CHAPTER 4

MATHEMATICAL MODELS

The use of mathematics in solving real-world problems has become widespread mainly due to the increasing computational ability of digital computers and computing methods, both of which have simplified the processing of lengthy and complicated problems. In this chapter different mathematical models related to diffusion dispersion are briefly discussed.

4.1 MATHEMATICAL MODELS

According to Dumont (1986), mathematical modelling processes are generally non-linear by nature and depend on multi-variables. Mainly, there are three approaches of modelling: physical, process and statistical modelling, that describe the pulp washing process. The present study focuses on the physical models. These models serve the purpose of describing the washing process in terms of mass transfer and fundamental fluid flow principles, which take place at a microscopic level during the process of displacement washing of a pulp fiber bed. The longitudinal dispersion, mass transfer coefficients, and porous structure of fiber are the key parameters involved in these models (Kim, 1989).

An overview of various models used to describe pulp washing has been presented by Pekkanen and Norden (1985). Extensive study has been carried out by Lapidus and Amundson (1952); Kuo (1960); Brenner (1962); Pellett (1964); Sherman (1964); Grähs (1974); Neretnieks (1976); Perron and Lebeau (1977); Raghavan and Ruthven (1983); Viljakainen (1985); Kim (1989); Trinh, et al (1989); Al-Jabari, et al (1994); Towers and Scallan (1996); Kukreja (1996); Potůček (1997); Sridhar (1999); Liao and Shiau (2000); Szukiewicz (2000); Liu and Bhatia (2001); Tervola (2006); and Kukreja and Ray (2009). Thee pulp washing models in the form of BVPs with different initial and boundary conditions were studied and the effect of various industrial parameters on washing operation was discussed.

Kukreja (1996) and Ganaie et al. (2014) considered some basic assumptions for a systematic investigation of a porous structure pulp fiber bed as detailed below:

- Macroscopically uniform bed
- Uniform cylindrical size of particles
- The Diameter of the particle fibre is taken small in comparison with the axial distance

- Independence cake thickness and radius of particle from the intra-fiber diffusion coefficient
- Interrelation of the particle porosity, consistency of fibers, and bed porosity.

Besides, the washing process is mainly associated with the diffusion-dispersion phenomenon. Okhovat et al. (2014) revealed that sufficient efforts are put on by the researchers to examine the behavior of the diffusion-dispersion phenomenon experimentally or through simulation. Many studies were conducted by the researchers to simulate the models used to express the process of the pulp and paper industry with advanced techniques (Arora et al., 2006). This has aided in improving the efficiency the industry. Keeping this in view and to further benefit the industry, the present study endorses the technique of QHCM to obtain the numerical solution of the one-dimensional linear, non-linear, and 2-dimensional models of pulp washing.

4.2 LINEAR MODEL - 1

Consider a diffusion-dispersion problem with Dirichlet's boundary conditions as:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x}, \tag{4.1}$$

To keep the mathematical complexity as small as possible, the boundary conditions are defined at two points only. One at the entry level of the bed (x = 0) and the other at the exit level of the bed ($x = L$). Between 0 and L, no condition is imposed.

At the initial stage, the bulk fluid concentration is assumed to be equal to inlet solute concentration or the concentration of solute at the inlet is taken equal to the concentration of solute in the wash liquor. In other words, at the entry level of the bed, no loss of solute is assumed from the bed with the introduction of displacing fluid.

At the exit level, an unacceptable conclusion is avoided by assuming that the concentration of solute passes through a minimum (or maximum) in the interior of the medium,

$$\left.\begin{aligned} c &= c_e & &at \;\; x = 0 \\ \frac{\partial c}{\partial x} &= 0 & &at \;\; x = L \end{aligned}\right\} \text{ for all t >0,} \tag{4.2}$$

where c = c (z, t) is the concentration of solute in liquor, the point from where the displacing fluid is introduced is at distance (x), time (t), axial dispersion coefficient (D_L), average interstitial velocity (u), and cake thickness (L) are the parameters.

The initial concentration of fluid is considered the same as the concentration of inlet solute.

i.e., $c(x, 0) = c_0$. (4.3)

where c_0 is the inlet solute concentration.

The first task in solving the model equation is the conversion of an equation into dimensionless form and then transforming the equation by using a suitable variable transformation. The reason behind this conversion is to give this equation a more flexible mathematical treatment.

The dimensionless form of the model and boundary conditions is:

$$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial X^2} - \frac{\partial C}{\partial X} \qquad \text{in} \quad \Omega \in (0,1), \tag{4.4}$$

Boundary conditions:

$$\left.\begin{aligned} C &= 0 & \quad at \ \ X = 0 \\ \frac{\partial C}{\partial X} &= 0 & \quad at \ \ X = 1 \end{aligned}\right\} \quad \text{for all} \quad T \geq 0, \tag{4.5}$$

Initial condition:

$$C(X,0) = 1. \tag{4.6}$$

where $C = \frac{c - c_s}{c_0 - c_s}$ is the dimensionless concentration of solute, $T = \frac{ut}{L}, X = \frac{x}{L}$ are dimensionless time and axial distance respectively. Also, $Pe = \frac{uL}{D_L}$ (the dimensionless parameter) is a ratio of advection to diffusion known as the *Pe*. It is a key parameter that influences the chemical reaction, and the optimum choice of the *Pe* is considered for obtaining good results.

Grähs (1974) solved the above problem with OCM and found the analytic solution to this problem. However, Arora et al. (2005) efficiently solved the model with the OCFE method with a Lagrangian basis and achieved better than the results obtained through OCM. Besides, Gupta et al. (2012) used CSCM to solve the model and experienced improvement in the results as compared to OCFE. In a study, Mittal et al. (2013) obtained the numerical solution to this problem with CHCM and found the technique more suitable than OCFE. While solving the same model using QHCM and comparing the results with that of CHCM, Kaur et al. (2018) obtained better results and in less CPU time.

