dispersion coefficient (D_L) and convection (uL). The industrial parameters such as bed efficiency and displacement ratio were also estimated.

Chaplya et al. (2013) solved the mathematical model for the prediction of pollution spread in the porous structure of soil related to the process. The diffusion problem for a two-phase layer with a diffusion coefficient involving the mechanism of advective mass transfer was considered. The first equation related to mass transport by diffusion and advection and the second assumes velocity as constant given as:

$$v\frac{\partial C_1}{\partial x} = D_1\left(\frac{\partial^2 C_1}{\partial x^2} + \frac{\partial^2 C_1}{\partial y^2}\right) \quad \text{and} \quad D_2\left(\frac{\partial^2 C_2}{\partial x^2} + \frac{\partial^2 C_2}{\partial y^2}\right) = 0\,, \tag{2.56}$$

Where D_1 and D_2 are diffusion coefficient, C_1 and C_2 are concentrations, v is advective velocity and x and y are directions. The study proposed the technique of integral transform for each domain to derive the analytic solution for a diffusion problem. The process of mass transfer was depended on various parameters like structure, porous media, and dispersion.

Robalo et al. (2013) studied the model based on the displacement washing operation describing the displacement of homogeneous solute by introducing a solvent as follows:

$$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial X^2} - \frac{\partial C}{\partial X} - \frac{\mu Bi}{Pe}C\,, \tag{2.57}$$

The Dirichlet and Neumann boundary conditions were used at the inlet and exit of the bed. The model also comprised the equation describing mass transfer in particles of the porous structure. The numerical solution of one-dimensional parabolic equation using the MFEM method was used to approximate polynomial in each finite element. The numerical outputs obtained were validated and compared with the existing analytic solution obtained by previous researchers. The study highlighted that MFEM gives an accurate solution for the model with a small number of spatial node points. Also, the CPU time used to complete the whole process was very less compared to previous techniques. It was observed that extra effort is needed to complete the process with an increase in *Pe*.

Jia et al. (2013) described the enhanced oil recovery practices which are solvent-based increasing the attention to the production of the crude oil reserves. The convection, dispersion, and molecular diffusion are considered the main mass transfer structures for crude oil and solvent vapor mixing. The models of advection-diffusion that describes the process of mass-transfer with different states of diffusion and flow velocity considered as:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x} - cv \right), \tag{2.58}$$

where, the concentration of solvent in the crude oil is represented by c, v represents the flow velocity, D represents the diffusion coefficient, and x represents the space variable.

The Dirichlet and Neumann boundary conditions were applied at the transition zone boundary and assumed that at the initial stage that the model is free of solvent. The semi-analytical solutions were derived for these models with the extraordinary approximation scheme and Laplace transformation. The numerical results were validated with the existing analytical solution and the value of *Pe* was helpful to estimate the results with more accuracy. Besides, the proximity of the solution profile was improved with the change due to the linear relation between D, v and *Pe*. The role of flow velocity was noticed much more than the diffusion coefficient in the mass-transfer procedure of crude oil–solvent.

Duque et al. (2014) used FEM with moving mesh to solve the equation involving adsorption for porous medium. The domain was partitioned into a finite number of elements and the interpolating polynomials such as Lagrange were used to estimate the solution for each finite element. Then derived system of ODEs was solved using the Gaussian quadrature. The better estimation was achieved by increasing the degree of interpolating polynomials and using an adequate grid with a small number of finite elements.

Kar et al. (2014) considered a radiative and dissipative visco-elastic flow problem for the porous stretched sheet. This phenomenon was mainly applicable to the polymer industry in sheets stretching with a dissipative environment and is described by the two-dimensional convective steady laminar flow equation for species concentration as:

$$u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}=D\frac{\partial^2 c}{\partial y^2}-K(c-c_\infty)\,, \tag{2.59}$$

where D is the diffusion coefficient and K is the chemical reactor parameter.

The Kummer's function (hypergeometric function) was applied to estimate the heat and mass transfer equations. It was observed that when diffusive fluid was low, the reduction in the rate of heat transfer was due to the presence of porous structure, heat source, and radiation. On the other hand, the rate of mass transfer was reduced when the diffusing species are heavier, the chemical reaction rate is higher, suction is stronger, and a porous matrix structure is present.

