CHAPTER 3

METHODOLOGY

The methods established to solve the mathematical models are viewed as a backbone in the pulp industry. The breakthrough in this area is the development of methods to find the solution to these models. The main task of researchers is to develop methods that are more reliable and accurate, so that the industry can use these methods to reduce the complexity and optimally utilize its available resources. The accuracy is not the only main concern of the problem, but the stability of the method, CPU time needed for the complete process, ease of use, and the suitable numerical scheme are other vital concerns. Two types of solutions are available in the literature to solve these models:

- Analytic Solution
- Numerical Solution

3.1 THE ANALYTIC SOLUTION

Roininen and Alopaeus (2011) explained that the possibility of the existence of analytic solutions holds only for linear equations, but it is tedious to derive an analytic solution for nonlinear equations. Achieving an analytic solution is not an easy task for nonlinear models specially. However, analytical solutions play a major role in verifying the results derived using numerical methods. Neretnieks (1976); Zheng and Gu (1996) and Liao and Shiau (2000) explored the analytical solutions of the model equations of fixed bed adsorber. Further, Brenner (1962); Kukreja (1996); Zheng and Gu (1996); Potůček, (1997); and Kukreja and Ray (2009) obtained the analytic solution of these models using Laplace transform. Further, Tervola (2006) used a modified asymptotic formula and Fourier series method based on the Laplace transform to solve the pulp-washing model.

The detailed study of these methods revealed that the analytic solution is complex and less suitable for nonlinear problems (Mittal et al., 2013). Further, due to difficulty in attaining the analytic solution of models, less development is observed in this direction. However, the complicacy in deriving the analytic solution gave rise to the idea of approximation techniques. The approximation techniques are also helpful in finding the solution to nonlinear models and the calculations are made easy using different software.

3.2 THE NUMERICAL SOLUTION

Mittal et al. (2013) stated that a lot of work is done by researchers in the direction of approximation. However, there are some certain drawbacks due to which the existing methods do not serve the purpose of more accuracy of the solution. A few studies highlighting the methods along with their shortcomings are given here under:

Fiadeiro and Veronis (1977); Dehghan (2004); Sari et al. (2010); and Tatari and Dehghan (2009) used the technique of finite difference method (FDM) to solve the models of diffusion-dispersion. However, Mittal and Kukreja (2015) described in their study that it is not an easy task to select a suitable step size in the FDM and this is the main drawback of this method. The method is not much stable because choosing a strict step size is the main necessity of this method for the stability of the solution. Nevertheless, the accuracy of the numerical solution is not so high. The discretization of even a few PDEs by the method of lines can lead to an extremely large system of ODEs; the numerical solution of which may have high cost and storage implications. Al-Jabari et al. (1994); Sridhar (1999); Liu and Bhatia (2001); and Sharma et al. (2011) solved the models numerically with Galerkin/Petrov Galerkin method. However, Arora et al. (2005) presented that the Galerkin method is unsuitable for large systems because the integration process becomes very tedious in this method. Also, the equations turn stiff for large values of parameters. This causes an increase in the oscillations. Therefore, the study tried weighted residual methods for the discretization process of two-point BVPs.

Fan et al. (1971) explained that the computational time and convergence features of a numerical scheme are also important, which depends on the selection of step-size of the integration scheme. The inappropriate step size can make the integration procedure inaccurate or divergent. The integration scheme sometimes does not provide accurate results, when the step size is too large. Further, Villadsen and Stewart (1967); Lee (1979); Al-Jabari et al. (1994); and Onah (2002) suggested the orthogonal collocation method (OCM) for numerical simulation of the models because it is simple and easily adaptable to the computer codes. Methods like FDM and OCM are not suitable in case of small step size and give oscillations (Shiraishi, 2001). Liu and Bhatia (2001); and Arora et al. (2005) illuminated that one cannot achieve better-converging results, when more collocation points are used. To overcome this situation, the orthogonal collocation on finite elements (OCFE) method comes into existence to handle the situation (Arora et al., 2006).