4.3 LINEAR MODEL - 2

Brenner (1962); and Sherman (1964) proposed the procedure of a mathematical model for displacement washing as detailed below:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x}, \tag{4.7}$$

At the entry level, the difference in concentration of solute in liquor and weak wash liquor multiplied by the ratio of axial dispersion coefficient to the interstitial velocity is equal to the concentration gradient at the inlet.

However, Brenner (1962) imposed following boundary conditions at the entry (x = 0) and exit of the bed (x = L).

$$\left.\begin{aligned} u(c - c_e) &= D_L \frac{\partial c}{\partial x} \quad && at \;\; x = 0 \\ \frac{\partial c}{\partial x} &= 0 && at \;\; x = L \end{aligned}\right\} \text{for all } t \geq 0. \tag{4.8}$$

The initial condition is the same as the linear model 1.

The dimensionless form of the above-given model is

$$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial X^2} - \frac{\partial C}{\partial X} \qquad \text{in} \qquad \Omega \in (0,1), \tag{4.9}$$

with boundary conditions as:

$$\left.\begin{aligned} Pe\,C &= \frac{\partial C}{\partial X} \quad && at \;\; X = 0 \\ \frac{\partial C}{\partial X} &= 0 && at \;\; X = 1 \end{aligned}\right\} \text{for all } T \geq 0. \tag{4.10}$$

Potůček (1997); Singh et al. (2008); and Kukreja and Ray (2009) have studied the model of pulp washing in detail by considering the present equation. Tervola (2006) explained that the advection-dispersion model presented by Brenner (1962) is perhaps the most acceptable for practical applications among all mathematical models described for pulp washing. The analytic solution of the above-discussed problem derived by Brenner (1962) is given as:

For small values of Pe:

$$C_e = \exp\left\{Pe\left(\frac{1}{2}-\frac{T}{4}\right)\right\}\sum_{k=1}^{\infty}\left[\frac{16\lambda_k\sin(2\lambda_k)}{16\lambda_k{}^2+Pe^2+4Pe}\right]\exp\left(\frac{-4\lambda_k{}^2T}{Pe}\right). \tag{4.11}$$

For large values of Pe:

$$C_e = 1-\frac{1}{2}\operatorname{erfc}\left\{(1-T)\sqrt{\frac{Pe}{4T}}\right\}-\left[\left\{3+\frac{Pe}{2}(1+T)\right\}\exp\left\{-\frac{Pe(1-T)^2}{4T}\right\}\sqrt{\frac{PeT}{\pi}}\right]+$$
$$+\left[\frac{1}{2}+\frac{Pe}{2}(3+4T)+\left(\frac{Pe}{4}\right)^2(1+T)^2\right]\exp(Pe)erfc\left\{(1+T)\sqrt{\frac{Pe}{4T}}\right\} \tag{4.12}$$

In a study, Arora et al. (2005, 2006) solved this problem numerically with the OCFE technique and validated the results with an analytic solution. Likewise, Gupta and Kukreja (2012) and Ganaie et al. (2013) explained the model problem using CSCM and CHCM respectively and found superior results. When Kaur et al. (2021) solved this model equation with QHCM, the results derived were found to be better than those obtained via CHCM.

4.4 LINEAR MODEL - 3

Arora et al. (2006) studied the pulp fiber bed washing model based on the phenomena of longitudinal mixing and assumed it to be governed by the equation (dimensionless form) given as

$$\frac{\partial C}{\partial T}=\frac{1}{Pe}\frac{\partial^2 C}{\partial X^2}-\frac{\partial C}{\partial X}-\frac{\mu Bi}{Pe}C, \tag{4.13}$$

where T is the time from commencement of displacement, X is the distance from the point of introduction of displacing fluid, $C = C(X,T)$ is solute concentration in liquor, $Bi = \frac{kL^2}{D_L}$ and represents the Biot number (Bi) which relates to the mass transfer resistance inside and at the surface of the body whereas $\mu = \varepsilon/(1-\varepsilon)$ is the ratio of the volume available for flow to the total volume and ε represents the porosity.

The boundary and initial conditions are the same as Linear model-1.

Zheng and Gu (1996) obtained the exact solution which is given hereunder:

$$C_e = \exp\left(\frac{-\mu BiT}{Pe}\right)\left[\begin{array}{l} 1-\frac{1}{2}erfc\left(\frac{\sqrt{Pe}(1-T)}{2\sqrt{T}}\right)+\sqrt{\frac{PeT}{\pi}}\exp\left(\frac{Pe(2T-T^2-1)}{4T}\right)- \\ \left(\frac{3+Pe+PeT}{2}\right)\exp(Pe)erfc\left(\frac{\sqrt{Pe}(1+T)}{2\sqrt{T}}\right) \end{array}\right]. \qquad (4.14)$$

Besides, Arora et al. (2006) compared the relative error of the OCM and OCFE methods by using the above model and observed that both the error norms are decreasing with the increase in the number of elements. Some other authors like Gupta and Kukreja (2012); Ganaie et al. (2013); and Robalo et al. (2013) solved the model with CSCM, CHCM, and moving finite element methods respectively for achieving improved results in less CPU time.

4.5 LINEAR MODEL - 4

The diffusion-dispersion model involving retardation coefficient is given as:

$$R_d \frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial X^2} - \frac{\partial C}{\partial X}, \qquad (4.15)$$

The boundary and initial conditions are same as given in linear model-1.

