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Numerical Procedure for the Solution of Non-Linear Pulp Washing Models

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Abstract: The pulp washing is a process in which soluble and insoluble materials which are adsorbed on the fiber surface are removed with the introduction of external fluid. The state of diffusion, adsorption, dispersion, desorption occurs throughout the process of solute removal and is described by the mathematical models. In the present study, a non-linear model of pulp washing is solved using a hybrid collocation scheme with the experimental data of a paper mill. The study highlights the effect of peclet number (the ratio of advection to diffusion) for the case of perfect mixing and displacement. Besides, the effect of dispersion coefficient and interstitial velocity on exit solute concentration are also discussed. The results reveal that medium range of peclet number increases the washing efficiency.
Keywords: pulp washing, non-linear model, dispersion coefficient, peclet number

1. INTRODUCTION

Pulp washing is a procedure of removal of soluble and insoluble materials which get adsorbed on the surface of particle with the introduction of external fluid. The development of a mathematical model is a sudden need to justify the performance of diffusion, adsorption, dispersion, desorption occurs throughout in the process of solute removal. Some models used to express such phenomena are presented in the form of two-point boundary value problems (BVPs) by various authors in the literature. [7] enlightened that process of diffusion and dispersion have its application in many fields of problems in real world. [16] explained that this is a process in which the axial dispersion coefficient serves as a strong tool. The axial dispersion coefficient is a robust factor that serves the part of diffusion coefficient as well as dispersion. Though, the particle geometry, the wash liquor, fibre surface/ pores and the bulk fluid and boundary conditions which describes the exchange of solute between the surface of fiber performs a major role towards this. Besides, [7] clarified that dispersion coefficient and interstitial velocity are generally considered as important parameters in the diffusion–dispersion process associated with pulp washing. In some situations, one or both parameters are considered as constant. However, in some procedures like enhanced oil recovery (EOR) both parameters vary with space and time.

The study of [6] also highlighted on the use of diffusion-dispersion equations to describe most of the physical phenomena. [1] revealed that dispersion coefficient strongly affects the solvent concentration during the vapex experiment, a phenomenon based on recovery of heavy oil solvent. The authors also explained that dispersion is the main factor that support engineers to derive the results for the best solvent concentration in optimizing oil production using vapex experiment. The concentration gradients are reduced when the diffusion diminishes and this causes the decrease in dispersion. The authors derived remarkable results in contrast to the diffusion coefficient in heavy oil propane. [5] supported that the phenomenon of longitudinal mixing is governed by the diffusion-dispersion equation and illuminated the complete process of mathematical model of displacement washing. [21] proposed the approximation technique to derive the exact solution over the entire range of parameters for this equation. In addition, many factors such as chemical and physical properties, enzyme reactions, and flow characteristics effect the reactor performance. The authors also estimated the range of mass transfer coefficient, axial dispersion coefficient, Reynolds numbers and kinetic parameters to predict the concentrations of the outlet flow.

[2] highlighted that numerous innovative techniques and algorithms are available in the literature for these equations. Many difficulties come across in finding the analytical solutions, the mostly seen is nonlinearities. There are also many other reasons due to which the difficulties occur in finding the numerical solutions. The two main reasons based on the nature of the equation containing partial derivatives of the first and second order in space. Secondly, construction of the suitable mesh to achieve an improved approximation of the problem. However, it is not an easy job to construct an appropriate mesh and sometimes due to the selection of mesh structure the problem is not solved. [10] explained that the model is rather complex because of nonlinear in nature and therefore to derive the exact solution is not an easy task.