Okhovat et al. (2014) considered the 2-dimensional, incompressible, isothermal, steady state convection-diffusion models to examine the mass transfer performance of the structure and solved the equations simultaneously. The combination of computational fluid dynamics (CFD) and a mathematical model was developed to explore the erosion-corrosion phenomenon applicable in two-phase fluid transport pipelines. The behaviors of the detaching and re-fixing impacts of flow lines were examined and results were compared with experiments in practical geometry and good agreements with the experimental results was noticed in this work.

Gupta et al. (2015) solved a 2-dimensional model for the particle phase and fluid phase. The particle diffusion model was virtuous to represent the solute accumulation on the fiber surface described as:

$$D_F\left(\frac{\partial^2 q}{\partial r^2}+\frac{1}{r}\frac{\partial q}{\partial r}\right)-\frac{\partial q}{\partial t}-C_F\,\frac{(1-\omega)}{\omega}\frac{\partial n}{\partial t}=0\ , \tag{2.60}$$

with adsorption isotherm as:

$$n=\frac{qN_i}{C_F k^{-1}+q}\,. \tag{2.61}$$

The boundary conditions used to describe the solute exchange between the fiber surface and the bulk fluid are related to mass transfer rates given as:

$$\frac{\partial q}{\partial r}=0 \quad \text{at} \quad r=0 \quad \text{and} \quad -D_F\left(\frac{\partial q}{\partial r}\right)=\frac{k_f\omega}{K}\left(q\,|_{r=R}-c\right) \quad \text{at} \quad r=R\,. \tag{2.62}$$

where c (z, t) is solute concentration in fluid, q (z, t, r) is solute concentration inside the pores, *n* (z, t, r) is adsorbed solute concentration on the fibre, C_F is fibre consistency, D_F is intrafibre diffusion coefficient, K is the volumetric equilibrium constant (dimensionless), k_f is film resistance mass transfer coefficient, ω is particle porosity, *r* is particle solute radial position, *R* is fibre radius, $k = k_1 / k_2$ and k_1, k_2 are mass transfer coefficients and *t* is time.

The one-dimensional axial dispersion model connected with solute concentration of intrapore at the fiber surface with axial distance (z) was used to represent the fluid phase is given as:

$$u\frac{\partial c}{\partial x} + \frac{\partial c}{\partial t} + \frac{2}{R}\left(\frac{1-\varepsilon}{\varepsilon}\right)D_F\left(\frac{\partial q}{\partial r}\right)_{r=R} = D_L\frac{\partial^2 c}{\partial x^2}, \qquad (2.63)$$

with boundary condition

$$uc - D_L\frac{\partial c}{\partial x} = 0 \quad \text{at} \quad x = 0 \qquad \text{and} \qquad \frac{\partial c}{\partial x} = 0 \quad \text{at} \quad x = L, \qquad (2.64)$$

where u was the interstitial velocity, *L* was the packed bed thickness, D_L was the longitudinal dispersion coefficient, ε was the cake porosity and *x* represent the thickness of the packed bed (variable).

The CSCM was used to solve the model equation and validated the derived results with the laboratory data of Arora and Potůček (2012). The convergence of order two was attained with CSCM. The results were derived the numerical results for various values of *Pe* and *Bi*. The study expressed the range of *Pe* for the experimental data used was lying from 18–26 and supported that not much effect of interstitial velocity was noticed on the concentration of solute. There was a decrease in viscosity and porosity when the interstitial velocity and axial dispersion coefficient was increased simultaneously, and the washing operation was not much affected by *u*. Further, the greater value of porosity made the exit solute concentration curve nearer to zero and thus the washing operation efficiency was increased. The distribution ratio was increased when the value of $\psi = \frac{R^2 u}{LD_F}$ is decreased. The retention time was increased in this situation and subsequently, more time was taken by concentration profiles to attain the steady state condition. The minimum relative error validates the accuracy of CSCM and produces smooth and stable solutions.

Mittal and Kukreja (2015) used the OCFE technique with cubic Hermite as a basis function in place of the Lagrangian basis. This study explored the 2D model used by Gupta et al. (2015) related to the solute removal process which involves axial and radial domains. The roots of shifted Legendre polynomials were used as collocation points in the radial direction and roots of shifted Chebyshev polynomials were used in the axial direction. The study found better results than the previous investigators in solving the pulp washing models.

Potůček and Hájková (2016) used the stimulus-response method to solve the pulp washing model applied by Potucek (1997) and explored the dispersed plug flow model which describes the displacement process of the black liquor from the pulp fibre bed. The washing experiment performed lies within the logical limits of plug flow with infinite diffusion for a fully stirred vessel. It was noticed that the washing curve with a long tail was obtained when there was short time contact between the fibers and wash liquid. The low average interstitial velocity was taken and the long-time contact of wash liquid with the fibers was noticed. The range of the *Pe* between 6 and 41 was considered and it was noticed that the dependency of *Pe* was little on the wash yield.