Liao and Shiau (2000) derived the analytic solution for this problem. Roininen and Alopaeus (2011) also applied the moment method to solve the model. Also, Arora et al. (2006, 2014) solved this model using OCFE and presented the relative error of the numerical solution for different values of Pe and R_d. It was observed that for better washing, the retardation coefficient (removal rate of adsorbed solute on the particle surface) must be greater than 1.

After validating the results for linear models, the present technique is applied to solve the non-linear models, which are used to describe the effect of some important parameters on the washing process.

4.6 NONLINEAR MODEL - 1

Consider a non-linear equation expressing the behavior of miscible liquids during diffusion-dispersion phenomena. The washing behavior of pulp fibers in the one-dimensional transport phenomenon of porous media involves axial dispersion and molecular diffusion. Kukreja (1996) explored the transport equation describing material balance across the bed in one dimension is defined as:

$$D_L \frac{\partial^2 c}{\partial x^2} = u \frac{\partial c}{\partial x} + \frac{\partial c}{\partial t} + C_F \frac{(1-\varepsilon)}{\varepsilon} \frac{\partial n}{\partial t}, \qquad (4.16)$$

Here, the first term represents diffusion dispersion, and the other terms represent convective flow, the concentration gradient of fluid, and the concentration gradient of particles respectively. Mathematically, u and D_L are functions of x, while c and n and functions of both x and t and c and n are the concentration of solute in liquor and fiber respectively. It is assumed that the deposition rate of solute is of second order in the forward direction and detachment rate is of the first order in the reverse direction.

The boundary conditions of this model are considered as same that of linear model-2.

Initially, bulk fluid concentration is taken equal to inlet solute concentration, *i.e.*,

$$c(x,0) = n(x,0) = c_i \text{ for } 0 < x < L/u. \qquad (4.17)$$

A non-linear Langmuir adsorption isotherm is considered in this model.

The Langmuir isotherm- Fogelberg and Fugleberg (1963) gives detailed information on non-linear Langmuir type adsorption isotherm for equilibrium between the solute concentration on the fibers and in the liquor. This isotherm assumes that the deposition (adsorption) rate is second order in the forward direction and the detachment (desorption) rate is first order in the backward direction, *i.e.*,

$$\frac{k_1 c}{C_F}(N_i - n) - k_2 n = \frac{\partial n}{\partial t}, \qquad (4.18)$$

at equilibrium, it simplifies to

$$n = \frac{A_0 c}{1 + B_0 c}. \qquad (4.19)$$

where $A_0 = \frac{kN_i}{C_F}$ and $B_0 = \frac{k}{C_F}$ are Langmuir constants.

The dimensionless form of the model is:

$$\frac{1}{Pe} \frac{\partial^2 C}{\partial X^2} = \frac{\partial C}{\partial T} + \frac{\partial C}{\partial X} + \frac{\mu C_F A_0}{\left[1 + B_0 \left\{c_s + C\left(c_0 - c_s\right)\right\}\right]^2} \frac{\partial C}{\partial T}, \qquad (4.20)$$

The boundary conditions in the dimensionless form are:

$$\left.\begin{aligned} PeC = \frac{\partial C}{\partial X} \qquad\qquad & at \quad X = 0 \\ \frac{\partial C}{\partial X} = 0 \qquad\qquad & at \quad X = 1 \end{aligned}\right\} \text{ for all } \quad t \geq 0, \tag{4.21}$$

The initial condition is:

$$C(X,0) = 1 \quad \text{at} \quad T = 0, \tag{4.22}$$

where $C = \dfrac{c - c_s}{c_0 - c_s}$ is the dimensionless concentration of solute in liquor, $N = \dfrac{n - c_s}{c_0 - c_s}$ is the dimensionless concentration of solute in fiber, $T = \dfrac{ut}{L}, X = \dfrac{x}{L}$ are dimensionless time and axial distance respectively. Also, $Pe = \dfrac{uL}{D_L}$ is the Peclet number and $\mu = \varepsilon / (1 - \varepsilon)$ is the ratio of the volume available for flow to the total volume and ε represents the porosity.

Arora et al. (2005) efficiently solved the model with the OCFE method with a Lagrangian basis. Besides, Gupta and Kukreja (2012) used CSCM to solve the model and experienced improvement in the results than OCFE. Thereafter, Mittal et al. (2013) obtained the numerical solution to this problem with CHCM. Besides, Kaur et al. (2021) solved this model using QHCM and compared the results with CHCM. The results achieved were effective and in less CPU time.

4.7 NONLINEAR MODEL - 2

The flow of external fluid through a packed bed of fiber based on axial dispersion and particle diffusion is described by a one-dimensional dispersion plug flow model (Potůček, 1997). The mathematical equation of the model is as follows:

$$D_L \frac{\partial^2 c}{\partial x^2} = u \frac{\partial c}{\partial x} + \frac{\partial c}{\partial t} + C_F \left(\frac{1-\varepsilon}{\varepsilon} \right) \frac{\partial n}{\partial t}, \tag{4.23}$$

with boundary conditions same as considered in the linear model-1. The initial condition and adsorption isotherm are the same as considered in nonlinear model-1

The dimensionless form of the model is:

$$\frac{1}{Pe} \frac{\partial^2 C}{\partial X^2} = \frac{\partial C}{\partial T} + \frac{\partial C}{\partial X} + \frac{\mu C_F A_0}{\left[1 + B_0 \left\{ c_s + C\left(c_0 - c_s\right) \right\}\right]^2} \frac{\partial C}{\partial T}. \tag{4.24}$$

The initial and boundary conditions (dimensionless) are the same as linear model-1. Kumar et al. (2010) explored this model with the technique of 'pdepe' solver in MATLAB and proved that the results derived are the same as the nonlinear model-1. However, Mittal and Kukreja (2015) solved this model using CHCM and proved that the numerical results of exit solute concentration for nonlinear model-1 are better than this model.

