Advances and Applications in Mathematical Sciences
Volume 20, Issue 11, September 2021, Pages 2549-2557

A COMPUTATIONALLY EFFICIENT ALGORITHM FOR SOLUTION OF MATHEMATICAL MODELS OF DISPLACEMENT WASHING

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Abstract

An efficient numerical technique for the solution of a mathematical model related to pulp washing is described along with the effect of various industrial parameters. The linear and non-linear models are solved using quintic Hermite collocation method with Dirichlet's and mixed Robin's boundary conditions. Results obtained using MATLAB ode15s are compared with analytic and other literature data. The method is found to be stable using stability analysis and convergence criteria. The present method is more convenient, simple and refined for solving two-point boundary value problems and the results are more robust than earlier ones.

2010 Mathematics Subject Classification: 97Mxx.
Keywords: Pulp washing, Quintic Hermite, Peclet number, Collocation points.
Received October 13, 2020; Accepted November 5, 2020

I. Introduction

In paper industry, pulp washing is a foremost process, which has to be performed in an eco-friendly and efficient manner. In this practice, wash liquor is introduced to remove the solute residing in irregular void matrix of the packed bed. With the introduction of bulk fluid, the adsorbed solute is removed. Several investigators [1-11, 13-20] studied the pulp washing models in the form of boundary value problems (BVPs) with different conditions and obtained solution with various methods. In the present study, quintic Hermite collocation method (QHCM) is used to find the solution of two linear and a non-linear model. The continuity condition of trial function and its derivatives at the grid points is satisfied, which in turn reduces the number of equations. This technique is very effective as it reduces mathematical complexity and give better results. To check the accuracy of the method, the linear models are solved with QHCM and results are compared with the previous techniques with the help of 2D plots in tabular and graphical forms. Afterwards the method is used to solve the non-linear model and results for some important parameters affecting the pulp washing process are also presented in this work. The procedure used for collocation points, stability analysis and convergence criteria are also discussed. The model equations, in dimensionless form, related to pulp washing are described in Table 1.

II. Method

In the present study, the QHCM is used to solve the BVPs. In this method, quintic Hermite polynomials are used as a basis function in collocation techniques. The domain $0 \leq \eta \leq 1$ is divided into finite number of sub parts called elements by inserting $\eta_1, \eta_2, \ldots \eta_{N+1}$ points such that $\eta_1 = 0$ and $\eta_{N+1} = 1$ with $h_k = \eta_{k+1} - \eta_k$. A new variable $u = (\eta - \eta_k)/h_k$ is introduced such that u varies from 0 to1 when η varies from η_k to η_{k+1}. Thereafter, OCM with quintic Hermite as a basis function within each element is applied. Zeros of 4th order shifted Legendre polynomial are taken as interior collocation points.

Table 1. Dimensionless form of mathematical models related to pulp washing.

Model Type	Model Equation (Dimensionless form)	Booundary Condition (for all $T \geq 0$)	Initial Condition	Adsorption Isotherm
Linear-1	$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z}$ in $\Omega \in (0, 1)$	$C = 0$ at $Z = 0$ $\frac{\partial C}{\partial Z} = 0$ at $Z = 1$	$c(Z, 0) = 1$	–
Linear-2	$\frac{\partial C}{\partial T} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2}$ $- \frac{\partial C}{\partial Z}$ *in* $\Omega \in (0, 1)$	$PeC = \frac{\partial C}{\partial Z}$ at $Z = 0$ $\frac{\partial C}{\partial Z} = 0$ at $Z = 1$	$c(Z, 0) = 1$	–
Non-linear	$\frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} = \frac{\partial C}{\partial T} + \frac{\partial C}{\partial Z}$ $+ \frac{\mu^C F^A 0}{[1 + B_0\{c_s + C(c_0 - c_3)\}]^2}\frac{\partial C}{\partial T}$ in $\Omega \in (0, 1)$	$PeC = \frac{\partial C}{\partial Z}$ at $Z = 0$ $\frac{\partial C}{\partial Z} = 0$ at $Z = 1$	$c(Z, 0) = 1$	$n = \frac{A_0 c}{1 + B_0 c}$

