

MODELLING OF DISPLACEMENT WASHING OF PULP FIBERS USING THE HERMITE COLLOCATION METHOD

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Abstract - A non-linear mathematical model for displacement washing of pulp fibers with suitable boundary conditions is presented. Model equations are divided into two phases: particle phase and external fluid phase. The Hermite collocation method (HCM) is employed to solve the non-linear model equations. The validity and efficiency of the proposed model is demonstrated by comparing the numerical results with the experimental ones. Stability of the proposed method is checked by evaluating L_2 and L_∞ norms at different time intervals. Industrial parameters such as displacement ratio and wash yield have been calculated to check the validity of the model. Numerical values obtained from the model equations are presented in terms of 2D graphs.

Keywords: Cubic Hermite polynomials; Peclet number; Biot number; Wash yield; Displacement ratio; Bed porosity.

INTRODUCTION

Applications of mathematical techniques for the solution of mass transfer problems in the field of chemical and process industries has always been the centre of study for mathematicians, as well as for chemical engineers. The diffusion dispersion problems arising from packed bed reactors have always motivated the scientists for the development of new models (Pellet, 1966; Grähs, 1974; Neretnieks, 1974, 1976; Perron & Lebeau, 1977; Al-Jabari *et al.*, 1994; Kukreja *et al.*, 1995; Eriksson *et al.*, 1996; Potůček, 1997; Potůček & Pulcer, 2004; Arora *et al.*, 2006, 2008). It has given rise to the use of a variety of analytical and numerical techniques for the solution of these models such as Laplace transforms (Brenner, 1962; Pellett, 1966; Rasmuson & Neretnieks, 1980; Liao & Shiau, 2000; Aminikhah, 2012), orthogonal collocation method (Villadsen & Stewart, 1967; Michelsen &

Villadsen, 1971; Raghvan & Ruthven, 1983; Adomaitis & Lin, 2000; Solsvik & Jakobsen, 2012), orthogonal collocation on finite elements (Carey & Finlayson, 1975; Ma & Guiochon, 1991; Arora *et al.*, 2005, 2006, 2008), Galerkin method (Liu & Bhatia, 2001; Onah, 2002; Bhrawy & El-Soubhy, 2010; Nadukandi *et al.*, 2010; Shen *et al.*, 2011; Zhu *et al.*, 2011; Solsvik & Jakobsen, 2012), Tau method (El-Daou & Al-Matar, 2010; Vanani & Aminataei, 2011; Solsvik & Jakobsen, 2012), Least Square method (Sporleder *et al.*, 2010; Toledo *et al.*, 2011; Wu, 2012; Solsvik & Jakobsen, 2012), spline collocation (Kadalbajoo *et al.*, 2008; Khuri & Sayfy, 2009; Pedas & Tamme, 2011; Rashidinia & Ghasemi, 2011; Dhawan *et al.*, 2012). In diffusion rate processes, usually the diffusion within particles pores and diffusion in the fluid phase between particles is considered. Diffusion dispersion problems in spherical catalyst particles have been studied widely as

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compared to particles having cylindrical geometry, e.g., fibers. Due to the highly porous nature and complex particle geometry of pulp fibers and rigidity in the computational approach, the majority of investigators have preferred the study of glass beads and granular particles instead of pulp fibers. The rate of removal of the soluble impurities from the pores of the particles is slower than that from the interstices of the particles, due to the relatively small pore size. Therefore, diffusion through the pores of particles is expected to control the overall washing rate (Pellett, 1966; Han, 1967).

The objective of the present study was to develop a mathematical model for the analysis of washing of the porous structure of particles, especially fibers. The prime motive of washing is to remove the soluble impurities adsorbed on the particle surface using external aid. For porous particles the solute must diffuse out before it is dispersed by the flowing liquid. The solute from the irregular void channels of the bed is displaced and coupled with diffusion-like dispersion of washing liquid in the direction of flow. Due to the adsorption of solute on the fiber surface, mass transfer occurs through the particle pores to particle surface and from particle surface to external fluid.

Dilution/extraction and displacement washing are basically two types of pulp-washing operations. In the former case the pulp slurry is diluted and thoroughly mixed with wash liquor and then filtered for thickening. In the latter case the liquor in the pulp bed is displaced with wash liquor. However, if the same amount of wash liquor is used, displacement washing is better than dilution/extraction (Potůček, 1997).

MODEL DEVELOPMENT

Fluid concentration in packed beds of porous particles is mainly based on two types of mechanisms. One is related to the transfer rate between fluid and particles and is given explicitly by the differential

$$\text{equation } \frac{\partial q}{\partial t} = f(n, q).$$

This type of mechanism has been discussed widely for both linear and non-linear isotherms (Brenner, 1962; Sherman, 1964; Grähs, 1974; Potůček, 1997; Potůček & Pulcer, 2004; Arora & Potůček, 2012). In the second type of rate mechanism, the function $f(n, q)$ is replaced by an integral equation signifying the solid phase diffusion into the interior of the particles. In this paper, second type of rate mechanism

has been followed for a Langmuir adsorption isotherm to study the displacement washing of fluid flow through the packed bed of particles.

The packed bed, in the present study, is divided into two zones, namely a zone of flowing liquor and the zone of porous material. The packed bed is composed of unbleached Kraft pulp fibers having cylindrical geometry. The schematic representation of pulp fibers is given in Figure 1.

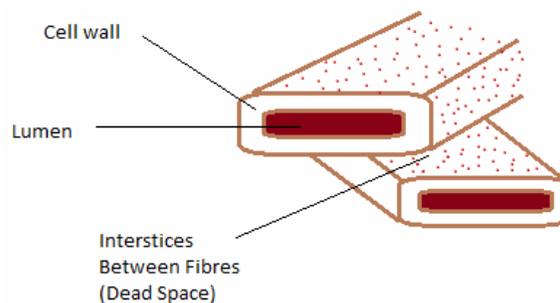


Figure 1: Schematic representation of fibers.