4.8 NONLINEAR MODEL - 3

In this case, the nonlinear model-1 is considered along with linear adsorption isotherm. The linear isotherm assumes that point-wise equilibrium inside the particle, i.e.,

$$n = kc\,. \tag{4.25}$$

Some authors like Brenner (1962); Sherman (1964); Potůček (1997); Kumar et al. (2010); and Ganaie et al. (2013) also used linear adsorption isotherm for finding solutions to the model.

The dimensionless form of the model is:

$$\frac{1}{Pe}\frac{\partial^2 C}{\partial X^2} = \frac{\partial C}{\partial T} + \frac{\partial C}{\partial X} + k\mu\frac{\partial C}{\partial T}\,. \tag{4.26}$$

Kumar et al. (2010); and Ganaie et al. (2013) solved this model with "pdepe" solver and CHCM respectively.

4.9 DISCRETIZED FORM OF MODELS

The linear and non-linear model equations along with initial and boundary conditions are solved by discretizing the dimensionless form of the model. Discretization is a process in which the differential equation reaches the true solution at the collocation points. In this process, the approximate function using the quintic Hermite polynomial as explained in chapter 3 is derived and the diagonalized form of different models are given hereunder:

4.9.1 Discretized Form of Linear Model - 1

$$\sum_{q=1}^{6}\frac{da_{q+3(k-1)}}{dt}H_q^k(u_r) = \frac{1}{Peh_k^2}\sum_{q=1}^{6}a_{q+3(k-1)}H_q^{k''}(u_r) - \frac{1}{h_k}\sum_{q=1}^{6}a_{q+3(k-1)}H_q^{k'}(u_r)\,, \tag{4.27}$$

where $r = 2,3,4,5$ (interior collocation points) and $k = 1,2,...,N$ (number of elements)

The boundary condition at initial point $x = 0$, *i.e.*, $X = 0$ gives

$$\sum_{q=1}^{6} a_q H_q^k(0) = 0 \Rightarrow a_1 = 0, \qquad (4.28)$$

The boundary condition for the element at x = L, i.e., $X = 1$ gives

$$\frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(m-1)} H_q^{k'}(1) = 0 \Rightarrow a_{3m+2} = 0, \qquad (4.29)$$

4.9.2 Discretized Form of Linear Model - 2

$$\sum_{q=1}^{6} \frac{da_{q+3(k-1)}}{dt} H_q^k(u_r) = \frac{1}{Peh_k^2}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k''}(u_r) - \frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k'}(u_r), \qquad (4.30)$$

where $r = 2,3,4,5$ (interior collocation points) and $k = 1,2,...,N$ (number of elements)

The boundary condition at initial point $x = 0$, *i.e.*, $X = 0$ gives

$$Pe\sum_{q=1}^{6} a_q H_q^k(0) - \frac{1}{h_1}\sum_{q=1}^{6} a_q H_q^{k'}(0) = 0 \Rightarrow Pea_1 - a_2 = 0, \qquad (4.31)$$

The boundary condition for the element at x = L, i.e., $X = 1$ gives

$$\frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(m-1)} H_q^{k'}(1) = 0 \Rightarrow a_{3m+2} = 0. \qquad (4.32)$$

4.9.3 Discretized Form of Linear Model - 3

$$\sum_{q=1}^{6} \frac{da_{q+3(k-1)}}{dt} H_q^k(u_r) = \left(\begin{array}{r} \frac{1}{Peh_k^2}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k''}(u_r) - \frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k'}(u_r) \\ -\frac{\mu B_i}{Pe}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k}(u_r) \end{array} \right) \qquad (4.33)$$

where $r = 2,3,4,5$ (interior collocation points) and $k = 1,2,...,N$ (number of elements)

The boundary condition at initial point $x = 0$, *i.e.*, $X = 0$ gives

$$\sum_{q=1}^{6} a_q H_q^k(0) = 0 \Rightarrow a_1 = 0, \qquad (4.34)$$

The boundary condition for the element at x = L, i.e., $X = 1$ gives

$$\frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(m-1)} H_q^{k'}(1) = 0 \Rightarrow a_{3m+2} = 0 \,. \tag{4.35}$$

4.9.4 Discretized Form of Linear Model - 4

$$R_d \sum_{q=1}^{6} \frac{da_{q+3(k-1)}}{dt} H_q^{k}(u_r) = \frac{1}{Peh_k^2}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k''}(u_r) - \frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k'}(u_r)\,, \tag{4.36}$$

where $r = 2,3,4,5$ (interior collocation points) and $k = 1,2,...,N$ (number of elements)

The boundary condition at initial point x = 0, *i.e.*, X = 0 gives

$$\sum_{q=1}^{6} a_q H_q^{k}(0) = 0 \Rightarrow a_1 = 0\,, \tag{4.37}$$

The boundary condition for the element at x = L, i.e., X = 1 gives

$$\frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(m-1)} H_q^{k'}(1) = 0 \Rightarrow a_{3m+2} = 0 \,. \tag{4.38}$$

4.9.5 Discretized Form of Non-Linear Model - 1

$$\sum_{q=1}^{6} \frac{da_{q+3(k-1)}}{dt} H_q^{k}(u_r) = \left[\frac{\left[1 + B_0\left\{(C_0 - C_s)\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k}(u_r) + C_s\right\}\right]^2}{\mu C_F A_0 + \left[1 + B_0\left\{(C_0 - C_s)\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k}(u_r) + C_s\right\}\right]^2}\right] \times \left(\frac{1}{Peh_k^2}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k''}(u_r) - \frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(k-1)} H_q^{k'}(u_r)\right), \tag{4.39}$$

where $r = 2,3,4,5$ (interior collocation points) and $k = 1,2,...,N$ (number of elements)