Jiwari et al. (2018) considered the one-dimensional advection-diffusion-reaction model to study tumor invasion and tumor angiogenesis. The model deals with the progression carried by tumor that aims to describe the linkage of the nutrient supply and blood network to examine further growth. An extensive range of solution profiles affected by a wide range of diffusion coefficients describing the natural phenomenon of tumor angiogenesis was explained in the study. It applied the numerical algorithm established for the differential quadrature method (DQM) in which the derivatives are replaced by a weighted sum which is then transformed into a system of differential equations, i.e., ODEs. The system attained is solved with the 4^{th} order Runge-Kutta method. The results of four numerical examples were tested to prove the efficiency and accuracy of using the present algorithm. The technique of DQM-based approach gave high accuracy with minimum computational cost.

Kaur et al. (2018) solved the linear and nonlinear model equations of pulp washing explored by Mittal et al. (2013) using the quintic Hermite collocation method (QHCM). The study proved the accuracy of this method over CHCM.

Mishra et al. (2019) presented a numerical technique of orthogonal spline collocation (OSC) for the solution of the semi linear reaction-diffusion equation described by BVPs for discretization in the spatial domain of time-dependent problems. The optimal accuracy of the method was proved and its advantages over FEM and FDM due to the continuous approximation of the solution (and its first derivative) over the entire spatial domain of the problem were also discussed. The advantage of not involving the calculation of integrals was explained and this is fit to use for high-order approximations of all types of boundary conditions. Additionally, this method yielded super convergent approximations of the solution and its first derivatives.

Bu and Bak (2020) used a backward semi-Lagrangian scheme (BSL) to solve the nonlinear advection-diffusion–dispersion equation. The BSL revealed better stability and believes to use more steps in temporal grid size than in the spatial. The scheme of a high order to measure stability and accuracy with the help of six numerical experiments was attained. The study estimated the computational errors using the L_2 norm and the maximum norm and proved the method as more accurate, and efficient with less computational costs in comparison with other methods.

Jannesari and Tatari (2020) presented a study on the adaptive element free Galerkin (EFG) algorithm based on the moving least squares (MLS) to find the results for convection-diffusion equations. The study also revealed that the situation of oscillatory numerical solutions can be avoided by the selection of *Pe* which should be chosen according to the need to attain stability. The relative error, L_2 error, and CPU time by dividing the domain into different elements were compared to prove the efficiency of the presented method.

Kaur et al. (2021) discussed in detail the QHCM technique. Furthermore, the model equations were solved used by Arora et al. (20006a) and proved the superiority of QHCM over OCFE and CHCM was noticed. The stability of the method using both Euclidean and maximum norms authors was also tested. The study also confirmed that less CPU time was consumed with QHCM as compared to previously existing ones. Moreover, the effect of important parameters like *Pe*, D_L, *u*, and *L* on the washing process were also discussed.

Hajaji et al. (2021) considered the quintic spline approximation to estimate the space derivative and the time derivative part was approximated using difference approximation. The combination of quintic spline techniques and the finite difference method gave improved results than the finite difference methods. The technique was numerically stable and simple for providing approximation order with high accuracy.

Singh et al. (2021) used the OCFE method to solve the PDEs by employing quintic Hermite polynomials. The BVPs of order three and PDEs (linear and nonlinear) were also solved, and the technique was suggested to find special solutions for the phenomena like travelling waves. The stability of high order with Gauss points as collocation points was achieved in this method using quintic polynomials and proved the method to be super convergent.

Mehrpouya and Salehi (2021) proposed a robust numerical method to derive an accurate solution to the complex five BVPs by using an orthogonal collocation scheme to discretize the problem and converted this to algebraic equations. The system of equations was solved using the collocation method and the method proved to acquires better numerical results even when small discretization points were used.

2.3 SUMMARY

The chapter highlights the contribution of various researchers in the field of mathematical modeling and application of convection-diffusion, advection-diffusion, adsorption-desorption in different areas including, oil extraction, tumor invasions, prediction of pollution spread in soil, fluid dynamics, paper industry, polymer industry, etc. Different numerical/analytic techniques used by previous researchers to solve linear and non-linear models along with their findings like, Laplace transform, Fourier transform, Galerkin method, FDM, OCM, OCFE and many more. Besides, the results related to these studies are also summarized in this chapter.