[4] solved the nonlinear model describing the washing behavior of pulp fibers in the one-dimensional transport phenomenon of porous media involving axial dispersion and molecular diffusion using orthogonal collocation finite element method with Lagrange polynomials as basis function. [20] proposed the technique of MATLAB "pdepe" solver to investigate the diffusion model based on longitudinal mixing with varying boundary and initial conditions that are mostly suitable for displacement washing based on particle diffusion and axial dispersion. They derived the results with better accuracy with negligible error. [18] explored the non-polynomial spline method for solution of two-point BVPs of order two with Dirichlet and Neumann boundary conditions. They also proved that the method gives better accuracy and less than half the errors than the quadratic and cubic spline methods. [16] applied cubic Hermite collocation method (CHCM) in which basis function is approximated using cubic Hermite polynomials as the trial function. These polynomials satisfy the continuity condition of solution and its first derivative at the boundary of each element. This helps in saving the computational time and effort in comparison with Lagrange basis where additional continuity condition is assumed. [18] used stimulus response method to solve the dispersed plug flow model explored by [17] which describes the displacement process of the residing solute from the pulp fibre bed. The authors explained that the breakthrough curve

is extremely affected by the pores network and discharge of of solute from walls fiber into the wash liquid.

This paper considers the nonlinear model used to describe the diffusion –dispersion process in pulp washing. The model is solved using quintic Hermite collocation method (QHCM). Owing to its accuracy and consumption of less CPU time, the technique is applied in the present study [12]. Firstly, the study considers the model for different values of dispersion coefficient and interstitial velocity. The other case is studied when both parameters are variables and peclet number takes various values from very small to vary large. The numerical results are validated with the experimental data of [9].

2. NUMERICAL SIMULATION OF NONLINEAR PULP WASHING MODEL

The washing behavior of pulp fibers in the one-dimensional transport phenomenon of porous media involves axial dispersion and molecular diffusion. [15] discovered the transport equation depicting material balance across the bed is defined as:

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

Here, u (interstitial velocity) & D_L (dispersion coefficient) are functions of x, while c & n (functions of both x & t) are the concentration of solute in liquor & fiber respectively. Here, the deposition rate of solute of order two is considered in the forward direction and first order detachment rate is assumed in the reverse direction.

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

At the point of outlet of the bed, the unacceptable conclusions can be avoided by assuming the concentration gradient to be zero so that the boundary conditions defined at entry i.e z = 0 and at the exit i.e. z = L are expressed as:

$$u(c-c_e) = D_L\frac{\partial c}{\partial z} \text{ at } z=0 \text{ and } \frac{\partial c}{\partial z}=0$$

at z=L for all $t \geq 0$

The initial condition is assumed as:

$$c(z,0) = n(z,0) = c_i$$

However, [5] also imposed the same boundary and initial conditions.

The solute concentration (n) adsorbed on fibers surface and the solute concentration (c) of the flowing liquor is associated with Langmuir adsorption isotherms described as:

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

where $A_0 = \frac{kN_i}{C_F}$ and $B_0 = \frac{k}{C_F}$

where A_0 and B_0 are Langmuir constants.

[3,4,8,14,16] used different numerical techniques to find the solution of this model.

The mathematical model is transformed into dimensionless form as:

$$\frac{1}{Pe}\frac{\partial^2 U}{\partial Z^2} = \frac{\partial U}{\partial T} + \frac{\partial U}{\partial Z} + \frac{\mu C_F A_0}{\left[1+B_0\left\{c_s + U\left(c_0 - c_s\right)\right\}\right]^2}\frac{\partial U}{\partial T}$$

with boundary conditions as:

$$\left.\begin{aligned} PeU &= \frac{\partial U}{\partial Z} && at\ \ Z=0 \\ \frac{\partial U}{\partial Z} &= 0 && at\ \ Z=1 \end{aligned}\right\} \text{ for all } t \geq 0$$

And initial condition as:

$$U(Z,0) = 1 \quad at\ T=0 \quad \text{at} \quad T=0$$

Where $U = \frac{c-c_s}{c_0-c_s}$ (dimensionless solute concentration in liquor), $N = \frac{n-c_s}{c_0-c_s}$ (dimensionless solute concentration in fiber), $T = \frac{ut}{L}$ (dimensionless time) and $Z = \frac{z}{L}$ (axial distance) . Also, $Pe = \frac{uL}{D_L}$ and $\mu = \varepsilon/(1-\varepsilon)$ is the ratio of the volume available for flow to the total volume and ε represents the porosity.

The detailed explanation of the method used in this study is available in [13].