Flow of fluid through the bed is represented by the external fluid concentration $c(x, t)$. Intraparticle and interparticle solute concentrations are represented by $n(r, x, t)$ and $q(r, x, t)$, respectively. Particle and bed porosities are described by β and ε , respectively. Movement of solute within particle pores is defined by Fick's law. The representation of different zones of the packed bed is given in Figure 2.

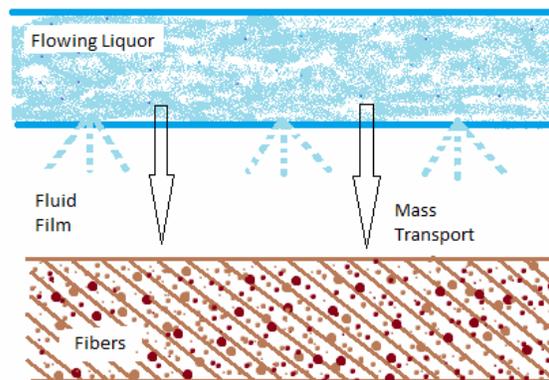


Figure 2: Schematic representation of different zones.

Properties of the Mathematical Model

The proposed model is based on certain features which are discussed below:

- The system is isothermal and the bed is macroscopically uniform.
- The particles (fibers) are porous and of uniform cylindrical size.

c) Pore radius and particle length are very small as compared to the axial distance.

d) The dispersion in the fluid is described by an axial dispersion coefficient and diffusion in particles is described by an intraparticle diffusion coefficient and both are independent of axial distance, pore radius and solute concentration.

e) The adsorption equilibrium between interparticle and intraparticle solute concentrations is assumed to be Langmuir.

f) The average solute concentration is defined over the bed cross section.

Model for the Particle Phase

The diffusion equation describing the movement of solute within particle pores as defined by Pellett (1966), is given by:

$$D_F \left(\frac{\partial^2 w}{\partial r^2} + \frac{1}{r} \frac{\partial w}{\partial r} \right) = \frac{\partial w}{\partial t} \quad (1)$$

where w is the local intraparticle solute concentration and does not distinguish between the solute adsorbed on the particle surface and the solute within the particle pores. To distinguish between these two, the surface diffusion effects are assumed to be negligible. The transport of solute within the particles is effectively described by a diffusion equation involving both the concentration of solute adsorbed on the particle surface and the intrapore solute concentration. The driving force for diffusion is assumed to be the intrapore concentration gradient and therefore the intraparticle diffusion equation takes the following form:

$$D_F \left(\frac{\partial^2 q}{\partial r^2} + \frac{1}{r} \frac{\partial q}{\partial r} \right) = \frac{\partial q}{\partial t} + \frac{(1-\beta)}{\beta} \frac{\partial n}{\partial t} \quad (2)$$

The local solute concentration applies to particles at any radial distance ' r ', which gives $w = \beta q + (1-\beta)n$, and local equilibrium is assumed to prevail in the individual intraparticle pores.

Adsorption Isotherms

Immense literature is available for a linear adsorption isotherm (Sherman, 1964; Pellett, 1966; Neretnieks, 1974; Perron & Lebeau, 1977; Rasmuson & Neretnieks, 1980; Kukreja *et al.*, 1995; Potůček, 1997; Potůček & Pulcer, 2004). This is due to the fact that a linear adsorption isotherm linearises the

differential equation describing the behavior of fluid flow and condenses the mathematical complexities. Crotagino *et al.* (1987), Trinh *et al.* (1989), Al-Jabari *et al.* (1994) are among the prominent names to follow the study of the Langmuir adsorption isotherm. However, these authors discussed the bulk fluid phase only. In the present study, the intrapore solute concentration and the concentration of solute adsorbed on the particle surface are related by a Langmuir adsorption isotherm in the particle phase. The mass balance equation for the adsorption isotherm is:

$$\frac{\partial n}{\partial t} = k_1 \frac{q}{C_F} (N_0 - n) - k_2 n \quad (3)$$

Model for the Bulk Fluid

The transport phenomenon in the porous media with a bed porosity ε is described by a one-dimensional axial dispersion model involving an axial dispersion coefficient (Rasmuson & Neretnieks, 1980). The mass balance equation for the bulk fluid is:

$$D_L \varepsilon \frac{\partial^2 c}{\partial x^2} = u \varepsilon \frac{\partial c}{\partial x} + \varepsilon \frac{\partial c}{\partial t} + (1-\varepsilon) \frac{\partial q}{\partial t} \quad (4)$$

where \bar{q} is defined as the volume average concentration in the particles. To correlate the intrapore solute concentration and the bulk fluid concentration, it is necessary to define a relation between these two in terms of axial distance.

$$\bar{q} = \frac{2}{R^2} \int_0^R q(r, x, t) r dr \quad (5)$$

Rasmuson & Neretnieks (1980) and Raghvan & Ruthven (1983) have related the particle phase and bulk fluid phase by defining the condition at the particle boundary. Therefore, Eq. (5) reduces to the following form:

$$\frac{\partial \bar{q}}{\partial t} = \frac{2k_f \beta}{KR} (c - q|_{r=R}) \quad (6)$$

Using Eq. (6) in Eq. (4), the latter takes the form:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} - 2 \left(\frac{1-\varepsilon}{\varepsilon} \right) \frac{k_f \beta}{KR} (c - q|_{r=R}) \quad (7)$$

Initial and Boundary Conditions

The concentration gradient is assumed to be zero at the centre of the particle, *i.e.*,

$$\frac{\partial q}{\partial r} = 0, \quad \text{at } r = 0 \text{ and } t > 0 \quad (8)$$

It is assumed that external mass transfer resistance exists at $r = R$ and mass transfer to the particle surface is controlled by the film resistance mass transfer coefficient.

$$-D_F \left(\frac{\partial q}{\partial r} \right) = \frac{k_f \beta}{K} (q|_{r=R} - c) \quad \text{at } r = R \text{ and } t > 0 \quad (9)$$

It signifies the relation between Eq. (6) and Eq. (9).