Fang et al. (2002) compared the finite element, finite difference, and finite volume method (FVM) and suggested that the finite element method (FEM) is slightly more beneficial than other methods. However, Roininen and Alopaeus (2011) used OCFE and the moment method with cubic polynomials and achieved better accuracy with less CPU time. It was noted in the study that the time needed to solve the reactor model of one-dimensional using OCFE is about half than the FVM and moment method. From the above discussion, it is observed that different methods have been used by the previous researchers to find the numerical solution of the models. However, owing to accuracy, few methods are discussed hereunder:

3.2.1 Orthogonal Collocation Method

Villadsen and Stewart (1967) explained that the collocation method is applied after converting the nonlinear differential equation into linear to achieve an approximate solution. The trial-function expansion is a technique that is extensively used to solve the BVPs, and the main target is to determine the expansion coefficients with the use of weighted-residual methods. This straightforward approach can be readily adapted for a general computer program. Further, Fan et al. (1971) described the three categories of collocation methods such as interior, boundary, mixed and applied the mixed collocation method to solve the axial dispersion model represented by nonlinear differential equations and suggested that the selection of optimal step size depends on many parameters such as *Pe*. It was demonstrated that this technique needs very short computational time and is free of stability difficulties. Kill et al. (1995) described that FDM needs more computation time to solve the problems as compared to OCM. It was also suggested that OCM is an effective solution technique for the problems of moving boundary faced in heat and mass transfer processes. The differential equations are transformed into the equations in time when it is applied to the space variables. In this method, the residual is forced to vanish at the collocation points, which are the zeros of the orthogonal polynomials. Soliman and Ibrahim (1999) proved the proficiency of the collocation method with derived numerical results. Also, it was stated that the method is ideally applicable to chemical reaction and diffusion problems and is of high accuracy with Jacobi polynomials.

Shiraishi (2001) enlightened that the orthogonal collocation method provides numerical solutions of high accuracy over the wide ranges of parameters for the axial dispersion model, which is extensively used for tubular flow reactors with the combined effect of the chemical reaction and reactant flow. To overcome the shortcomings, an effective numerical scheme with an accuracy of super high order by using the Taylor's series solution for BVP was proposed. Further, Carrara et al. (2003) stated that this method is based on the approximation of a solution using a series. The collocation method is used to solve the mathematical model describing the dispersion flow in the reactor represented by a second order PDE. The solution at the collocation points is attained by determining the unknown coefficient of the polynomials. The computer programs are developed to approximate the collocation equation which is expressed in terms of solution at grid points and collocation points. Hasegawa et al. (1996) derived a highly accurate numerical solution for this model using OCM with Lagrange's interpolation. Further, Mittal and Kukreja (2015) observed the oscillations in results using OCM for large values of the parameters, which do not yield good results, even with more collocation points. The situation of this type is handled with the method of OCFE, which is a combination of the orthogonal collocation method and FEM.

3.2.2 Orthogonal Collocation Finite Element Method

This approach is gaining popularity in contrast with the conventional finite difference method due to the compactness of the results (Carey and Finlayson, 1975). This is a method, which is combination of the two approaches (OCM and FEM) with the use of orthogonal polynomial expansions suited better for collocation technique. Carey and Finlayson (1975) proved that the technique is mainly useful for chemical engineering problems and is very elegant and a simple technique that gained popularity because it is easily adaptable to computer programs and takes less computational time. Ma and Guiochon (1991) supported that this technique permits the achievement of more accurate results in calculations for diffusion problems and is beneficial for local estimation and grid refinement. Likewise, Onah (2002) used OCFE to check the asymptotic behavior of parabolic PDE and Liu and Jacobsen (2004) proposed the method of OCFE by evaluating and minimizing the resulting residuals with proper mesh discretization and solved the reaction-convection-diffusion problem for bifurcation analysis of systems.

