Research Article

Application of Mathematica Software to Solve Pulp Washing Model

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The removal of the bulk liquor surrounding the pulp fibers using less concentrated liquor is known as pulp washing. In the present study, a pulp washing model involving diffusion-dispersion through packed beds of finite length is presented. Separation of variables is applied to solve system of governing partial differential equations and the resulting equations are solved using Mathematica. Results from the present case are compared with those of previous investigators. The present case is giving better results than the previous investigators.

1. Introduction

The objective of pulp and paper industry to produce its target production with high efficiency and less environmental load can only be met by initiating a meticulously planned research on mathematical methods. Pulp washing plays an important role in reduction of black liquor solids in the pulp being carried forward for further processing. The efficiency of washing depends on the degree of mixing, rate of desorption, diffusion-dispersion of dissolved solids, and chemicals from the fibrous matrix. Modeling of pulp washing is done mainly using three approaches, namely, (a) process modeling (b) physical modeling, and (c) statistical modeling.

A complete review of the various process models used to describe pulp washing has been presented by [1]. Initially researchers like in [2, 3] proposed the models based on axial dispersion. Pellett [4] introduced a mathematical model combining the effects of particle diffusion and axial dispersion. A detailed model related to mass transfer in fibrous particle was given by [5]; it was also restricted for axial dispersion only. Comprehensive models involving physical features of the fibers such as fiber porosity and fiber radius were presented by [6, 7].

Extensive study of axial dispersion model has been carried out by [8–26]. The model has been solved using analytic and numerical techniques like Laplace transform

technique [2–4, 10, 15, 23, 26], finite difference technique [25], orthogonal collocation method [5, 7, 12], orthogonal collocation on finite elements [6, 20, 21], Galerkin/Petrov Galerkin method [8, 19], Hermite collocation method by [11, 17, 24] and Spline collocation method [13].

The accuracy of the analytic solution undoubtedly exceeds the limit of applicability of the theory to real situations. Moreover, it is highly desirable to have a simple and consistent model of the transport phenomenon based on essential features of real situation. Keeping this modest goal in mind axial dispersion model is solved along with linear adsorption isotherm. The method of separation of variables is first applied on partial differential equation and then Laplace transform is taken of the equations. Finally the mathematical expressions are solved using Mathematica software to obtain solute concentration at any location and time.

2. Model Based on Axial Dispersion

The displacement washing model based on the axial dispersion and particle diffusion describing the washing zone is given by

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial z} + \mu \frac{\partial n}{\partial t} = D_L \frac{\partial^2 c}{\partial z^2} \quad (1)$$

with adsorption isotherm

$$n = kc. \quad (2)$$

This equation represents the basis for the mathematical models of displacement washing, where t is the time from the commencement of the displacement, z is the distance from the point of introduction of the displacing fluid, $c = c(z, t)$ is the solute concentration, D_L is longitudinal dispersion coefficient, u is the average interstitial velocity of the fluid, and L is thickness of the packed bed.

On account of unusual nature of displacement process, appropriate boundary conditions have been extensively discussed in the literature [2, 6, 27, 28]. Accordingly, the boundary conditions at the inlet and outlet of the bed are

$$\begin{aligned} c &= c_s \quad \text{at } z = 0, \\ \frac{\partial c}{\partial z} &= 0 \quad \text{at } z = L \end{aligned} \quad (3)$$

and initial condition is given by

$$c(z, 0) = n(z, 0) = c_i \quad \text{for } 0 < z < \frac{L}{u}. \quad (4)$$

Conversion of Model into Dimensionless Form. Equations (1) to (4) can be put in dimensionless form using dimensionless variables:

$$\begin{aligned} C &= \frac{c - c_s}{c_i - c_s}; \quad N = \frac{n - c_s}{c_i - c_s}; \\ Z &= \frac{z}{L}; \quad T = \frac{ut}{(1 + \mu k)L}. \end{aligned} \quad (5)$$

The dimensionless time, T , corresponds physically to the number of pore displacements introduced into the medium since the start of the experiment.

By these means, (1) reduces to

$$\frac{\partial C}{\partial T} + \frac{\partial C}{\partial Z} = \frac{1}{\text{Pe}} \frac{\partial^2 C}{\partial Z^2}, \quad (6)$$

where $\text{Pe} = uL/D_L$ is the Peclet number. The boundary conditions are now of the form

$$C(0, T) = 0 \quad \text{at } Z = 0 \quad \text{for } T > 0, \quad (7)$$

$$\frac{\partial C}{\partial Z}(1, T) = 0 \quad \text{at } Z = 1 \quad \text{for } T > 0 \quad (8)$$

while the initial condition is

$$C = 1 \quad \text{at } T = 0 \quad \text{for } 0 < Z \leq 1. \quad (9)$$

Now, our main aim is to estimate $C = C(Z, T)$ satisfying (7)–(9), which will eventually lead to exit solute concentration $C_e = C_e(T) = C(1, T)$.