The boundary condition at initial point x = 0, *i.e.*, X = 0 gives

$$Pe\sum_{q=1}^{6} a_q H_q^{k}(0) - \frac{1}{h_1}\sum_{q=1}^{6} a_q H_q^{k'}(0) = 0 \Rightarrow Pea_1 - a_2 = 0\,, \tag{4.40}$$

The boundary condition for the element at x = L, i.e., X = 1 gives

$$\frac{1}{h_k}\sum_{q=1}^{6} a_{q+3(m-1)} H_q^{k'}(1) = 0 \Rightarrow a_{3m+2} = 0 \,. \tag{4.41}$$

4.9.6 Discretized Form of Non-Linear Model – 2

$$\sum_{q=1}^{6}\frac{da_{q+3(k-1)}}{dt}H_q^k(u_r)=\left[\frac{\left[1+B_0\left\{(C_0-C_s)\sum_{q=1}^{6}a_{q+3(k-1)}H_q^k(u_r)+C_s\right\}\right]^2}{\mu C_F A_0+\left[1+B_0\left\{(C_0-C_s)\sum_{q=1}^{6}a_{q+3(k-1)}H_q^k(u_r)+C_s\right\}\right]^2}\right]\times\left(\frac{1}{Peh_k^2}\sum_{q=1}^{6}a_{q+3(k-1)}H_q^{k''}(u_r)-\frac{1}{h_k}\sum_{q=1}^{6}a_{q+3(k-1)}H_q^{k'}(u_r)\right), \quad (4.42)$$

where $r = 2,3,4,5$ (interior collocation points) and $k = 1,2,...,N$ (number of elements)

The boundary condition at initial point x = 0, *i.e.*, X = 0 gives

$$\sum_{q=1}^{6}a_q H_q^k(0)=0 \Rightarrow a_1 = 0, \quad (4.43)$$

The boundary condition for the element at x = L, i.e., X = 1 gives

$$\frac{1}{h_k}\sum_{q=1}^{6}a_{q+3(m-1)}H_q^{k'}(1)=0 \Rightarrow a_{3m+2}=0. \quad (4.44)$$

4.9.7 Discretized Form of Non-Linear Model - 3

$$\sum_{q=1}^{6}\frac{da_{q+3(k-1)}}{dt}H_q^k(u_r)=\frac{1}{(1+k\mu)}\left[\frac{1}{Peh_k^2}\sum_{q=1}^{6}a_{q+3(k-1)}H_q^{k''}(u_r)-\frac{1}{h_k}\sum_{q=1}^{6}a_{q+3(k-1)}H_q^{k'}(u_r)\right] \quad (4.45)$$

where $r = 2,3,4,5$ (interior collocation points) and $k = 1,2,...,N$ (number of elements)

The boundary condition at initial point x = 0, *i.e.*, X = 0 gives

$$Pe\sum_{q=1}^{6}a_q H_q^k(0)-\frac{1}{h_1}\sum_{q=1}^{6}a_q H_q^{k'}(0)=0 \Rightarrow Pea_1 - a_2 = 0, \quad (4.46)$$

The boundary condition for the element at x = L, i.e., X = 1 gives

$$\frac{1}{h_k}\sum_{q=1}^{6}a_{q+3(m-1)}H_q^{k'}(1)=0 \Rightarrow a_{3m+2}=0. \quad (4.47)$$

By the technique of QHCM, the above system of linear and non-linear PDEs is reduced to the system of ODEs. The equations are written in the form as: $Du = Mu$

where D is the differential operator and u is the vector of collocation solutions of order $4N$. M is the square matrix of order $4N \times 4N$. The system is solved using MATLAB ode 15s system solver.

4.10 TWO-DIMENSIONAL (2-D) MODELS

Raghavan and Ruthvan (1983) described the 2-D model of displacement washing and solved the same with the OCM. The study also exhibited the model involving axial dispersion coefficient, particle diffusion, film resistance mass transfer coefficient, bed porosity, and pore radius of particles to study the flow of fluid for two phases through a packed bed of porous particles. The present method is extended to solve the 2-D model representing the displacement washing with particle and bulk fluid phases. Arora and Potuček (2012) explained the mechanism of mass transfer, which relates to the material transfer rate between fibers and fluid. Because of the porous nature of fibers, solute residing inside the pores of fibers comes out when the external fluid is introduced. The axial dispersion, mass transfer, and fluid concentration inside and outside the particles contribute the main role in the process. The concentration of external fluid is considered as a function of time and axial distance whereas the concentration of inter-particle solute and concentration of solute adsorbed on the surface of the particle is considered as a function of time, axial distance, and pore radial distance. The unsteady state PDEs describing different phases for the bulk fluid and particle diffusion presented below as:

4.10.1 Mathematical Equations for the Particle Diffusion

The existing solute in the pores of fibers is drawn out when the external fluid is introduced in the porous structured bed. The solute present on the fiber surface is represented by the particle diffusion model. The equation for particle phase in terms of radial direction can be written as:

$$D_F\left(\frac{\partial^2 q}{\partial r^2}+\frac{1}{r}\frac{\partial q}{\partial r}\right)-\frac{\partial q}{\partial t}-C_F\,\frac{(1-\beta)}{\beta}\frac{\partial n}{\partial t}=0\,, \qquad (4.48)$$

The intra-pore concentration is denoted by q (r, x, t) and n (r, x, t) represents the solute concentration on the particle surface. The particles are cylindrical in nature with R as the pore radius and β as the particle porosity. The axial dispersion (D_L) and effective diffusivity don't depend on the concentrations of solute and cake thickness. The relation between bulk fluid and intra-pore diffusion at the particle surface is governed by the fluid film mass transfer coefficient

k_f. The intra-fiber diffusion coefficient (D_F) is considered only in the particle diffusion phase. This is true because the solid-phase diffusion effects are small and can be neglected. So, the transport inside the fiber is better explained by the diffusion in the solution phase only.