Arora et al. (2006) supported that the OCFE is one of the most appropriate and simplest in the category of these methods. In this method, OCM is associated with the FEM. The OCM provides the accuracy and FEM gives stability to the results. Also, in OCFE, the time variable and its differential operator are expressed in terms of the space variable. In this procedure, the continuity of the trial function including the first derivative at the boundaries of the elements, or the nodal points is a mandatory condition. The orthogonal polynomial such as Lagrange's interpolation is used to approximate the solution and residuals are set equal to zero at the collocation points. The system of equations so derived are solved with MATLAB ode15s system solver. Thereafter, the method was applied to test the validity of several problems and derived better results.

Arora et al. (2006) and Ganaie et al. (2013) solved the diffusion-reaction problem with mixed boundary and Dirichlet boundary conditions and shows that the results are more stable and convergent than the OCM.

3.2.3 Spline Collocation Method

Potůček (1997) used the cubic B-spline method to solve the one-dimensional axial dispersion model and validated the experimental results of a paper mill. Further, Bialecki and Fairweather (2001); Kadalbajoo and Awasthi (2008); Gupta et al. (2012); Mittal and Jain (2012), and Nazir et al. (2016) used the spline collocation method to solve the diffusion models and obtained better results than previous techniques such as OCFE. It error bounds, super convergence properties, and consistency along with the stability of the method was also established. In a study, Caglar et al. (2006) used the cubic B-spline interpolation for the solution of two-point BVPs and compared the results with FEM, FDM, and FVM. The results so derived proved the B-spline interpolation method has better accuracy. Likewise, Ramadan et al. (2007) explored the spline method for the solution of two-point BVPs with Dirichlet and Neumann boundary conditions and noticed better accuracy. Also, Dhawan and Kapoor (2011) focused on B-spline functions along with FEM to solve the ADE numerically and observed a major reduction in the computational cost while solving the problem. The satisfactory results were derived with the good agreement and more accuracy.

Liu et al. (2011) presented an interpolation method based on the quartic spline functions for solving the two-point BVP and proved the accuracy of 4^{th} and 6^{th} order near the boundary and at the boundary for the linear case. Further, Mittal and Jain (2012) explored the collocation method with cubic B-splines as a basis function to solve the nonlinear Burgers' equation by taking Dirichlet's boundary conditions. The efficiency of the method was confirmed and an improved solution as compared to the existing ones was achieved. Likewise, Arora et al. (2016) solved Burgers' equation using Hermite splines polynomials and proved the stability and efficiency of the method by comparing the results with previously existing techniques.

3.2.4 Cubic Hermite Collocation Method

Finlayson (1980) explained the cubic Hermite collocation method (CHCM) in detail. In this technique, the cubic Hermite polynomials are used to approximate the trial function. These polynomials are C^1 continuous. In other words, these polynomials have the property of continuity of solution and first derivative at the boundary of each element. Owing to this property, the additional requirement of continuity condition at nodal points is abolished. This helps in saving the computational time, cost, and effort in comparison with the Lagrange basis. It was also proved that the results obtained using this method are better in comparison to the previous methods. Finlayson (1980) proved in his work that nearly one-third of computational cost is decreased in this procedure. Further Mittal et al. (2013) and Ganaie and Kukreja (2014) applied this method to solve different BVPs that are linear as well as nonlinear with different boundary conditions and proved that the results are improved than the OCFE and OCM techniques. The studies provide the numerical results using CHCM are nearer to an analytic solution with better accuracy than previously existing results of OCM and OCFE.

It is observed from the earlier paragraphs that numerous authors applied varied techniques to obtain accuracy in optimum time for solving the mathematical models. However, in its pursuit, one must perform tedious numerical calculations at several points and this process consumes more time. To overcome this situation, the QHCM is applied for solving mathematical models related to industrial practices in the present study.