Discretized form obtained using QHCM is given as:

$$\sum_{q=1}^{6}\frac{da_{q+3(k-1)}}{dt}H_q^k(u_r) = \left[\frac{\left[1+B_0\left\{\left(c_0-c_s\right)\sum_{q=1}^{6}a_{q+3(k-1)}H_q^k(u_r)+c_s\right\}\right]^2}{\left[\mu C_F A_0 + \left[1+B_0\left\{\left(c_0-c_s\right)\sum_{q=1}^{6}a_{q+3(k-1)}H_q^k(u_r)+c_s\right\}\right]^2\right]}\right] \times \left(\frac{1}{Peh_k^2}\sum_{q=1}^{6}a_{q+3(k-1)}H_q^{k''}(u_r) - \frac{1}{h_k}\sum_{q=1}^{6}a_{q+3(k-1)}H_q^{k'}(u_r)\right)$$

where 'r' represents interior collocation points and $2 \leq r \leq 5,\ r \in N$. Also, 'k' represents number of elements in which domain is divided and takes value between 1 & N.

Boundary condition at Z = 0, *i.e.*, u = 0

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

$$Pea_1 - a_2 = 0$$

At Z = 1, i.e., u = 1 is

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

The system of equations obtained from the above is solved with MATLAB's ode 15s and the obtained results are validated using experimental data of [9].

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3. NUMERICAL RESULTS

In this section, the numerical results for different values of parameters such as dispersion coefficient, interstitial velocity and peclet number (Pe) are discussed in detailed. The range of Pe for perfect displacement and perfect mixing is also discussed in this part.

3.1 Effect of dispersion coefficient (DL)

The model is solved using present method and numerical results are derived for exit solute concentration by taking different values of dispersion coefficient. The results are presented in figure 1. The axial dispersion coefficient makes its major effect on concentration profile. It is noticed that more time is taken by solute to leach out for large value of DL as compared to small value of DL due to porous nature of pulp. In this situation the adsorbed solute on pulp fiber is not properly detached that causes delay in washing. The more value of axial dispersion makes the Pe diminishes and due to this more back mixing take place less amount of the black liquor is removed from the solute. Also, the breakthrough curves become broadens when the axial dispersion coefficient increases. In this case, less time is taken and higher result can be achieved for recovery of black liquor. Dispersion can be made greater in case when the miscible fluids flow through the porous structure. The other reason of existence of fluid dispersion is that fluid in large pores travel more quickly than fluid in small pores with same pressure gradient. [10] illuminated that mostly small amount of DL or higher Pe is preferred to achieve the target of effectual washing.

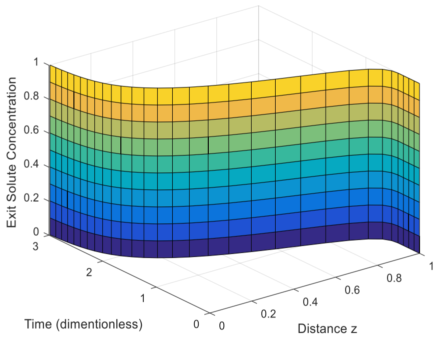

Fig.1 (a)

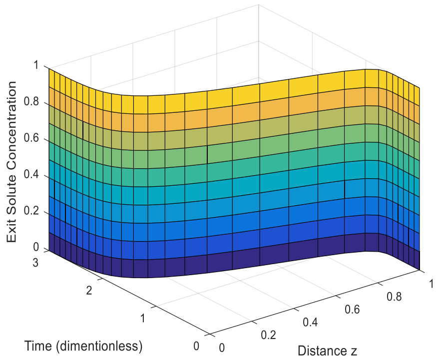

Fig.1 (b)

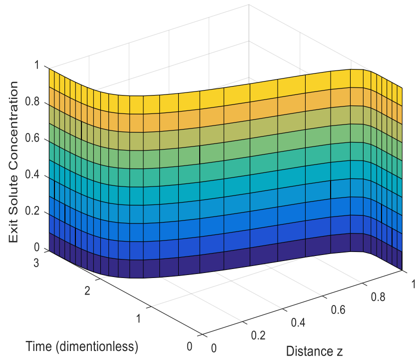

Fig.1 (c)