3. Solution of Model

Method of separation of variables is applied to solve (6). This method transforms the PDE into a system of ODEs, each of which depends only on one of the functions and the solution is given as product of the functions.

Equation (6) can be separated in terms of variables Z and T by assuming that $C(Z, T) = X(Z)Y(T)$ and then substituting $\partial C/\partial Z = X'Y$ and $\partial C/\partial T = XY'$ in it, as follows:

$$\frac{X'' - \text{Pe } X'}{X} = \frac{\text{Pe } Y'}{Y} = -p^2 \text{ (constant)}. \quad (10)$$

Individual solutions of expression (10) are given by

$$X(Z) = \exp\left(\frac{\text{Pe } Z}{2}\right) [c_1 \cos(\alpha Z) + c_2 \sin(\alpha Z)], \quad (11)$$

$$Y(T) = c_3 \exp\left(-\frac{p^2 T}{\text{Pe}}\right). \quad (12)$$

Application of boundary condition $X = 0$ at $Z = 0$ in (11) gives $c_1 = 0$ and the boundary condition $\partial X/\partial Z = 0$ at $Z = 1$ gives $\text{Pe} \tan \alpha + 2\alpha = 0$.

Therefore the solution $C(Z, T) = X(Z)Y(T)$ is given by

$$C(Z, T) = A \exp\left(\frac{\text{Pe } Z}{2}\right) \sin(\alpha Z) \exp\left(-\frac{p^2 T}{\text{Pe}}\right). \quad (13)$$

Equation $\text{Pe} \tan \alpha + 2\alpha = 0$ is a transcendental equation; it will have infinite many root; therefore the solution (13) will depend on n ; that is,

$$\begin{aligned} C(Z, T) &\sim C_n(Z, T) = X_n(Z) Y_n(T) \\ &= A_n \exp\left(\frac{\text{Pe } Z}{2}\right) \sin(\alpha_n Z) \\ &\quad \times \exp\left(-\frac{p_n^2 T}{\text{Pe}}\right). \end{aligned} \quad (14)$$

Using the principle of superposition, we get

$$\begin{aligned} C(Z, T) &= \sum_{n=1}^{\infty} C_n(Z, T) \\ &= \sum_{n=1}^{\infty} A_n \exp\left(\frac{\text{Pe } Z}{2}\right) \sin(\alpha_n Z) \exp\left(-\frac{p_n^2 T}{\text{Pe}}\right). \end{aligned} \quad (15)$$

Applying the initial condition $C(Z, 0) = 1$, we find that

$$\sum_{n=1}^{\infty} A_n \sin(\alpha_n Z) = \exp\left(-\frac{\text{Pe } Z}{2}\right); \quad (16)$$

therefore A_n represents the Sturm-Liouville problem for $\exp(-\text{Pe } Z/2)$ and is given by

$$A_n = \frac{\int_0^1 e^{-\text{Pe } Z/2} \sin(\alpha_n Z) dZ}{\int_0^1 \sin^2(\alpha_n Z) dZ}. \quad (17)$$

Finally, the solute concentration at any location and time in the bed can be written as

$$C(Z, T) = \frac{\sum_{n=1}^{\infty} \int_0^1 e^{-Pe Z/2} \sin(\alpha_n Z) dZ}{\int_0^1 \sin^2(\alpha_n Z) dZ} \times \exp\left(\frac{Pe Z}{2} - \frac{p_n^2 T}{Pe}\right) \sin(\alpha_n Z), \quad (18)$$

where α_n ($n = 1, 2, 3, \dots$) are the positive roots, taken in order of increasing magnitude, of the transcendental equation $Pe \tan \alpha_n + 2\alpha_n = 0$ and $p_n = \sqrt{(4\alpha_n^2 + Pe^2)/4}$.

It is important to mention that (6) is also solved analytically by Grahs [5] and Kukreja [14]. Their solutions are given below.

Applying separation of variables, Grahs [5] found the concentration of solute as

$$C(Z, T) = \exp\left\{\frac{Pe}{2}\left(Z - \frac{T}{2}\right)\right\} \times \left[\sum_{n=1}^{\infty} \frac{4\alpha_n^2 \sin(\alpha_n Z) \exp(-\alpha_n^2 T/Pe)}{\{2\alpha_n - \sin(2\alpha_n)\}((Pe/4) + \alpha_n^2)} \right], \quad (19)$$

where α_n are the positive roots of $Pe \tan \alpha_n + 4\alpha_n = 0$.

Using Laplace transform, Kukreja [14] found the concentration of solute as

$$\frac{c - c_s}{c_i - c_s} = \sum_{n=1}^{\infty} 4\alpha_n^2 \exp\left(p_n T + \frac{Pe Z}{2}\right) \times \sum_{n=1}^{\infty} \frac{[Pe \sin\{(Z-1)\alpha_n\} - 2\alpha_n \cos\{(Z-1)\alpha_n\}]}{Pe p_n (Pe^2 + 4\alpha_n^2 + 2Pe) \sin(\alpha_n)}, \quad (20)$$

where $Pe \tan \alpha_n + 2\alpha_n = 0$ and $p_n = -(4\alpha_n^2 + Pe^2)/4Pe$.