Boundary conditions: The boundary conditions depending on the mass transfer rate explain the exchange of solute between the bulk fluid and the fiber surface. Neretnieks (1976) and Raghavan and Ruthvan (1983) assumed the boundary condition describing the relation of bulk fluid phase and particle phase as:

$$\frac{\partial q}{\partial r}=0 \qquad \text{at} \qquad r=0, \tag{4.49}$$

$$k_f \beta\left(q\big|_{r=R}-c\right)=-KD_F\left(\frac{\partial q}{\partial r}\right) \qquad \text{at} \qquad r=R. \tag{4.50}$$

Adsorption Isotherm: It is the relation of intra-fiber and inter-fiber concentrations of solute and is described by Langmuir kinetics. The deposition rate and detachment rate is assumed as of second order in the forward direction and in the reverse direction respectively given by the following equation:

$$\frac{\partial n}{\partial t}=k_1\frac{q}{C_F}(N_i-n)-k_2 n, \tag{4.51}$$

where k_1 is deposition and k_2 is detachment rate constants. The monovalent adsorption equation at equilibrium reduces to Langmuir adsorption isotherm as under:

$$n=\frac{qkN_i}{C_F+qk}. \tag{4.52}$$

4.10.2 Mathematical Equations for the Bulk Fluid

The model equation for the fluid phase is represented by the one-dimensional axial dispersion model associated with the axial distance (x) and the concentration of intra-pore solute with the fiber surface is described by Arora and Potuček (2012) as follows:

$$u\varepsilon\frac{\partial c}{\partial x}+\varepsilon\frac{\partial c}{\partial t}+\frac{2(1-\varepsilon)}{R}D_F\left.\frac{\partial q}{\partial r}\right|_{r=R}=D_L\varepsilon\frac{\partial^2 c}{\partial x^2}, \tag{4.53}$$

The fluid flow of the pulp fibre bed is expressed with the bulk fluid concentration, and it is denoted by c (x, t).

***Boundary conditions*:** The rate of change of inside pores solute concentration with respect to the radial position of the particle is assumed to zero, i.e.,

$$\frac{\partial q}{\partial r} = 0 \qquad \text{at } r = 0, \tag{4.54}$$

and the rate of change w.r.t particle boundary radial position is supposed to be regulated by film resistance mass transfer coefficient, i.e.,

$$-D_F \frac{\partial q}{\partial r} = \frac{k_f w}{k}(q \mid r = R - c) \qquad \text{at } r = R, \tag{4.55}$$

Also, at the entry of the bed, loss of solute is considered negligible from the bed in the axial direction ($x = 0$) at the point of introduction of the displacing fluid:

$$uc - D_L \frac{\partial c}{\partial x} = 0 \qquad \text{at } x = 0, \tag{4.56}$$

Similarly, the rate of change of concentration is taken as zero at the exit point of the bed in the axial direction (z = L) and given as:

$$\frac{\partial c}{\partial x} = 0 \qquad \text{at } x = L, \tag{4.57}$$

***Initial condition*:** It is presumed that initially, the solute concentration of bulk fluid and solute concentration of intra-pore are identical to the solute concentration inside the vat. Also, the solute concentration that is adsorbed on fibers is assumed to be equal to the solute concentration that is adsorbed on the inside vat of the fibers

$$C = q = C_i \quad \text{and} \quad n = N_i \qquad \text{at } t = 0. \tag{4.58}$$

Arora and Potůček (2012) solved these models using OCFE and derived the effect of Pe and Bi on exit solute concentration, displacement ratio, and bed efficiency from the models. The excellent results with quadratic convergence using the technique of OCFE with Lagrangian basis were found. Mittal and Kukreja (2015) explored a 2-D model related to the solute removal process which involves axial and radial domains with the OCFE technique by using cubic Hermite as a basis function in place of the Lagrangian basis. The roots of shifted Legendre polynomials were used as collocation points in the radial direction and roots of shifted Chebyshev polynomials in the axial direction. However, Gupta et al. (2015) solved the same model for particle phase and fluid phase for the diffusion-dispersion phenomenon using CSCM.

4.10.3 Dimensionless Form of 2-D Model

The model equations alongwith boundary conditions, and initial conditions are converted into dimensionless form as under:

$$\left(\frac{\partial^2 Q}{\partial \varsigma^2}+\frac{1}{\varsigma}\frac{\partial Q}{\partial \varsigma}\right)=\frac{\partial Q}{\partial \varsigma}+N_1\frac{(1-\beta)}{\beta}\frac{\partial N}{\partial \tau}, \tag{4.59}$$

$$\frac{\partial Q}{\partial \varsigma}=0 \text{ at } \varsigma=0, \tag{4.60}$$

$$\frac{\partial Q}{\partial \varsigma}=Bi(C-Q) \quad \text{ at } \varsigma=1, \tag{4.61}$$

$$\frac{\partial N}{\partial \tau}=\frac{R^2 k_1}{D_F}\left(C_1 Q(1-N)-\frac{N}{K}\right) \quad , \tag{4.62}$$

$$\frac{\partial C}{\partial \tau}=\frac{\psi}{Pe}\frac{\partial^2 C}{\partial \zeta^2}-\psi\frac{\partial C}{\partial \zeta}-\theta Bi\left(C-Q|_{\eta=1}\right), \tag{4.63}$$