A lot of work has been done by the researchers in the direction to solve the models and attain the accuracy of the numerical technique in a minimum time. In its pursuit, the QHCM is implemented in the present study to derive the numerical solution of mathematical models associated with the industry. According to Dyksen and Lynch (2000), the subsidiary condition of continuity of first and second derivatives at the boundary of each element is not required in these polynomials therefore, the number of equations is reduced considerably. This technique is a combination of the OCM and FEM in which the quintic Hermite polynomials are used as a trial function in discretizing process for the model of diffusion dispersion phenomena. These polynomials have a special property that the continuity condition of a trial function and its first and second derivative at the grid points is satisfied, which makes the resulting solution with continuous derivative throughout the domain (Arora et al., 2016). According to Kaur et al. (2021), QHCM is a weighted residual method in which Hermite interpolating polynomials which are of the order five are considered to approximate the trial function. This is a generalized form of the Lagrange interpolation polynomials. Further, in a study, Kaur et al. (2018) explained that the quintic Hermite polynomials reduce the number of equations and the mathematical complexity, which is the main advantage of the method. Kaur et al. (2018, 2021) explained that this is a technique that gives more accurate results in less time. This technique is also helpful in reducing the mathematical complexity and number of equations. Hereunder, the procedure related to QHCM is explained in detail:

The domain $0 \le \zeta \le 1$ is partitioned into a finite number of parts by introducing $\zeta_1, \zeta_2, ..., \zeta_{N+1}$ points such that $\zeta_1 = 0$ and $\zeta_{N+1} = 1$ with $h_k = \zeta_{k+1} - \zeta_k$. Introducing a new variable $u = (\zeta - \zeta_k)/h_k$ such that u varies from 0 to1 when ζ varies from ζ_k to ζ_{k+1}. Then OCM with quintic Hermite as the basis function within each element is applied.

The approximate solution $c(u,t)$ at the r^{th} collocation point in the k^{th} element is given by:

$$c_{kr}(u,t) = \sum_{q=1}^{6} a_{q+3(k-1)}^{kr}(t) H_q^k(u); \; k = 1,2,...,N+1; \; r = 2,3,4,5. \tag{3.1}$$

using Eq. (3.1) one gets:

$$\frac{\partial c_{kr}}{\partial u} = \frac{1}{h_k} \sum_{q=1}^{6} a_{q+3(k-1)}^{kr}(t) \frac{dH_q^k(u)}{du}, \tag{3.2}$$

$$\frac{\partial^2 c_{kr}}{\partial u^2} = \frac{1}{h_k^2} \sum_{q=1}^{6} a_{q+3(k-1)}^{kr}(t) \frac{d^2 H_q^k(u)}{du^2}, \tag{3.3}$$

$$\frac{\partial c_{kr}}{\partial t} = \sum_{q=1}^{6} \frac{da_{q+3(k-1)}^{kr}(t)}{dt} H_q^k(u), \tag{3.4}$$

where the standard quintic Hermite basis functions H_q^p's are given by:

$$P_j(\zeta) = H_{3q-2}^p(\zeta) = \begin{cases} \left(\frac{\zeta - \zeta_{k-1}}{h_{k-1}}\right)^3 \left(6\left(\frac{\zeta - \zeta_{k-1}}{h_{k-1}}\right)^2 - 15\left(\frac{\zeta - \zeta_{k-1}}{h_{k-1}}\right) + 10\right); & \zeta \in [\zeta_{k-1}, \zeta_k] \\ \left(1 - \frac{\zeta - \zeta_k}{h_k}\right)^3 \left(1 + 3\left(\frac{\zeta - \zeta_k}{h_k}\right) + 6\left(\frac{\zeta - \zeta_k}{h_k}\right)^2\right); & \zeta \in [\zeta_k, \zeta_{k+1}] \\ 0; & otherwise \end{cases} \tag{3.5a}$$