Figure 1 (a) Exit solute concentration for DL=2.10E-03, (b) Exit solute concentration for DL=5.20E-04 (c) Exit solute concentration for DL=2.60E-04

3.2 Influence of interstitial velocity (u)

Interstitial velocity plays an important role in washing process. The output results for different values of u are presented in figure 2. The rate of increase of interstitial velocity depends upon many factors such as the bed porosity and geometry of particle. However, black liquor can be removed in better way when flow rates is small. Whereas the high flow rates make the washing operations poor because black liquor solids take more time to leach out from pulp fibre. The concentration profiles are little affected by interstitial velocity because of the simultaneous increase in axial dispersion. But, small interstitial velocity affects the concentration. Overall, not much significant effect is noticed on exit solute concentration profiles at exit level when the interstitial velocity is very high.

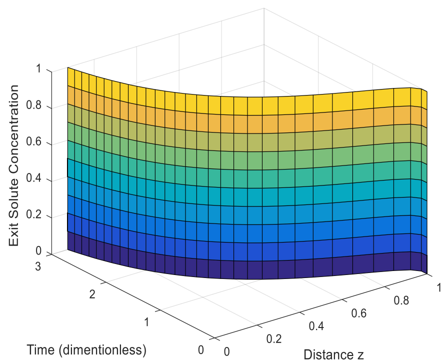

Fig. 2(a)

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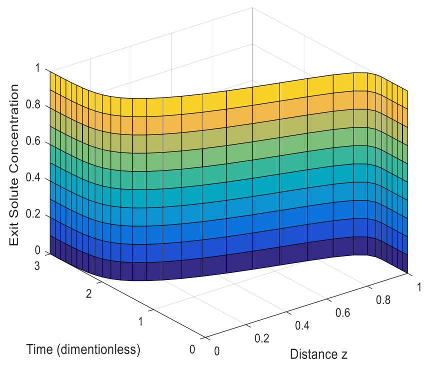

Fig. 2(b)

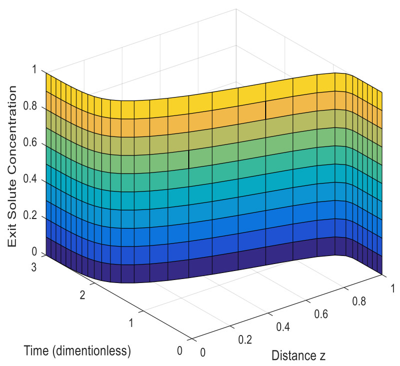

Fig. 2(c)

Figure: - 2(a) Exit solute concentration for u=2.10E-02, (b) Exit solute concentration for u=3.86E-02
(c) Exit solute concentration for u=4.83E-02

3.3 Limiting case of peclet number (Pe)

The Pe is defined as the ratio of advection to diffusion. Diffusion coefficient is dominant in the case when Pe is small and the advection is dominant when Pe is large. Advection shows that the substance is transported by a fluid in a specific direction because of bulk motion. [11] explained that Pe is the main challenging parameter in approximating the convection diffusion problems. This provides a measure to determine the ratio of advection and diffusion. The advection dominate diffusion in case of Pe>1 and diffusion dominates advection in the situation when Pe is less than 1[14].

3.3.1 Perfect mixing case:

The state of perfect mixing is represented by the model in case when Pe is going to be vanished and this is a situation when the bed performs like a perfect mixing chamber. The concentration profiles at exit level for small values of Pe is presented in figure 3. In this case, the solute takes more time to remove out of fiber interstices. When Pe is small, back mixing effect is more because axial dispersion coefficient is increased when the cake thickness and interstitial velocity are assumed as constant. In this case, more time is taken by solute to diffuse out of the pores of particle. In this case, the interstitial velocity plays more important role than diffusion coefficient. The concentration profile turns into more broaden in shape and washing time drops very rapidly. In this state, the original contents present is shoved out with the introduction of displacing fluid. In contrary, the diffusion coefficient plays a prominent role when Pe is very small because the interstitial velocity becomes small and the concentration profiles converges slowly. The solute takes large time to come out from the pores of particle in case when value of Pe is small. This is not an ideal state for industrial practice. [8] also discussed the limiting case of Pe to be zero for the situation of displacement washing.