At the inlet and creek of the bed, Danckwart's boundary conditions were applied.

$$uc - D_L \frac{\partial c}{\partial x} = 0 \quad \text{at } x = 0 \quad (10)$$

$$\frac{\partial c}{\partial x} = 0 \quad \text{at } x = L \text{ and } t > 0 \quad (11)$$

$$\text{Initially, } c = q = C_0 \text{ and } n = N_0 \quad (12)$$

Rearranging and introducing dimensionless variables given in the nomenclature, the mathematical Equations (2), (3) and Equations (7) to (12) can be converted into the following form:

$$\frac{\partial^2 Q}{\partial \eta^2} + \frac{1}{\eta} \frac{\partial Q}{\partial \eta} = \frac{\partial Q}{\partial \tau} + \mu N_1 \frac{\partial N}{\partial \tau} \quad (13)$$

$$\frac{\partial N}{\partial \tau} = P_1 (C_1 Q (1 - N) - k^* N) \quad (14)$$

$$\frac{\partial C}{\partial \tau} = \frac{\psi Bi}{Pe} \frac{\partial^2 C}{\partial \xi^2} - \psi Bi \frac{\partial C}{\partial \xi} - \theta Bi (C - Q|_{\eta=1}) \quad (15)$$

$$\frac{\partial Q}{\partial \eta} = 0, \quad \text{at } \eta = 0 \text{ and } \tau > 0 \quad (16)$$

$$\frac{\partial Q}{\partial \eta} = Bi (C - Q|_{\eta=1}), \quad \text{at } \eta = 1 \text{ and } \tau > 0 \quad (17)$$

$$C - \frac{1}{Pe} \frac{\partial C}{\partial \xi} = 0, \quad \text{at } \xi = 0 \text{ and } \tau > 0 \quad (18)$$

$$\frac{\partial C}{\partial \xi} = 0, \quad \text{at } \xi = 1 \text{ and } \tau > 0 \quad (19)$$

$$\text{Initially, } C = Q = N = 1, \quad (20)$$

for all $\xi(0,1)$ and $h(0,1)$

HERMITE COLLOCATION METHOD

Orthogonal collocation is one of the weighted residual methods used to solve the system of boundary value problems. In this technique the residual is set equal to zero at collocation points. For a stiff system of equations, the method of orthogonal collocation does not give good results for small values of the parameters. To overcome this problem, Carey & Finlayson (1975) proposed the conjunction of finite elements with the orthogonal collocation method, termed as orthogonal collocation on finite elements (OCFE). In this technique, the trial function is approximated by using Lagrangian interpolating polynomials as base functions. With Lagrangian interpolating polynomials as base functions, an additional condition of continuity has to be imposed to make the approximating function continuous at the node points. To overcome this problem, the Hermite collocation method (HCM) was proposed, which is the combination of Hermite interpolating polynomials and the orthogonal collocation technique. In the Hermite collocation method cubic Hermite interpolating polynomials are used as base functions to approximate the trial function (Dyksen & Lynch, 2000; Lang & Sloan, 2002; Jung, 2003; Liu *et al.*, 2005; Ma *et al.*, 2006; Finden, 2007; Mazroui *et al.*, 2007; Han, 2009; Ricciardi & Brill, 2009; Gülsu *et al.*, 2011; Yalçınbaş *et al.*, 2011; Orsini *et al.*, 2011). To apply the collocation technique, the residual is set equal to zero at the collocation points. In Hermite interpolating polynomials, the additional condition of continuity at node points is not required due to the structure of Hermite interpolating polynomials, as the Hermite interpolating polynomials possess C^1 continuity. Therefore, the Hermite collocation method has the property to transform the mixed collocation method into an interior collocation method, which reduces the number of collocation equations.

The proposed model was solved using HCM by applying Hermite collocation on the radial and axial domain. In the proposed model, cubic Hermite polynomials were employed to discretize the approximating function. The cubic Hermite basis is defined (Dyksen & Lynch, 2000) as:

$$P_j(\xi) = \begin{cases} 3 \left(\frac{\xi_{j+1} - \xi}{\xi_{j+1} - \xi_j} \right)^2 - 2 \left(\frac{\xi_{j+1} - \xi}{\xi_{j+1} - \xi_j} \right)^3 & \xi_j \leq \xi \leq \xi_{j+1} \\ 3 \left(\frac{\xi - \xi_{j-1}}{\xi_j - \xi_{j-1}} \right)^2 - 2 \left(\frac{\xi - \xi_{j-1}}{\xi_j - \xi_{j-1}} \right)^3 & \xi_{j-1} \leq \xi \leq \xi_j \\ 0 & \text{elsewhere} \end{cases} \quad (21)$$

$$\bar{P}_j(\xi) = \begin{cases} \frac{(\xi_{j+1} - \xi)^2}{\xi_{j+1} - \xi_j} - \frac{(\xi_{j+1} - \xi)^3}{(\xi_{j+1} - \xi_j)^2} & \xi_j \leq \xi \leq \xi_{j+1} \\ \frac{(\xi - \xi_{j-1})^2}{\xi_j - \xi_{j-1}} + \frac{(\xi - \xi_{j-1})^3}{(\xi_j - \xi_{j-1})^2} & \xi_{j-1} \leq \xi \leq \xi_j \\ 0 & \text{elsewhere} \end{cases} \quad (22)$$

The piecewise cubic Hermite basis functions are designed such that:

$$P_j(\xi_i) = \delta_{ji}, P_j'(\xi_i) = 0, \bar{P}_j(\xi_i) = 0, \bar{P}_j'(\xi_i) = \delta_{ji}.$$

Orthogonal collocation is applied within each sub-domain in the radial and axial direction by introducing new variables η^* and ζ , respectively, in such a way that $\zeta = \frac{\xi - \xi_\gamma}{h_\gamma}$, where $h_\gamma = \xi_{\gamma+1} - \xi_\gamma$ such that $\zeta = 0$ when $\xi = \xi_\gamma$ and $\zeta = 1$ when $\xi = \xi_{\gamma+1}$, and $\eta^* = \frac{\eta - \eta_\ell}{h_\ell}$, where $h_\ell = \eta_{\ell+1} - \eta_\ell$ such that $\eta^* = 0$ when $\eta = \eta_\ell$ and $\eta^* = 1$ when $\eta = \eta_{\ell+1}$.