$$Q_j(\zeta) = H^p_{3q-1}(\zeta) = \begin{cases} -h_{k-1}\left(\dfrac{\zeta-\zeta_{k-1}}{h_{k-1}}\right)^3\left(1-\dfrac{\zeta-\zeta_{k-1}}{h_{k-1}}\right)\left(4-3\dfrac{\zeta-\zeta_{k-1}}{h_{k-1}}\right); & \zeta\in[\zeta_{k-1},\zeta_k] \\ h_k\left(1-\dfrac{\zeta-\zeta_k}{h_k}\right)^3\left(\dfrac{\zeta-\zeta_k}{h_k}\right)\left(1+3\dfrac{\zeta-\zeta_k}{h_k}\right); & \zeta\in[\zeta_k,\zeta_{k+1}] \\ 0; & otherwise \end{cases} \quad (3.5b)$$

$$R_j(\zeta) = H^p_{3q}(\zeta) = \begin{cases} \dfrac{1}{2}h_{k-1}\left(\dfrac{\zeta-\zeta_{k-1}}{h_{k-1}}\right)^3\left(1-\dfrac{\zeta-\zeta_{k-1}}{h_{k-1}}\right)^2; & \zeta\in[\zeta_{k-1},\zeta_k] \\ \dfrac{1}{2}h_k\left(1-\dfrac{\zeta-\zeta_k}{h_k}\right)^3\left(\dfrac{\zeta-\zeta_k}{h_k}\right)^2; & \zeta\in[\zeta_k,\zeta_{k+1}] \\ 0; & otherwise \end{cases} \quad (3.5c)$$

where only one function and its first and second order derivatives from six nodes is one and others are zero at the boundary of the domain.

In another way, $P_j(\zeta_i)=\delta_{ij}$, $P_j^{'}(\zeta_i)=0$, $P_j^{''}(\zeta_i)=0$, $Q_j(\zeta_i)=0$, $Q_j^{'}(\zeta_i)=\delta_{ij}$, $Q_j^{''}(\zeta_i)=0$, $R_j(\zeta_i)=0$, $R_j^{'}(\zeta_i)=0$, $R_j^{''}(\zeta_i)=\delta_{ij}$ for $i, j=1,2,...,6$.

In particular, for k^{th} element $[\zeta_k,\zeta_{k+1}]$, the quintic Hermite basis functions $P_j(\zeta_i)$, $Q_j(\zeta_i)$, $R_j(\zeta_i)$ are expressed as given:

$$\left.\begin{array}{ll} H_1^k(\xi)=\left(1+3\xi+6\xi^2\right)(1-\xi)^3 , & H_2^k(\xi)=\xi(1-\xi)^3(1+3\xi) \\ H_3^k(\xi)=\dfrac{1}{2}\xi^2(1-\xi)^3 , & H_4^k(\xi)=\xi^3\left(6\xi^2-15\xi+10\right) \\ H_5^k(\xi)=\xi^3(1-\xi)(3\xi-4) , & H_6^k(\xi)=\dfrac{1}{2}\xi^3(1-\xi)^2 \end{array}\right\} \quad (3.6)$$

Such that $H_1(\xi)=H_4(1-\xi),\ H_2(\xi)=-H_5(1-\xi),\ H_3(\xi)=H_6(1-\xi)$

3.2.5 Collocation Points

The residuals are equated to zero at collocation points. The collocation points play a major role in the discretization process and the residuals are made satisfied at these points to reach the exact solution. The selection of collocation points is a very important aspect that one has to bear in mind while applying any numerical technique.

Fan et al. (1971) stated that a computational approach that comprises a collocation method is based on the selection of collocation points and explained that the choice of collocation points is very important in the collocation technique. The addition of collocation points helps in making the approximation of high order accuracy. The collocation points make the error minimize and yield satisfactory results. Further, Finlayson (1980) in his study, preferred roots of Chebyshev interpolation polynomials as collocation points to minimize the residuals. In addition, Arora et al. (2006) mentioned that Jacobi, Legendre, and Chebyshev polynomials are the type of orthogonal polynomials that can be followed as a trial function and collocation points are zeros of these polynomials.