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

$$c_{kj}(u, t) = \sum_{p=0}^{6} a^{kj}_{p+3(k-1)}(t) H^k_p(u) \text{ where } k = 1, 2, m \text{ and } j = 2, 3, 4, 5. \tag{1}$$

$$\frac{\partial c_{kj}}{\partial u} = \frac{1}{h_k}\sum_{l=1}^{6} a^{kj}_{p+3(k-1)} \frac{dH^k_p}{du} \tag{2}$$

$$\frac{\partial^2 c_{kj}}{\partial u^2} = \frac{1}{h_k^2}\sum_{p=1}^{6} a^{kj}_{p+3(k-1)} \frac{d^2 H^k_p}{du^2} \tag{3}$$

$$\frac{\partial c_{kj}}{\partial t} = \sum_{l=1}^{6} \frac{da^{kj}_{p+2(k-1)}}{dt} H^k_p \tag{4}$$

where the standard quintic Hermite basis functions H_p^k's is given by:

$$H_{3p-2}^k(\eta) = \begin{cases} \left(\frac{\eta - \eta_{k-1}}{h_{k-1}}\right)^3 \left(6\left(\frac{\eta - \eta_{k-1}}{h_{k-1}}\right)^2 - 15\left(\frac{\eta - \eta_{k-1}}{h_{k-1}}\right) + 10\right); \eta \in [\eta_{k-1}, \eta_k] \\ \left(1 - \frac{\eta - \eta_k}{h_k}\right)^3 \left(1 + 3\left(\frac{\eta - \eta_k}{h_k}\right) + 6\left(\frac{\eta - \eta_k}{h_k}\right)^2\right); \eta \in [\eta_k, \eta_{k+1}] \\ 0; \text{ otherwise} \end{cases} \tag{5a}$$

$$H_{3p-1}^k(\eta) = \begin{cases} -h_{k-1}\left(\frac{\eta - \eta_{k-1}}{h_{k-1}}\right)^3 \left(1 - \frac{\eta - \eta_{k-1}}{h_{k-1}}\right)\left(4 - 3\frac{\eta - \eta_{k-1}}{h_{k-1}}\right); \eta \in [\eta_{k-1}, \eta_k] \\ h_k\left(1 - \frac{\eta - \eta_k}{h_k}\right)^3 \left(\frac{\eta - \eta_k}{h_k}\right)\left(1 + 3\frac{\eta - \eta_k}{h_k}\right); \eta \in [\eta_k, \eta_{k+1}] \\ 0; \text{ otherwise} \end{cases} \tag{5b}$$

$$H_{3p}^k(\eta) = \begin{cases} \frac{1}{2}h_{k-1}\left(\frac{\eta - \eta_{k-1}}{h_{k-1}}\right)^3 \left(1 - \frac{\eta - \eta_{k-1}}{h_{k-1}}\right)^2; \eta \in [\eta_{k-1}\eta_k] \\ \frac{1}{2}h_k\left(1 - \frac{\eta - \eta_k}{h_k}\right)^3 \left(\frac{\eta - \eta_k}{h_k}\right); \eta \in [\eta_k, \eta_k + 1] \\ 0; \text{ otherwise} \end{cases} \tag{5c}$$

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. Using QHCM, discretized form of linear and non-linear models obtained using (1) to (4) can be written in the form $Du = Mu$, where D is differential operator and u is vector of collocation solutions of order m. M is square matrix of order $4m \times 4m$. The system is solved using MATLAB.

A. Stability analysis and convergence criteria. The stability analysis is studied using Euclidean and supremum norms are given below:

$$\| L \|_2 = \sqrt{h \sum_{j=1}^{N} E^2} \text{ and } \| L \|_\infty = \max_j E$$

where E is the point-wise error such that $E = | u_j^{exacl} - (u_N)_j |$ exact and u_j^{exacl}, $(u_N)_j$ are the exact and numerical solution respectively.

III. Results and Discussion

Hereunder the stability, convergence and efficiency of the linear and nonlinear models is checked and compared with the previous techniques in the next paragraphs.

A. Linear model 1. The QHCM results from model 1 for exit solute concentration are presented in Table 2. The numerical results are compared with the analytic results given by [8] and [15] obtained using the Cubic Hermite Collocation Method (CHCM)) for Peclet number 1, 10 and 40. The solution profiles are obtained by dividing the whole domain into 30 elements. The results obtained using QHCM are good in agreement with exact ones in comparison to CHCM. The stability analysis for QHCM and CHCM is presented using $\| L \|_2$ and $\| L \|_\infty$ norms in Table 2. Clearly QHCM results are better than CHCM.

Table 2. Comparison of exit solute concentration w.r.t. exact and numerical solutions.