$$C-\frac{1}{Pe}\frac{\partial C}{\partial \zeta}=0 \text{ at } \zeta=0, \tag{4.64}$$

$$\frac{\partial C}{\partial \zeta}=0 \quad \text{ at } \zeta=1, \tag{4.65}$$

$$C = Q = N = 1 \text{ at } \tau=0. \tag{4.66}$$

where

$$C=\frac{c}{C_0},\ C_1=\frac{C_0}{C_F},\ N_1=\frac{N_0}{C_1},\ Q=\frac{q}{C_0},\ N=\frac{n}{C_0},\ \zeta=\frac{z}{L},\ \varsigma=\frac{r}{R},$$

$$Bi=\frac{k_f wR}{KD_F},\ \tau=\frac{tD_F}{R^2},\ \theta=\frac{2(1-\varepsilon)}{\varepsilon},\ \psi=\frac{R^2 u}{LD_F},\ Pe=\frac{uL}{D_L},\ k=\frac{k_1}{k_2}$$

are dimensionless parameters.

4.10.4 Numerical Procedure for 2-D Model

In the present technique, the unknown solution function is approximated using quintic Hermite interpolation as a trial function. These polynomials have the property of continuity of the first and second derivatives at nodal points that help to derive the solution at a steep gradient. The domain is partitioned into a finite number of elements and afterward, the collocation method is employed within each element for the assumed trial function. In this case, the residuals derived for the approximate solution of model equations are satisfied at interior collocation points and the boundary conditions are satisfied at extreme node points. The radial domain is divided into N subdomains with $\varsigma_1 = 0$ and $\varsigma_{N+1} = 1$. Each part of the subdomain is transformed onto [0, 1] by using transformation $u = (\varsigma - \varsigma_l)/h_l$, where $l = 1, 2, ..., N$ and $h_l = \varsigma_{l+1} - \varsigma_l$. Similarly, the axial domain is partitioned into υ subparts with $\varsigma_1 = 0$ and $\varsigma_{\upsilon+1} = 1$. Each part of the subdomain is transformed onto [0, 1] by using transformation as $v = (\varsigma - \varsigma_m)/h_m$, where $m = 1, 2, ..., \upsilon$ and $h_m = \varsigma_{m+1} - \varsigma_m$. The interior collocation points are considered as roots of 4th order shifted Legendre polynomials.

Let $Q_l^m(u, v, \tau)$ represent the estimated solution of $Q(u, v, \tau)$ then:

$$Q_l^m(u,v,\tau) = \sum_{i,j=1}^{6} q_{i+3(l-1)}^{j+3(m-1)}(\tau) H_i^j(u,v), \tag{4.67}$$

The six quintic Hermite basis functions are given as follows:

$$\begin{aligned}
&H_1^k(\eta) = (1+3\eta+6\eta^2)(1-\eta)^3, \quad H_2^k(\eta) = \eta(1+3\eta)(1-\eta)^3 \\
&H_3^k(\eta) = \frac{1}{2}\eta^2(1-\eta)^3, \quad H_4^k(\eta) = (10-15\eta+6\eta^2)\eta^3 \\
&H_5^k(\eta) = (1-\eta)\eta^3(3\eta-4), \quad H_6^k(\eta) = \frac{1}{2}\eta^3(1-\eta)^2
\end{aligned} \tag{4.68}$$

where $H_4^k(1) = 1, H_1^k(0) = 1, H'^k_2(0) = 1, H'^k_5(1) = 1$ others are zero

$$\left.\begin{aligned}
&Q_l^m(1,v,\tau) = Q_{l+1}^m(0,v,\tau), && Q_l^m(u,1,\tau) = Q_l^{m+1}(u,0,\tau), \\
&\frac{\partial Q_l^m}{\partial v}(1,v,\tau) = \frac{\partial Q_{l+1}^m}{\partial v}(0,v,\tau), && \frac{\partial Q_l^m}{\partial u}(u,1,\tau) = \frac{\partial Q_{l+1}^m}{\partial u}(u,0,\tau).
\end{aligned}\right\} \tag{4.69}$$

Similarly, $$N_l^m(u,v,\tau) = \sum_{i,j=1}^{6} n_{i+3(l-1)}^{j+3(m-1)}(\tau) H_i^j(u,v), \tag{4.70}$$

and $$C^m(v,\tau) = \sum_{j=1}^{6} c^{j+3(m-1)}(\tau) H_j(v), \tag{4.71}$$

Substituting the approximate solutions into the model equations, the following residual equations are obtained:

$$R_Q(u,v,\tau)=\sum_{j=1}^{6}\frac{dq_{i+3(l-1)}^{j+3(m-1)}(\tau)}{d\tau}H_i^j(u,v)-\frac{1}{h_l^2}\sum_{i,j=1}^{6}q_{i+3(l-1)}^{j+3(m-1)}(\tau)\frac{\partial^2 H_i^j(u,v)}{\partial u^2}$$
$$-\frac{1}{(uh_l+\varsigma_l)h_l}\sum_{i,j=1}^{6}q_{i+3(l-1)}^{j+3(m-1)}(\tau)\frac{\partial H_i^j(u,v)}{\partial u}+N_1\left(\frac{1-\beta}{\beta}\right)\sum_{i,j=1}^{6}\frac{dn_{i+3(l-1)}^{j+3(m-1)}(\tau)}{d\tau}H_i^j(u,v), \quad (4.72)$$