In QHCM, the roots of 4th order shifted Legendre polynomials are taken as collocation points. According to Andrews (1984), these polynomials are a special case of Jacobi polynomials. Besides, Villadsen and Stewart (1967) discussed that the Chebyshev polynomials provide accurate results at the corner points of the domain. However, Douglas and Dupont (1973) expressed that Legendre polynomials provide more accuracy in numerical results when the points lie in the center of the domain. Furthermore, Arora et al. (2006) and Ganaie et al. (2014) used roots of Legendre polynomials as collocation points and derived better numerical results than using Chebyshev polynomials. Likewise, Parand and Rad (2012) and Gupta et al. (2015) showed that the results attained with the use of these polynomials are more accurate. Further, Arora et al. (2016) used the roots of 4th order shifted Legendre polynomial which is a particular case of Jacobi polynomial as interior collocation points. The recurrence relation satisfied by these equations is given as:

$$\begin{aligned}\left[\begin{array}{l}(\alpha^2-\beta^2)(1+\alpha+\beta+2n)+\\ \qquad x(\alpha+\beta+2n)(\alpha+\beta+2n+1)(\alpha+\beta+2n+2)\end{array}\right]P_n^{(\alpha,\beta)}(x)\\ =(2n+2)(1+\alpha+n+\beta)(2n+\alpha+\beta)P_{n+1}^{(\alpha,\beta)}(x)+\\ 2(n+\alpha)(n+\beta)(2+\alpha+\beta+2n)P_{n-1}^{(\alpha,\beta)}(x)\end{aligned} \tag{3.7}$$

with $P_0^{(\alpha,\beta)}(x)=1$ and $P_1^{(\alpha,\beta)}(x)=(\alpha+1)+0.5(x-1)(\alpha+\beta+2)$ for all $x\in[-1,1]$ and $n\in N$ is the degree of a polynomial. α and β are parameters assumed as zero as a particular case. The transformation $u=\frac{x+1}{2}$ is used to shift the zeros of polynomials from [-1,1] onto [0,1].

The interior collocation points, which are the roots of 4th order shifted Legendre polynomial given below as:

$$\xi_2 = \frac{1}{2} + \frac{1}{2}\sqrt{\frac{3}{7} + \frac{2\sqrt{30}}{35}}, \qquad \xi_3 = \frac{1}{2} + \frac{1}{2}\sqrt{\frac{3}{7} - \frac{2\sqrt{30}}{35}},$$
$$\xi_4 = \frac{1}{2} - \frac{1}{2}\sqrt{\frac{3}{7} + \frac{2\sqrt{30}}{35}}, \qquad \xi_5 = \frac{1}{2} - \frac{1}{2}\sqrt{\frac{3}{7} - \frac{2\sqrt{30}}{35}}. \tag{3.8}$$

The derived four roots lie between 0 and 1 taken as interior collocation points and serve the purpose of the discretization where the endpoints of the domain are 0 and 1.

3.2.6 Error Calculation

To verify the numerical results, error calculation is an important criterion for stability analysis. In the case of linear problems, the comparison of numerical and analytic results is made using the relative error, $\|L\|_\infty$ norm (supremum norm), and $\|L\|_2$ norm (Euclidean norm). These norms are defined as:

$$\|L\|_2 = \sqrt{h\sum_{j=1}^{N}\left|c_j^{exact} - (c_N)_j\right|^2} \quad \text{and} \quad \|L\|_\infty = \max_j \left|c_j^{exact} - (c_N)_j\right|,$$

where c_j^{exact} is the exact solution and $(c_N)_j$ is the numerical solution.
The relative error can be calculated as:

$$\frac{\left|c_j^{exact} - (c_N)_j\right|}{c_j^{exact}}. \tag{3.9}$$

Edoh et al. (2000); Arora et al. (2016) explained the convergence criteria and relative error for making the comparison of supremum and Euclidean norms to test the stability and efficiency of the method. Similarly, Bialecki and Fairweather (2000); Liu and Jacobsen (2004); Dhawan and Kapoor (2011) have also established the accuracy of these norms and checked the steady state condition based on residuals. Bu and Buk (2020) also estimated the computational errors using, the L_2 norm, the maximum norm, and the relative L_2 norm and proved the method to be more accurate, and efficient with less computational costs in comparison with other methods.