	Pe=1			Pe=10			Pe=40		
Time	Analytic	QHCM	CHCM	Analytic	QHCM	CHCM	Analytic	QHCM	CHCM
0	1.000E+00	1.000E+00	1.00E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00	1.000E+00
0.5	2.316E-01	2.314E-01	2.325E-01	8.879E-01	8.875E-01	8.860E-01	9.986E-01	9.984E-01	9.980E-01
1	3.784E-02	3.781E-02	3.780E-02	3.225E-01	3.220E-01	3.214E-01	4.108E-01	4.022E-01	4.044E-01
1.5	6.183E-03	6.180E-03	6.179E-03	7.612E-02	7.577E-02	7.589E-02	1.904E-02	1.901E-02	1.860E-02
2	1.010E-03	1.012E-04	1.013E-04	1.607E-02	1.603E-02	1.601E-02	3.077E-04	2.948E-04	2.931E-04
2.5	1.651E-04	1.650E-04	1.661E-04	3.284E-03	3.279E-03	3.273E-03	3.171E-06	3.025E-06	2.994E-06
3	2.697E-05	2.696E-05	2.763E-05	6.629E-04	6.621E-04	6.641E-04	2.623E-08	2.473E-08	2.218E-08
$\|L\|_\infty$	-	7.248E-04	9.561E-03	-	2.640E-03	3.140E-03	-	2.790E-01	2.949E-01
$\|L\|_2$	-	3.70E-04	8.090E-04	-	1.013E-03	2.103E-03	-	3.423E-03	8.023E-02

B. Linear model 2. The QHCM results of model 2 are compared with the analytic ones derived by [3] using Laplace transform and CHCM [7]. The relative error of the results is plotted in Figure 1. It is observed that the relative error is nearer to zero for QHCM, whereas for CHCM its magnitude is higher, indicating the superiority of present technique.

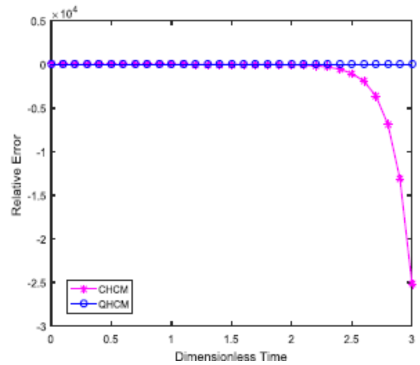
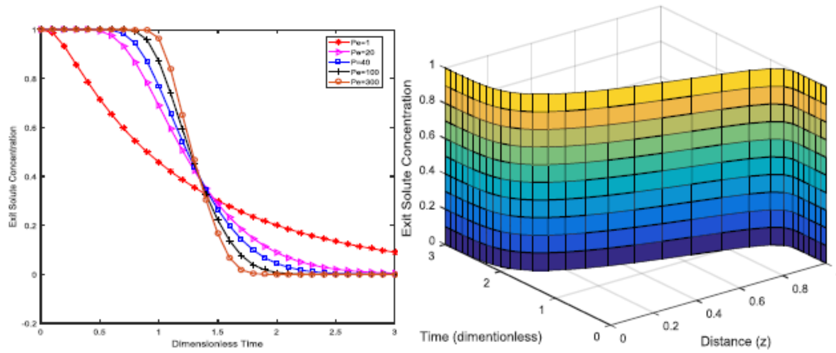


Figure 1. Comparison of Relative Error of CHCM and QHCM for Pe=40.

C. Non-linear model. The non-linear model is solved using QHCM. The model is simulated using the data of [8]. This data is related to the research experiments, which were performed for washing of wood pulp.

(1) Effect of Peclet number (Pe) on exit solute concentration: Solution profiles for the model are obtained in the form of breakthrough curves. Comparison of exit solute concentration for different Pe (number of elements = 32) is shown in Figure 2(a). It is observed that when Pe is small, more diffusion occurs and the solute instantly mixes. In this state the black liquor instantly starts coming out and more time is required to diffuse out the liquor from the bed in with the higher Pe. So, better washing can be obtained for $Pe > 30$ and real flow can be described in a better way at $Pe = 40$. This result is also supported by the study of [1, 12, 17]. The result for $Pe = 40$ in the form of surface plot given in Figure 2(b) also strengthen our result.



2(a) 2(b)

Figure 2. (a) Comparison of exit solute concentration (b) Surface plot for Pe=40.

IV. Conclusion

The numerical study helps to check the efficiency of the method for a problem with different boundary conditions. The QHCM used here provides the strong results. The solution approaches to a steady state condition when time increases. Additionally, the error analysis is calculated in terms of relative error and found to be least in comparison with previous technique i.e. CHCM. Stability of the method using QHCM is verified with both Euclidean norm and Supremum norms. The method is also applied to non-linear model of pulp washing. It is found that the exit solute concentration is greatly affected by Peclet number. The method is validated with the result of experiments. The effect of important parameter such as Peclet number on exit solute concentration in terms of breakthrough curves are also calculated. It can be concluded that, the QHCM is efficient, simple, less time consuming and gives accurate and faster results.

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