After rearranging the terms, $P_j(\xi)$ and $\bar{P}_j(\xi)$ take the following form (Finlayson, 1980):

$$\begin{aligned} H_1(\zeta) &= 1 - 3\zeta^2 + 2\zeta^3 \\ H_2(\zeta) &= h_\gamma \zeta (\zeta - 1)^2 \\ H_3(\zeta) &= \zeta^2 (3 - 2\zeta) \\ H_4(\zeta) &= h_\gamma \zeta^2 (\zeta - 1) \end{aligned} \quad (23)$$

Therefore, the approximating function for $C^\gamma(\zeta, \tau)$ can be defined as $C^\gamma(\zeta, \tau) = \sum_{i=1}^4 c_i^\gamma(\tau) H_i(\zeta)$, where the c_i^γ 's are continuous functions of τ . Similarly, the

approximating functions for $Q^{(\ell, \gamma)}(\eta, \zeta, \tau)$ and $N^{(\ell, \gamma)}(\eta, \zeta, \tau)$ can be defined in both the radial and axial directions. The structure of the $(\gamma - 1)^{th}$, γ^{th} and $(\gamma + 1)^{th}$ elements in the axial domain for Hermite collocation is defined in Figure 3.

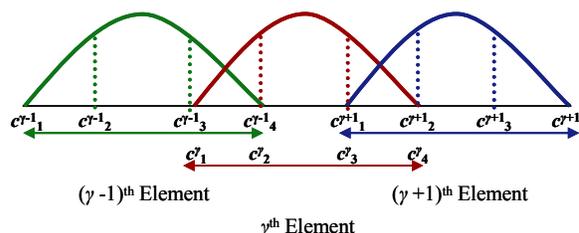


Figure 3: Structure of the $(\gamma - 1)^{th}$, γ^{th} and $(\gamma + 1)^{th}$ elements in Hermite collocation.

COLLOCATION POINTS

Choice of the collocation points is the basis of the collocation technique. These are chosen in such a way to keep the error minimum. Therefore, the interior collocation points in both the axial and radial direction are taken to be the roots of the shifted Legendre polynomial. The collocation points are taken to be $\zeta_2 = \frac{1}{2} - \frac{1}{2\sqrt{3}}$ and $\zeta_3 = \frac{1}{2} + \frac{1}{2\sqrt{3}}$ with 0 and 1 as boundary points by transforming the domain $[-1, 1]$ of a shifted Legendre polynomial of order 2 onto $[0, 1]$.

As given in the previous section, substituting

$$C^\gamma(\zeta, \tau) = \sum_{i=1}^4 c_i^\gamma(\tau) H_i(\zeta),$$

$$Q^{\ell, \gamma}(\eta, \zeta, \tau) = \sum_{i=1}^4 q_i^{\ell, \gamma} H_i(\eta),$$

$$N^{\ell, \gamma}(\eta, \zeta, \tau) = \sum_{i=1}^4 n_i^{\ell, \gamma} H_i(\eta), \text{ gives}$$

$$c_1^1(\tau) = \frac{1}{Pe} c_2^1(\tau), c_4^{s_2}(\tau) = 0 \text{ and } q_2^{(1, \gamma)}(\tau) = 0,$$

$$q_4^{(s_1, \gamma)}(\tau) = Bi \left[\sum_{i=1}^4 c_i^\gamma(\tau) H_{ji} - q_3^{(s_1, \gamma)}(\tau) \right] \text{ in the axial}$$

and radial domain, respectively. It converts the system of partial differential equations given in Eq. (13) to Eq. (20) into the system of ordinary differential equations. At the j^{th} collocation point, the system of equations can be expressed as:

$$\sum_{i=1}^4 \frac{dq_i^{(\ell,\gamma)}}{d\tau} H_{ji} = \frac{1}{h_\ell^2} \sum_{i=1}^4 q_i^{(\ell,\gamma)} B_{ji} + \frac{1}{\eta_j h_\ell} \sum_{i=1}^4 q_i^{(\ell,\gamma)} A_{ji} - \mu N_1 P_1 \left(C_1 \left(\sum_{i=1}^4 q_i^{(\ell,\gamma)} H_{ji} \right) \left(1 - \sum_{i=1}^4 n_i^{(\ell,\gamma)} H_{ji} \right) - k^* \sum_{i=1}^4 n_i^{(\ell,\gamma)} H_{ji} \right) \quad (24)$$

for all, $\ell = 1, 2, \dots, s_1$, $\gamma = 1, 2, \dots, s_2$

$$\sum_{i=1}^4 \frac{dn_i^{(\ell,\gamma)}}{d\tau} H_{ji} = P_1 \left(C_1 \left(\sum_{i=1}^4 q_i^{(\ell,\gamma)} H_{ji} \right) \left(1 - \sum_{i=1}^4 n_i^{(\ell,\gamma)} H_{ji} \right) - k^* \sum_{i=1}^4 n_i^{(\ell,\gamma)} H_{ji} \right) \quad (25)$$

for all, $\ell = 1, 2, \dots, s_1$, $\gamma = 1, 2, \dots, s_2$

$$\sum_{i=1}^4 \frac{dc_i^{(\gamma)}}{d\tau} H_{ji} = \frac{\psi Bi}{Pe h_\gamma^2} \sum_{i=1}^4 c_i^{(\gamma)} \bar{B}_{ji} - \frac{\psi Bi}{h_\gamma} \sum_{i=1}^4 c_i^{(\gamma)} \bar{A}_{ji} - \theta Bi \left(\sum_{i=1}^4 c_i^{(\gamma)} H_{ji} - \sum_{i=1}^4 q_i^{(m,\gamma)} H_{li} \right) \quad (26)$$

for all, $\ell = 1, 2, \dots, s_1$, $\gamma = 1, 2, \dots, s_2$

where B_{ji} and A_{ji} are discretization matrices for the second- and first-order derivatives, respectively, in the radial domain and \bar{B}_{ji} and \bar{A}_{ji} are discretization matrices for the second- and first-order derivatives, respectively, in the axial domain. The resulting system of differential equations can be put into the matrix form as $\mathbf{H}\bar{\mathbf{C}}' = \mathbf{M}\bar{\mathbf{C}}$, where \mathbf{H} is the matrix of Hermite functions, $\bar{\mathbf{C}}$ is the matrix of collocation functions and $\bar{\mathbf{C}}'$ is the matrix of the derivative of these collocation functions with respect to time and \mathbf{M} is the coefficient matrix.