3.3.2. Perfect displacement case:

In case when Pe is high, the dispersion is assumed to have negligible effect. The concentration profiles at exit level for large values of Pe is presented in figure 3. [8] verified that the dispersion coefficient becomes smaller with large value of Pe and more solute is diffused out from the pores of particle and the time for washing is reduced sharply in this case. the on exit solute concentration. The situation of perfect displacement is that in which the PDE is reduced to be of order one. In such a situation, the time for washing falls quickly and the solution profile grow into broaden. But this situation is not realistic because the diffusion coefficient cannot be zero and the interstitial velocity cannot be infinite. Ideally, all the solvable impurities are not easily removed from the pulp fiber bed. It is observed that mass transfer zone is steeper when value of Pe is high. This causes increase in the dispersion coefficient when the cake thickness and interstitial velocity are kept constant.

Practically, both the situations are not ideally applicable for industrial practice. For proficient washing operations, the value of Pe is considered to lie between the medium range [11]. This flow rate is intermediary range between the cases of perfect mixing (Pe=0) and perfect displacement (Pe= ∞). [4,5] also supported the medium range of Pe to be lie between 20 to 40.

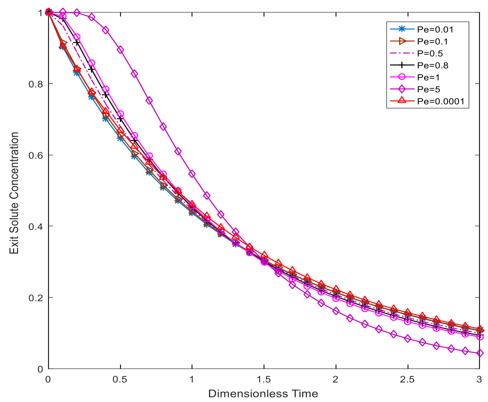

Fig.3(a)

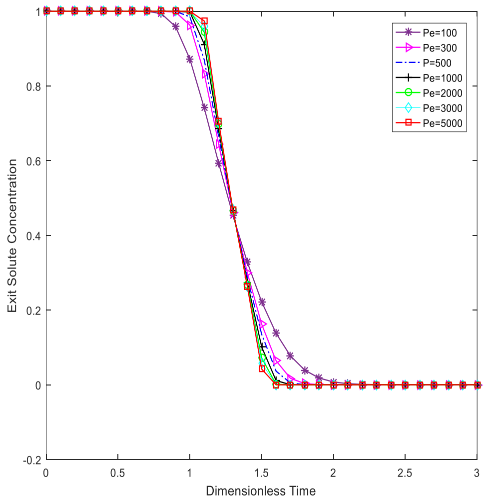

Fig.3(b)

Figure: - 3(a) Influence of small value of Pe on concentration profile

3(b) Influence of small value of Pe on concentration profile

4. CONCLUSION

It is observed that the concentration profiles for both the cases of variable and fixed dispersion coefficient are of fairly different shapes. The interstitial velocity perform a major role as compared to dispersion coefficient in the washing process. Further, the diffusion coefficient plays a leading role in the case when the interstitial velocity is very small. The value of Pe becomes small in this case and the concentration profiles slowly converge. Besides, the effect of axial dispersion in the bed is neglected when the Pe moves towards zero. When the value of Pe is larger, the case is called perfect displacement. However, a sharp decrease in time for washing is noticed when Pe increases. Also in real world situation, all the solvable impurities cannot be removed from the pulp fiber bed and industries have to consider an optimum range of Pe to retain a balance between the time of washing and removal of impurities. Thus, it can be concluded that an ideal range of Pe makes the industries to maintain a balance between the time of washing and the removal of impurities.

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