The solutions given by (18)–(20) are complex and time consuming. These equations are evaluated using Mathematica software. This technique is novel and elegant and can be conveniently handled by any nonmathematician also.

4. Results and Discussion

Solution of (18)–(20) are obtained using Mathematica by taking 22 mesh points within the dimensionless time and also in dimensionless distance x . For $Pe = 1$, the surface plots of the dimensionless concentration with respect to dimensionless distance ($0 \leq x \leq 1$) and dimensionless time ($0 \leq T \leq 1.2$) are shown in Figures 1, 2, and 3, respectively, for the present case (18), Grahs (19), and Kukreja (20). It can be observed from Figure 1 that the surface plot of (18) is very smooth at $T = 0$, whereas for (19) and (20) fluctuation is observed.

In Figures 4 to 6, exit solute concentration obtained from (18)–(20) is plotted, respectively. In Figure 5, the solution profile of (19) is starting from 1.3 approximately, which is highly impossible in pulp washing system, as the dimensionless concentration can never exceed 1. Smoothest profile can be seen in case of Figure 4.

FIGURE 1: Surface plot for the present case represented by (18).

FIGURE 2: Surface plot for Grahs [5] represented by (19).

FIGURE 3: Surface plot for Kukreja [15] represented by (20).

FIGURE 4: Exit solute concentration profile for present case.

FIGURE 6: Exit solute concentration profile by Kukreja [14].

FIGURE 5: Exit solute concentration profile by Grahs [5].

FIGURE 7: Absolute error between present case and Grahs [5].

In Figures 7 and 8, the absolute error obtained from (19) and (20) from (18) is plotted. The magnitude of error in case of (19) is 4 to 5 times higher than (20). This indicates more deviation between the present case and Grahs [5] as compared to Kukreja [14].

The results from the three investigators are summarized in Table 1. At $T = 0$ the error with Kukreja [14] is 2.92%, whereas with Grahs [5] it is 29.13%; ideally, these should have been 0.0%. Similarly, at $T = 0.1$, the error is found to be 6.25% while comparing the results with Kukreja [14] and for Grahs [5] it is 12.23%, which is again very high. It can further be seen in Table 1 that at $T = 0.5$ onwards the error is 0.0% with Kukreja [14] whereas with Grahs [5] it is reducing but persists continuously. Hence, this comparison shows that results of Kukreja [14] are matching with present case but those of Grahs [5] are showing significant error.

5. Conclusion

The investigation, based on diffusion model of longitudinal mixing in beds of finite length, is applicable to displacement washing with axial dispersion and particle diffusion. The present solution of the model as well as the solution proposed by Grahs [5] and Kukreja [14] involves complicated expressions. The application of Mathematica makes it convenient

TABLE 1: Comparison of solution of Grahs [5] and Kukreja [14] with the present case.

Time	Present case	Grahs [5]	Kukreja [14]	% error with [5]	% error with [14]
0.00	1.0000	1.2913	0.9708	29.13	2.92
0.10	0.9864	0.1087	0.9239	12.23	6.25
0.20	0.6866	0.8477	0.6805	16.11	0.61
0.30	0.4779	0.6203	0.4773	14.24	0.06
0.40	0.3326	0.4512	0.3326	11.86	0.00
0.50	0.2315	0.3279	0.2315	09.64	0.00
0.60	0.1611	0.2382	0.1611	07.71	0.00
0.70	0.1122	0.1731	0.1122	06.09	0.00
0.80	0.0781	0.1258	0.0781	04.77	0.00
0.90	0.0543	0.0914	0.0543	03.71	0.00
1.00	0.0378	0.0664	0.0378	02.86	0.00
1.10	0.0263	0.0482	0.0263	02.19	0.00
1.20	0.0183	0.0350	0.0183	01.67	0.00

to evaluate these expressions. The present results are more accurate than the output provided by Grahs [5] and Kukreja [14]. The algorithms based on Mathematica are novel and easy to set up. Therefore, the present technique provides a good

FIGURE 8: Absolute error between the present case and Kukreja [14].

alternate to the available techniques for dealing with such type of problems.

Nomenclature

- c : Concentration of the solute in the liquor, kg/m^3
 c_i : Initial solute concentration, kg/m^3
 c_s : Solute concentration of incoming fluid, kg/m^3
 c_e : Exit solute concentration from the bed, kg/m^3
 D_L : Longitudinal dispersion coefficient, m^2/s
 L : Cake thickness, m
 n : Concentration of the solute in the fiber, kg/m^3
 t : Time, s
 u : Liquor speed in cake pores, m/s
 z : Distance from point of introduction of solvent, m
 ε : Porosity of packed bed
 μ : Ratio of porosity, $(1 - \varepsilon)/\varepsilon$.

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