After application of HCM, for 5 elements in the radial domain and varying elements in the axial domain, '46s₂' number of differential equations appear, where s_2 is the number of elements in the axial domain. This system of differential equations is solved using MATLAB with the 'ode15s' system solver, which uses the backward differentiation formula to

solve the system of differential equations.

STABILITY ANALYSIS

The test of every numerical technique lies in how stable it is or how fast it converges. In present study, the stability analysis was made on the basis of the L₂-norm and L_∞-norm. In Table 1 to Table 4, the L₂-norm and L_∞-norm are presented for different values of Peclet number Pe and Biot number Bi at different time intervals. The average bed porosity ε and dimensionless parameter ψ are taken to be 0.6314 and 0.1, respectively. The values in Table 1 to Table 4 are found to be stable after 10 elements in the axial domain. However, the L_∞-norm is observed to be higher than the L₂-norm, but the stability in the results can be better judged by the L₂-norm as compared to the L_∞-norm.

Table 1: L₂-norm and L_∞-norm for $Pe=5$, $Bi=4.5$.

τ (-)	2 elements		5 elements		10 elements		12 elements	
	$\ \mathbf{C}\ _2$	$\ \mathbf{C}\ _\infty$						
0	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.50	0.935	1.035	0.920	1.363	0.903	1.502	0.900	1.523
1.00	0.772	0.927	0.791	1.045	0.787	1.100	0.787	1.116
1.25	0.696	0.877	0.727	0.964	0.729	0.994	0.728	1.002
1.75	0.554	0.735	0.600	0.795	0.606	0.835	0.607	0.838

Table 2: L_2 -norm and L_∞ -norm for $Pe=7$, $Bi=5.5$.

$\tau (-)$	2 elements		5 elements		10 elements		12 elements	
	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$
0	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.50	0.935	1.083	0.945	1.496	0.940	1.568	0.938	1.604
1.00	0.732	0.999	0.782	1.120	0.786	1.146	0.786	1.161
1.25	0.636	0.892	0.702	0.987	0.710	1.028	0.711	1.038
1.75	0.458	0.655	0.539	0.828	0.558	0.854	0.556	0.857

Table 3: L_2 -norm and L_∞ -norm for $Pe=10$, $Bi=6.7$.

$\tau (-)$	2 elements		5 elements		10 elements		12 elements	
	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$
0	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.50	0.923	1.232	0.956	1.541	0.960	1.663	0.960	1.675
1.00	0.666	0.980	0.758	1.127	0.769	1.195	0.770	1.200
1.25	0.536	0.783	0.656	1.050	0.673	1.073	0.674	1.078
1.75	0.320	0.440	0.450	0.790	0.473	0.846	0.476	0.852

Table 4: L_2 -norm and L_∞ -norm for $Pe=15$, $Bi=7.5$.

$\tau (-)$	2 elements		5 elements		10 elements		12 elements	
	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$	$\ C\ _2$	$\ C\ _\infty$
0	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.50	0.938	1.391	0.981	1.665	0.992	1.836	0.993	1.850
1.00	0.609	0.907	0.761	1.286	0.778	1.302	0.780	1.311
1.25	0.438	0.616	0.637	1.095	0.666	1.174	0.669	1.182
1.75	0.200	0.359	0.385	0.823	0.425	0.890	0.429	0.893

EXPERIMENTAL

Displacement washing experiments simulated under the laboratory conditions were performed in a cylindrical glass cell with inside diameter of 35 mm under constant bed height of 30 mm. The fiber pulp bed occupied the volume between the permeable septum and a piston, covered with 45 mesh screens to prevent fiber losses from the bed.

Pulp beds were formed from a dilute suspension of unbeaten unbleached Kraft pulp in black liquor. Pulp was obtained from a blend of softwoods containing approximately $\frac{3}{4}$ spruce and $\frac{1}{4}$ pine. After compressing to the desired thickness of 30 mm, the consistency, *i.e.*, mass concentration of moisture-free pulp fibers in the bed was about 12%. In order to characterise the pulp fibers used in the experiments, physical properties of Kraft pulp were determined. The Schopper-Riegler freeness had a value of 13.5°SR. The degree of delignification of the pulp was expressed by the kappa number of about 32. Using the Kajaani FS-100 instrument, the mean length of the fibers was also measured. The weighted average length was 3.35 mm, while the numerical average length was 1.46 mm. The specific surface of fibers having a coarseness of $0.15 \text{ m}^2 \text{ kg}^{-1}$ was $733 \text{ m}^2 \text{ kg}^{-1}$.

Distilled water was used as wash liquid and was distributed uniformly through the piston to the top of bed at the start of the washing experiment. At the same time, the displaced liquor was collected at atmospheric pressure from the bottom of the bed *via* the septum. The washing effluent was sampled at different time intervals until the effluent was colourless. Samples of the washing effluent leaving the pulp bed were analysed for alkali lignin using an ultraviolet spectrophotometer operating at a wavelength of 295 nm. In Table 5, the input values for three runs of experiments are given. Displacement washing experiments with composition of pulp fibers, including washing equipment, were described in detail in Arora & Potůček (2012).

Table 5: Experimental data of pulp fibers.