$$R_N(u,v,\tau)=\sum_{j=1}^{6}\frac{dn_{i+3(l-1)}^{j+3(m-1)}(\tau)}{d\tau}H_i^j(u,v)-\frac{R^2k_1}{D_F}\Bigg[C_1\sum_{i,j=1}^{6}q_{i+3(l-1)}^{j+3(m-1)}(\tau)H_i^j(u,v)\times$$
$$\left(1-\sum_{j=1}^{6}n_{i+3(l-1)}^{j+3(m-1)}(\tau)H_i^j(u,v)\right)-\frac{1}{k^*}\sum_{i,j=1}^{6}n_{i+3(l-1)}^{j+3(m-1)}(\tau)H_i^j(u,v)\Bigg], \quad (4.73)$$

$$R_C(v,\tau)=\sum_{j=1}^{6}\frac{dc^{j+3(m-1)}(\tau)}{d\tau}H_j(v)-\frac{\psi}{Peh_m^2}\sum_{j=1}^{6}c^{j+3(m-1)}(\tau)H_j''(v)+\frac{\psi}{h_m}\sum_{j=1}^{6}c^{j+3(m-1)}(\tau)H_j'(v)$$
$$+\theta Bi\left(\sum_{j=1}^{6}c^{j+3(m-1)}(\tau)H_j(v)-\sum_{i,j=1}^{6}q_{3i+1}^{j+3(m-1)}(\tau)H_j(v)\right). \quad (4.74)$$

The residuals R_Q, R_N and R_C are forced to vanish at collocation points. The evaluation of $Q(u,v,\tau)$ and $C(v,\tau)$ at boundary collocation points yields:

$$\sum_{j=1}^{6}q_{3l-1}^{j+3(m-1)}(\tau)H_j(v_s)=0, \quad (4.75)$$

$$\sum_{j=1}^{6}q_{3n+2}^{j+3(m-1)}(\tau)H_j(v_s)=-Bi(h_n)\left[\sum_{j=1}^{6}q_{3n+1}^{j+3(m-1)}(\tau)H_j(v_s)-\sum_{j=1}^{6}c^{j+3(m-1)}(\tau)H_j(v_s)\right], \quad (4.76)$$

where for $m=1,\ s=1,2,3,4,5$; $m=2,3,4....,\upsilon-1, s=2,3,4,5$ and $m=\upsilon,\ s=2,3,4,5$.

$$c^1(\tau)-\frac{1}{Pe}c^2(\tau)=0, \quad (4.77)$$

$$c^{3\upsilon+2}(\tau)=0, \quad (4.78)$$

Let the index set $A=H_i(u)\ \{(i,j)|i,j=1,2,3,4,5,6\}$. The condition $Q(u,v,0)=1$ implies:

$$\sum_{i,j=1}^{6}q_{i+3(l-1)}^{j+3(m-1)}(0)H_i(u)H_j(v)=1, \quad (4.79)$$

using the points $(u,v)\in D=\{(0,0),(1,0),(0,1),(1,1)\}$,

Also, $q_{i+3(l-1)}^{j+3(m-1)}(0)=1$, (4.80)

For $(\alpha,\beta)\in B=\{(1,1),(1,4),(4,1),(4,4)\}$, we get

$$\sum_{\alpha,\beta=1}^{6} q_{\alpha+3(l-1)}^{\beta+3(m-1)}(0)H_{\alpha}^{'}(u)H_{\beta}(v)=0\,, \tag{4.81}$$

$$\sum_{\alpha,\beta=1}^{6} q_{\alpha+3(l-1)}^{\beta+3(m-1)}(0)H_{\alpha}(u)H_{\beta}^{'}(v)=0\,, \tag{4.82}$$

$$\sum_{\alpha,\beta=1}^{6} q_{\alpha+3(l-1)}^{\beta+3(m-1)}(0)H_{\alpha}^{'}(u)H_{\beta}^{'}(v)=0\,, \tag{4.83}$$

One can easily see that $q_{\alpha+3(l-1)}^{\beta+3(m-1)}(0)=0$ for indices $(\alpha,\beta)\in A-B$. Similarly

$$n_{\alpha+3(l-1)}^{\beta+3(m-1)}(0)=\begin{cases}1, & (\alpha,\beta)\in B\\ 0, & (\alpha,\beta)\in A-B\end{cases} \tag{4.84}$$

The initial condition $C(v,0)=1$ implies:

$$c^{3m+1}(0)=1,\; c^{3m+2}(0)=0\,, c^{3m+3}(0)=0 \tag{4.85}$$

for $m=0,1,...,\upsilon$. The initial conditions:

$$c^{1}(0)=1,\; c^{2}(0)=0\,, c^{3}(0)=0\,,\; q_{3n+1}^{1}(0)=c^{1}(0)=0\,. \tag{4.86}$$

The derived system of the differential equation along with the boundary conditions are solved using MATLAB ode15s system solver.

4.11 SUMMARY

In this chapter, different mathematical models, and basic assumptions for a systematic exploration of a porous structured pulp fibre bed are discussed. The different mathematical models of pulp washing explored by various authors are also given. Further, one dimensional linear, nonlinear, and 2-D models along with different boundary conditions related to pulp washing are presented. Discretized form and detailed numerical procedure using QHCM of the method are reported.

Contents of this chapter are published in:

1. *Afrika Matematika, Vol. 32(5) 997-1019, 2021, ISSN: 2190-7668. (Scopus indexed).*
2. *Journal of Engineering Research, Vol. 10 (1A), 67-77, 2021, ISSN: 2307-1885 (SCIE).*
3. *Advances and Applications in Mathematical Sciences, 20(11) 2549-2557, 2021, ISSN: 0974-6803 (UGC-Care).*
4. *Advances in Intelligent Systems and Computing, Vol. 1412, 995-1009, 2022 Springer Nature, ISSN: 2194-5357(Scopus indexed).*