ABSTRACT

Introduction

Mathematical modeling is a process of representation of the real-life problems occurred in industrial practices into a set of mathematical equations. It plays an important role in understanding complex processes. Various processes in science and engineering such as in the field of oil extraction from underground reservoirs, flow problems, the problems associated with environmental pollution, diffusion-dispersion, advection-diffusion, heat transport problems, and many more are described by mathematical modeling. Since these models involve the rate of change of physical quantities, therefore, quantitative treatment of these models is usually expressed in the form of boundary value problems (BVPs). One such two-point BVP in the form of mathematical models used in industrial practices is associated with the pulp washing process. Pulp washing is concerned with detaching cellulose fibres from black liquor with the use of a minimal amount of wash liquor. The solute displacement from the pulp fiber bed is related to the diffusion-dispersion phenomena.

Various researchers have solved such models analytically and numerically using different techniques. The detailed study of these methods revealed that the analytic solution is complex and less suitable for nonlinear problems. Various authors have applied approximation techniques such as the finite difference method (FDM), Galerkin method, orthogonal collocation method (OCM), orthogonal collocation finite element method (OCFE), moving finite element method (MFEM), cubic spline collocation method (CSCM), cubic Hermite collocation method (CHCM) and many more for solving the mathematical models. These techniques have certain drawbacks owing to which, the existing methods did not serve the purpose of achieving the accuracy of the solution. Even, some methods take more time and effort in numerical simulation. To fill the gap in the literature and to achieve the research objectives, this study presents an effort in solving the mathematical model of pulp washing using the quintic Hermite collocation method (QHCM) to improve the accuracy using minimum time and effort.

Mathematical Models

The linear and non-linear associated with the pulp-washing process are solved using this technique, and the results obtained are compared with the analytic solution and other

previous methods. A summary of these models is given in Table 1. In addition, the range of important parameters suitable for efficient washing is determined. Thereafter, the numerical results using the present method are also validated using the experimental data of the paper mill.

Table 1: Linear and nonlinear model equations

Model type	Model Equation (Dimensionless)	Boundary Condition $for\ all\ T \geq 0$	Initial Condition	Adsorption Isotherm
Linear Model-1	$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z}$	$C = 0 \quad at \quad Z = 0$ $\frac{\partial C}{\partial Z} = 0 \quad at \quad Z = 1$	$C(Z,0) = 1$	-
Linear Model-2	$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z}$	$PeC = \frac{\partial C}{\partial Z} at \quad Z = 0$ $\frac{\partial C}{\partial Z} = 0 \quad at \quad Z = 1$	$C(Z,0) = 1$	-
Linear Model-3	$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z} - \frac{\mu Bi}{Pe} C$	$PeC = \frac{\partial C}{\partial Z} at \quad Z = 0$ $\frac{\partial C}{\partial Z} = 0 \quad at \quad Z = 1$	$C(Z,0) = 1$	-
Linear Model-4	$R_d \frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z}$	$C = 0 \quad at \quad Z = 0$ $\frac{\partial C}{\partial Z} = 0 \quad at \quad Z = 1$	$C(Z,0) = 1$	-
Nonlinear Model-1	$\frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} = \frac{\partial C}{\partial T} + \frac{\partial C}{\partial Z} +$ $\frac{\mu C_F A_0}{\left[1 + B_0\left\{c_s + C\left(c_0 - c_s\right)\right\}\right]^2}\frac{\partial C}{\partial T}$	$PeC = \frac{\partial C}{\partial Z} at \quad Z = 0$ $\frac{\partial C}{\partial Z} = 0 \quad at \quad Z = 1$	$C(Z,0) = 1$	$n = \frac{A_0 c}{1 + B_0 c}$
Nonlinear Model-2	$\frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} = \frac{\partial C}{\partial T} + \frac{\partial C}{\partial Z} +$ $\frac{\mu C_F A_0}{\left[1 + B_0\left\{c_s + C\left(c_0 - c_s\right)\right\}\right]^2}\frac{\partial C}{\partial T}$	$C = 0 \quad at \quad Z = 0$ $\frac{\partial C}{\partial Z} = 0 \quad at \quad Z = 1$	$C(Z,0) = 1$	$n = \frac{A_0 c}{1 + B_0 c}$
Nonlinear Model-3	$\frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} = \frac{\partial C}{\partial T} + \frac{\partial C}{\partial Z} + k\mu\frac{\partial C}{\partial T}$	$PeC = \frac{\partial C}{\partial Z} at \quad Z = 0$ $\frac{\partial C}{\partial Z} = 0 \quad at \quad Z = 1$	$C(Z,0) = 1$	$n = kc$

After considering the above-mentioned linear and non-linear models, the present method is extended to solve two-dimensional models of displacement washing with particle and bulk fluid phases.

Methodology

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 a system of equations satisfies the solution values at collocation points. The present technique i.e. QHCM, a weighted residual method that is a combination of the OCM and FEM is used to solve the models. In this process, quintic Hermite polynomials of order five are used to approximate the trial function. These polynomials have a special property that the continuity condition of a trial function, its first & second derivative at the grid points are automatically satisfied.

In QHCM, 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 to 1 when ζ varies from ζ_k to ζ_{k+1}. Then, OCM with quintic Hermite as the basis function is applied within each element.