Parameter	Value	Unit
Pe	7.921-10.651	-
ε	0.6075-0.6314	-
u	$(0.1300-0.2071) \times 10^{-3}$	m/s
Consistency	11.737-12.303	%
D_L	$(0.611-1.145) \times 10^{-6}$	m^2/s
β	0.7246	-
L	30×10^{-3}	m
R	$(10-25) \times 10^{-9}$	m

RESULTS AND DISCUSSION

It can be observed from Table 1 to Table 4 that stability occurs after 10 elements in the axial domain. Therefore, the theoretical effect of different parameters on the exit solute concentration will be discussed for 5 elements in the radial domain and 10 elements in the axial domain.

Effect of Peclet Number (Pe)

In Figure 4, the theoretical effect of Peclet number is shown on the exit solute concentration for $Bi = 5$ and $\varepsilon = 0.6314$. It can be observed from this figure that, as the value of Peclet number increases, *i.e.*, for $Pe \geq 20$, solution profiles converge rapidly to the steady-state condition and follow a Gaussian shape curve. However, for small values of Peclet number, *i.e.*, $Pe = 5$, solution profiles take a long time to converge to a steady-state condition. This is due to the fact that, for small values of Pe , the axial dispersion coefficient (D_L) is large. It causes more back mixing and, as a result, fewer impurities are washed out and a long time in the washing operation is required. Therefore, high Pe is preferred for better washing operations at small intervals of time. For $Pe = 20$ and $Pe = 30$, no considerable effect is observed on solution profiles. It authenticates the fact that better washing operations can be achieved for $Pe \leq 30$ (Al-Jabari *et al.*, 1994; Arora *et al.*, 2006).

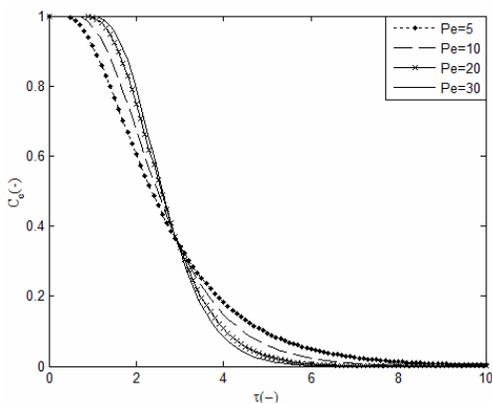


Figure 4: Behaviour of the solution profile for different values of Pe with $Bi = 5$ and $\varepsilon = 0.6314$.

Effect of Biot Number (Bi)

Biot number (Bi) signifies the mass transfer resistances inside and on the surface of the particle. Theoretical effects of Biot number on the solution profiles are shown in Figure 5 for $Pe = 10$ and $\varepsilon = 0.6314$. For small values of Biot number, *i.e.*, $Bi = 5$, solution profiles take a long time to converge to the steady-

state condition as compared to large values of Biot number, *i.e.*, $Bi = 15$, where the solution profile converges for τ nearly equal to 3. This is due to the fact that, for high Bi , the mass transfer rate increases, resulting in more removal of impurities adsorbed on the particle surface and hence better washing operations can be achieved.

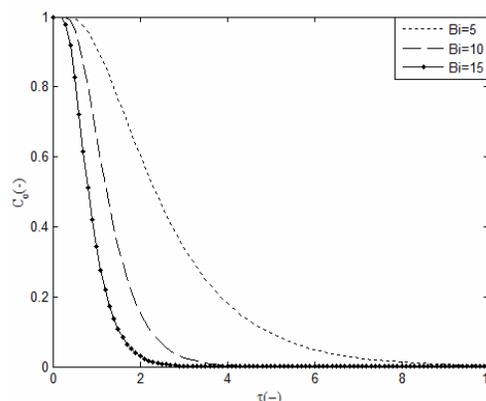


Figure 5: Behaviour of the solution profile for different values of Bi with $Pe = 10$ and $\varepsilon = 0.6314$.

Effect of the Dimensionless Parameter ψ

The effect of pore radius of the particle, film resistance mass transfer coefficient and interstitial velocity can be observed effectively by studying the effect of the dimensionless parameter ψ on the solution profiles. In Figure 6 the theoretical effect of ψ is shown for $Pe = 10$, $Bi = 6.7$ and $\varepsilon = 0.6314$.

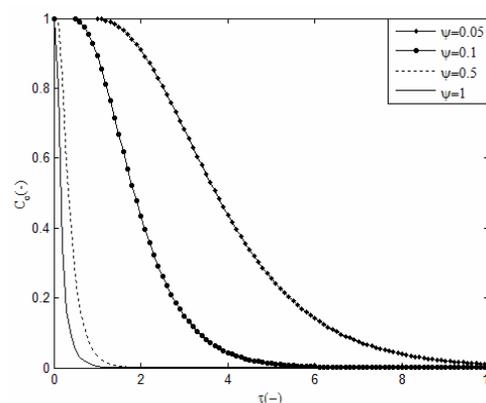


Figure 6: Behaviour of the solution profile for different values of the dimensionless parameter ψ for $Pe = 10$, $Bi = 6.7$ and $\varepsilon = 0.6314$.

It is observed from this figure that, for $\psi = 0.05$, more time is elapsed to converge to the steady-state condition, as compared to the value of $\psi = 0.5$. This is due to the fact that, with the increase in the value of ψ , the pore radius of particles swells, which in-

creases the diffusion in the particle pores, resulting in better removal of impurities adsorbed on the particle surface and hence better washing operations can be attained. For $\psi > 0.5$ no significant effect can be analysed on the solution profiles.

Effect of Bed Porosity (ε)

The packed bed porosity, ε is the most significant and perceptive factor which affects the solution profiles extensively. As the value of bed porosity increases, permeability increases causing the amount of solute removed from interparticle voids by the convective mechanism to increase, and the washing process runs very rapidly. The effect of bed porosity ε for $Pe = 10$ and $Bi = 6.7$, is shown in Figure 7. It can be easily observed from the figure that the solution profiles converge to the steady-state condition more rapidly for $\varepsilon = 0.8120$ as compared to $\varepsilon = 0.5561$.