3.2.7 Convergence Criteria

According to Edoh et al. (2000), it is not an easy task to calculate the residual for non-linear BVPs. In the case of non-linear problems, the numerical results are verified using the convergence technique. However, the stability analysis for these models can be checked based on numerical results. Farrell and Hegarty (1991) suggested the method to derive the rate of convergence for the non-linear problem as given below:

$$\upsilon = \min(\upsilon^n) \text{ for } \upsilon^n = \frac{\log(\rho^n) - \log(\rho^{2n})}{\log(2)} . \tag{3.10}$$

where $\rho^n = \max \left\| \overline{c^n} - \overline{c^{2n}} \right\|_\infty$ and $\overline{c^n}$ is the numerical value at n node points.

Also, Arora et al. (2005) used this result to check the stability of numerical techniques for the non-linear BVPs. Some authors such as Arora et al. (2016) used the rate of convergence to prove the convergence of the method.

3.2.8 Algorithm of the Method

Step 1. The domain $0 \le \zeta \le 1$ is divided into N number of elements as

$$0 = \zeta_1 \le \zeta_2 \le .... \le \zeta_{N+1} = 1.$$

Step 2. The transformation $u = \dfrac{\zeta - \zeta_k}{h_k}$ is used such that $0 \le u \le 1$ whenever $\zeta_k \le \zeta \le \zeta_{k+1}$

Step 3. The trial function represented at r^{th} collocation point for $2 \le r \le 5$ and k^{th} element ($1 \le k \le N$) given as:

$$c_{kr}(u,t) = \sum_{q=1}^{6} a_{q+3(k-1)}^{kr}(t) H_q^k(u),$$

Step 4. The derivatives are $\dfrac{\partial c_{kr}}{\partial u} = \dfrac{1}{h_k} \sum_{q=1}^{6} a_{q+3(k-1)}^{kr}(t) \dfrac{dH_q^k}{du}$,

$$\frac{\partial^2 c_{kr}}{\partial u^2} = \frac{1}{h_k^2} \sum_{q=1}^{6} a_{q+3(k-1)}^{kr}(t) \frac{d^2 H_q^k}{du^2} ,$$

$$\frac{\partial c_{kr}}{\partial t} = \sum_{q=1}^{6} \frac{d a_{q+2(k-1)}^{kr}(t)}{dt} H_q^k ,$$

Step 5. The model is discretized using steps 3 and 4.

Step 6. Then the system of differential algebraic equations is obtained from step 5 as $A\dfrac{dX}{dt} = BX$

Step 7. The derived system of equations is solved numerically by using MATLAB ode 15s system solver.

3.3 SUMMARY

Two methods for solving the mathematical models viz. analytic and numerical are explained in this chapter. The possibility of the existence of analytic solutions holds only for linear equations, whereas it is cumbersome to derive an analytic solution for nonlinear equations. The complicacy in deriving the analytic solution gave rise to the idea of approximation techniques such as FDM and the Galerkin method. There were still some difficulties in finding the solution, which gave rise to other methods like OCM, OCFE, CHCM, and SCM. Further, to improve accuracy in less time, the QHCM is discussed in detail and suggested for solving the mathematical model related to pulp washing. This technique is a combination of the OCM and FEM in which the quintic Hermite polynomials of the order five are used as a trial function in discretizing process. The roots of 4^{th} order shifted Legendre polynomials are taken as collocation points. Besides, the error calculation and method to check stability and convergence are also discussed in this chapter.