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

$$c_{pm}(u,t) = \sum_{q=1}^{6} a_{q+3(p-1)}^{pm}(t) H_q^p(u);\ p = 1,2,...,N;\ m = 2,3,4,5.$$

and

$$\frac{\partial c_{pm}}{\partial u} = \frac{1}{h_k} \sum_{q=1}^{6} a_{q+3(p-1)}^{pm} \frac{dH_q^p}{du},$$

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

$$\frac{\partial c_{pm}}{\partial t} = \sum_{q=1}^{6} \frac{da_{q+3(p-1)}^{pm}}{dt} H_q^p,$$

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

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

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

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

where only one function and its first and second-order derivatives from six nodes are 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 $i, j = 1, 2, ..., 6$.

The zeros of orthogonal polynomials such as 4th-order shifted Legendre polynomials are taken as interior collocation points.

By the technique of QHCM, the linear and non-linear models are reduced to the system of DAEs. The equations are written in the form: $Du = Mu$

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*×*4N*. The system is solved using MATLAB ode15s.

Results and Discussion

Four linear models related to pulp washing are solved with QHCM and the accuracy of the numerical results is tested with the help of the relative error and absolute error. The validity of the approach is tested by comparing the results with analytic solutions and previously published work. The stability is checked for linear models with the help of Euclidean and supremum norms. The comparisons of numerical solutions derived using QHCM with the previously existing methods such as OCFE, CHCM, MFEM, and CSCM are presented in terms of relative error, norms, and CPU time. The numerical results show more accuracy with a lesser number of equations and in minimum time as compared to the previous methods. Also, $Pe < 20$, $Bi < 5$ and $R_d > 1$ are of practical importance in the pulp-washing process.

After validating the results for linear models, the present technique is applied to solve three non-linear models. Numerical results obtained for 50 elements using QHCM are the same as compared to the results for 100 elements with CHCM for nonlinear models. It proves that better results are attained with less number of equations and in minimum time using the present technique. Besides, numerical results obtained via QHCM are verified using the experimental data of three paper mills available in the literature. The concentration of solute at the exit level using QHCM is quickly decreasing with time in comparison to the previous technique i.e. CHCM. The medium range of *Pe*, the small value of D_L & distribution ratio, the high porosity, increase in cake thickness makes the washing operation effective and help to achieve the target of washing with less quantity of water.

Interstitial velocity on account of an increase in axial dispersion does not affect the concentration profiles. Also, the variation in the D_L and u is observed when L is assumed constant. Bed efficiency is increased with a high value of *Pe* in comparison to the small value of *Pe*. Better washing is attained with the increase in displacement ratio owing to the high value of *Pe*. Furthermore, it is noticed that the results derived for the concentration of solute in the case of both nonlinear model-1 and 2 are the same when *Pe* is increased to 40. However, for *Pe* less than 40, the exit solute concentration for both models does not provide the same results. For nonlinear model-3, the exit solute concentration is more peaked when *Pe* is increased from 100. However, when *Pe* is small, the exit solute concentration profile is more curved with a slow rate of convergence.

The stability analysis for all the models based on the eigenvalues is derived and presented graphically. It is observed that all the eigenvalues are complex and lie in the stability region. For convergence analysis the result is proved by the theorem as given below:

Theorem: Let $\tilde{c}(z)$ be the collocation approximation from space of quintic Hermite interpolation polynomial to the solution $c(x)$ of the differential equation such that $c(z) \in C^6[0,1]$, Then the uniform error estimate is given by: $\left\| c(z) - \tilde{c}(z) \right\|_\infty \le Kn^{-4} \ln^6(n)$, where K is a positive constant.

The numerical results for the 2D model are validated with the experimental values of the paper mill available in the literature. The relative error is found to be very less using QHCM in comparison to OCFE and CSCM. The range of *Pe* lies between 10 to 20 for the improvement in washing. A small distribution ratio causes more bulging in pores. It is noticed that large values of *Bi* cause an increase in the mass transfer rate and indicate the fast convergence of the solution profiles as compared to small *Bi*.

The industrial data is collected from the prominent paper mill of Punjab (using wheat straw as a raw material) at the 4th stage of the pulp-washing process. The important industrial parameters such as bed porosity, fiber consistency, fiber porosity, interstitial velocity, and axial dispersion coefficient required to analyze the mathematical models are calculated using the raw data available from the industry with the expressions available in the literature. All these models are solved using this industrial data.

Conclusion and Recommendation

The relevant problems having applications associated with the pulp washing phenomenon are explored with the QHCM. The present technique is found to be efficient, economical in use, takes less CPU time, and is easy to implement. Besides, the numerical results derived using the present technique are compared with the previous techniques and are found to be superior and accurate. The range of various parameters used for pulp washing based on the data collected from the industry shows that the target of efficient washing is achieved for *Pe* between 10 and 20. It is noticed that the concentration profile at the exit level for the range of porosity between 0.941-0.961 has not much effect on the concentration profile. Further, the results derived for the concentration of solute at the exit level are not much affected by the range between 55.88 - 81.52 of fiber consistency. It is evident from the results of the study that various parameters used by the industry are optimal.

The computational cost of the model is reduced with the present technique. Therefore, the method worked well and can be widely employed to solve more problems related to the application areas of convection, advection, diffusion, and dispersion phenomena owing to its accuracy, simplicity, and less time-consuming property.