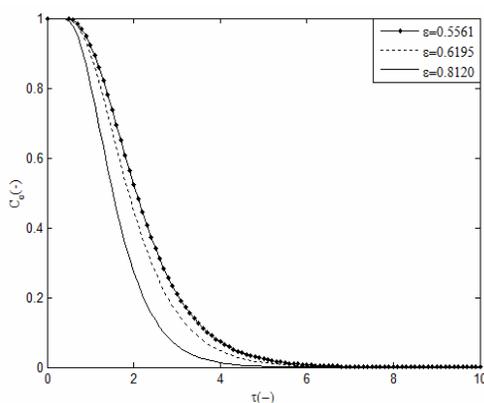


Figure 7: Behaviour of the solution profile for different values of ε with $Pe = 10$ and $Bi = 6.7$.

Wash Yield ($WY_{\tau=1}$)

The most significant solute removal parameter used in the industry is wash yield. It is the proportion of dissolved solids removed relative to the dissolved solids entering with the unwashed pulp. If the solute is split in a similar portion as the fluid, it is easy to analyse how much solute is left in the thickened pulp. Wash yield defined for $\tau = 1$ can be calculated using the following formula (Potůček, 1997):

$$WY_{\tau=1} = \frac{\int_0^1 C_e d\tau}{\int_0^{\tau} C_e d\tau} \quad (27)$$

Wash yield for $Pe = 9$, $Bi = 6$ and $\varepsilon = 0.6075$ was calculated at different time intervals for 5 elements in the radial domain and varying elements in the axial domain. Values of WY are given in Table 6. It is observed from this table that wash yield at any time lies within the range varying from 0.7 to 0.8 which is less than nearly seventy times the initial solute concentration. As time increases from $\tau = 5$, no considerable effect is observed and the values of $WY_{\tau=1}$ remain stable. For pulp fibers, the influence of Peclet number on wash yield can be linked by Equation (28) given by Potůček (2005), which agrees well with the values given in Table 6.

$$WY_{\tau=1} = 0.72Pe^{0.040} \quad (28)$$

Table 6: $WY_{\tau=1}$ for different elements of the axial domain and at varying time periods.

$\tau (-)$	2 elements	5 elements	10 elements	12 elements
2	0.7834	0.7680	0.7604	0.7592
3	0.7566	0.7394	0.7306	0.7294
4	0.7532	0.7355	0.7266	0.7252
5	0.7528	0.7349	0.7260	0.7247

COMPARISON OF EXPERIMENTAL AND NUMERICAL VALUES

Theoretically, one can vary a single parameter keeping the other parameters constant. However, practically, it is not possible to vary only a single parameter. As bed porosity changes, the pore radius of the particle, interstitial velocity and permeability vary, which varies the axial dispersion and intraparticle diffusion coefficient and, therefore, the Peclet number and Biot number also vary. In Figure 8 the behaviour of the solution profiles is shown for different values of Pe , Bi and ε . Although the range of bed porosity does not vary greatly, the solution profiles converge rapidly for $Pe = 10.651$ and $Bi = 6.7$ as compared to $Pe = 7.921$ and $Bi = 5.5$. It reflects the fact that, with the increase in Biot number, the pore radius of particles increases, which gives better washing results.

In Table 7, a comparison between experimental and numerical values is shown for different values of Pe , Bi and ε in terms of relative error:

$$\text{Relative error} = \frac{|C_{exp} - C_{num}|}{C_{exp}} \quad (29)$$

where C_{exp} is the experimental value and C_{num} is the numerical value. It is observed from this table that the minimum error is of the order 10^{-3} , which is less than 1% in all cases. It signifies the validity of the model for the washing cell.

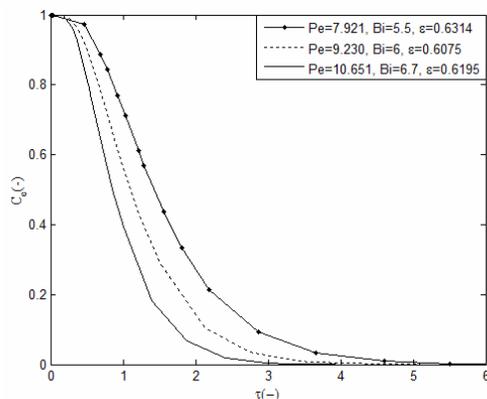


Figure 8: Behaviour of the solution profiles for different values of Pe , Bi and ε .

Table 7: Comparison of Experimental and Numerical values.

$Pe=7.921, Bi=5.5, \varepsilon=0.6314$			$Pe=9.230, Bi=6, \varepsilon=0.6075$			$Pe=10.651, Bi=6.7, \varepsilon=0.6195$		
Experimental	Numerical	Relative Error	Experimental	Numerical	Relative Error	Experimental	Numerical	Relative Error
1.0000	1.00000	0.0000	1.00000	1.0000	0.0000	1.0000	1.00000	0.0000
1.0000	1.00048	4.8000×10^{-4}	9.6737×10^{-1}	9.6929×10^{-1}	1.9766×10^{-3}	1.0000	1.00157	1.5700×10^{-3}
9.7173×10^{-1}	9.7029×10^{-1}	1.4838×10^{-3}	9.3008×10^{-1}	9.3093×10^{-1}	9.1202×10^{-4}	1.0000	1.00087	8.7000×10^{-4}
8.8734×10^{-1}	8.8681×10^{-1}	6.0321×10^{-4}	9.0763×10^{-1}	9.0996×10^{-1}	2.5747×10^{-3}	9.6433×10^{-1}	9.6509×10^{-1}	7.8795×10^{-4}
7.1077×10^{-1}	7.1074×10^{-1}	4.3998×10^{-5}	6.4407×10^{-1}	6.4714×10^{-1}	4.7762×10^{-3}	7.9303×10^{-1}	7.9107×10^{-1}	2.4727×10^{-3}
6.1286×10^{-1}	6.1219×10^{-1}	1.1040×10^{-3}	5.5085×10^{-1}	5.5074×10^{-1}	1.9326×10^{-4}	7.7146×10^{-1}	7.7267×10^{-1}	1.5696×10^{-3}
5.6985×10^{-1}	5.6967×10^{-1}	3.2013×10^{-4}	4.3051×10^{-1}	4.3232×10^{-1}	4.2148×10^{-3}	6.5989×10^{-1}	6.6091×10^{-1}	1.5424×10^{-3}
9.2175×10^{-2}	9.2648×10^{-2}	5.1268×10^{-3}	1.2712×10^{-2}	1.2817×10^{-2}	8.2313×10^{-3}	6.5948×10^{-2}	6.5857×10^{-2}	1.3774×10^{-3}
3.2773×10^{-2}	3.2812×10^{-2}	1.1700×10^{-3}	8.0508×10^{-3}	8.1164×10^{-3}	8.1460×10^{-3}	1.9909×10^{-2}	1.9781×10^{-2}	6.4219×10^{-3}
2.6628×10^{-3}	2.6742×10^{-3}	4.2687×10^{-3}	1.4407×10^{-3}	1.4476×10^{-3}	4.7769×10^{-3}	2.3642×10^{-3}	2.3717×10^{-3}	3.2002×10^{-3}
1.1471×10^{-3}	1.1368×10^{-3}	8.9802×10^{-3}	8.4746×10^{-4}	8.4127×10^{-4}	7.2967×10^{-3}	1.1199×10^{-3}	1.1133×10^{-3}	5.8375×10^{-3}
6.9644×10^{-4}	6.9108×10^{-4}	7.6962×10^{-3}	5.9322×10^{-4}	5.8904×10^{-4}	7.0502×10^{-3}	6.6363×10^{-4}	6.6479×10^{-4}	1.7630×10^{-3}
5.3257×10^{-4}	5.3132×10^{-4}	2.3370×10^{-3}	4.6610×10^{-4}	4.7017×10^{-4}	8.7198×10^{-3}	4.9772×10^{-4}	4.9464×10^{-4}	6.1858×10^{-3}

Displacement Ratio (DR)

Displacement ratio is the most perceptive factor in the washing theory. It is calculated from the average solute concentration of the solute using the following formula:

$$DR = 1 - C_{av} \quad (30)$$

In Figure 9, a comparison has been made for the displacement ratio calculated for different values of Pe , Bi and ε . It is observed from this figure that, with the increase in the value of Pe , Bi and ε , the solution profiles for DR converge more rapidly as compared to small values of Pe , Bi and ε . For different values of Pe , Bi and ε , the solution profiles converge at almost the similar times. This is because the bed porosity lies in same range in the three washing runs

(Arora & Potůček, 2012). However, the solution profile converges slightly faster for $Pe = 10.651$ as compared to other solution profiles.

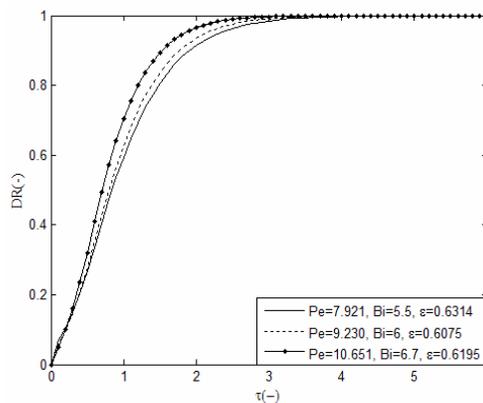


Figure 9: Behaviour of DR for different values of Pe , Bi and ε .

CONCLUSIONS

A mathematical model for the displacement washing process was presented and solved using HCM. Numerical results were compared with the experimental ones of a washing cell for different values of displacement washing parameters. It can be concluded from all the experimental and theoretical findings that the proposed mathematical model agrees fairly well with the experimental data, in view of significant aspects of dispersion, diffusion and different porosities. Comparison of numerical and experimental values presented in the tables and graphs validate this information.

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NOMENCLATURE

Bi	Biot number, dimensionless ($=k_f\beta R/KD_F$)
c	concentration of solute in the liquor (kg/m^3)
C	dimensionless concentration ($=c/C_0$)
C_0	solute concentration in the vat (kg/m^3)
C_1	dimensionless parameter ($=C_0/C_F$)
C_{av}	average solute concentration, dimensionless
C_e	exit solute concentration, dimensionless
C_F	fiber consistency (kg/m^3)
D_F	intrafiber diffusion coefficient (m^2/s)
D_L	axial dispersion coefficient (m^2/s)
DR	Displacement Ratio, dimensionless
K	volume equilibrium constant, dimensionless
k^*	mass transfer coefficient, dimensionless ($=k_2/k_1$)
k_1, k_2	mass transfer coefficient (1/s)
k_f	film mass transfer coefficient (m/s)
L	thickness of the bed (m)
n	concentration of solute adsorbed on the fibers (kg/m^3)
N	dimensionless concentration of solute adsorbed on fibers ($=n/N_0$)
N_0	initial concentration of solute adsorbed on the fibers (kg/m^3)
N_1	dimensionless parameter ($=N_0/C_0$)
P_1	dimensionless parameter ($=k_1R^2/D_F$)
Pe	Peclet number, dimensionless ($=uL/D_L$)

Q	dimensionless pore liquid concentration ($=q/C_0$)
q	pore liquid concentration (kg/m^3)
R	fiber radius(m)
r	radial position in particle (m)
t	time (s)
u	interstitial velocity through bed (m/s)
WY	wash yield, dimensionless
x	distance from point of introduction of solvent (m)

Greek Symbols

β	particle porosity, dimensionless
ε	porosity of cake, dimensionless
η	dimensionless radial coordinate ($=r/R$)
θ	$2(1-\varepsilon)/\varepsilon$
μ	$(1-\beta)/\beta$ (dimensionless)
ξ	dimensionless axial coordinate ($=x/L$)
τ	dimensionless time ($=tD_F/R^2$)
ψ	dimensionless parameter ($=KRu/k_f\beta L$)

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