CELLULOSE CHEMISTRY AND TECHNOLOGY

COMPARATIVE STUDY OF AXIAL DISPERSION MODEL USING CUBIC HERMITE COLLOCATION METHOD FOR LINEAR AND NONLINEAR ADSORPTION ISOTHERMS

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The transient behaviour of desorption phenomena of a solute through a packed bed of porous particles is characterized using the one dimensional axial dispersion model. Mass-transfer resistance due to pore diffusion/dispersion is considered in the model. The model is analyzed with respect to linear and nonlinear (Langmuir) adsorption isotherm, for same set of boundary and initial conditions. The model is solved numerically, using the cubic Hermite collocation method with Gauss Legendre quadrature points of order two, as collocation points. Linear and nonlinear cases are compared based on experimental data, from a paper mill, reported by previous investigators. The value of exit solute concentration for different parameters like Péclet number, axial dispersion coefficient, interstitial velocity and cake thickness is measured through the models. It is concluded that the nonlinear isotherm follows the actual desorption process more closely than the linear isotherm.

Keywords: diffusion, dispersion, Langmuir isotherm, leaching, numerical solution, packed bed

INTRODUCTION

The removal of solutes from a packed bed using a solvent is of great importance. The solute occupying the space between the interstices of fibres (as displaceable fluid) and in the pores of the fibres (as stagnant fluid) is shown in Fig. 1. The displacement of the solute from the void spaces of the bed takes place due to diffusion-dispersion in the direction of flow. Diffusion due to concentration gradient, dispersion due to back mixing and adsorption-desorption of solutes towards the fibre surface cause the stagnant fluid (containing solute) to move out of the particle voids. The solutes are subsequently displaced by the flowing fluid. This causes an asymptotic decline in the concentration of solute with time.

To analyze, simulate and optimize the solute removal from a packed bed, the development of a mathematical model is an imperative necessity. Models proposed by earlier investigators can be classified into three categories, namely macroscopic, microscopic and semi quantitative models. The macroscopic models can be categorized as black box type, because these models give outside description of the process based on material balances only.

The microscopic models[1-36] are concerned with the basic mechanism and are based on the fundamentals of fluid dynamics. Semi quantitative models are intermediate between these two models.

The microscopic model of packed bed gives importance to three physical rates:

1. axial dispersion of the bulk fluid (flowing liquor);
2. intrafiber Fick's second law of diffusion;
3. liquid phase mass transfer, which accounts for the transport of the solute from the fiber surface to the flowing liquid.

However, boundary conditions describing the solute exchange between the fiber surface and the bulk fluid also play an important role. In the following section, a general model based on the equation of continuity, diffusion-dispersion and kinetics of adsorption-desorption is discussed for two different adsorption isotherms.

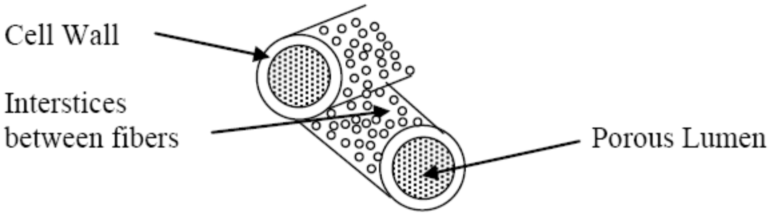

Figure 1: Schematic representation of fibers

DESCRIPTION OF THE PROBLEM

For a systematic analysis of a packed bed of porous particles it is assumed that:

1. the bed is macroscopically uniform;
2. particles are of uniform cylindrical size;
3. particle diameter is very small as compared to axial distance;
4. the intrafiber diffusion coefficient is independent of cake thickness and particle radius;
5. the consistency of fibers, particle porosity and bed porosity are interrelated to each other.

The material balance across any simple shell, in one dimensional form, can be written as:

$$D_L \frac{\partial^2 c}{\partial z^2} = u\frac{\partial c}{\partial z} + \frac{\partial c}{\partial t} + \frac{1-\varepsilon}{\varepsilon}\frac{\partial n}{\partial t}. \tag{1}$$

Here, the first term represents diffusion-dispersion, the other terms represent convective flow, concentration gradient of fluid and concentration gradient of particles, respectively. Mathematically, u and D_L are functions of z, while c and n are functions of both z and t.

The concentration of the solute adsorbed on fibers is linked with the concentration of the solute in the flowing liquor via linear and Langmuir adsorption isotherms. The linear isotherm assumes that pointwise equilibrium is attained instantaneously inside the particle, *i.e.*,

$$n = kc \tag{2a}$$

The Langmuir isotherm assumes that the deposition (adsorption) rate is second order in forward direction and the detachment (desorption) rate is first order in backward direction, *i.e.*,

$$\frac{\partial n}{\partial t} = k_1 \frac{c}{C_F}(N_i - n) - k_2 n$$

At equilibrium, it simplifies to:

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

where $A_0 = \frac{kN_i}{C_F}$ and $B_0 = \frac{k}{C_F}$ (2b)

Initially, bulk fluid concentration is taken equal to inlet solute concentration, *i.e.*,

$$c(z,0) = C_i \tag{3}$$

To keep the mathematical complexity as small as possible, the boundary conditions are defined at two points only. One at the top of the bed (z = 0) and the other at the bottom of the bed ($z = L$). Between 0 and L, no condition is imposed.

At the inlet of the bed (z = 0), there is a step change in the solute concentration. The difference of concentration gradient at the inlet concentration multiplied by the ratio of interstitial velocity to axial dispersion coefficient is equal to the concentration of weak wash liquor, *i.e.*,

$$uc - D_L \frac{\partial c}{\partial z} = uC_S \tag{4}$$

At the outlet of the bed ($z = L$), to avoid the unacceptable conclusions that the fluid will pass through the maximum or minimum in the interior of the bed, the concentration gradient is taken as zero, *i.e.*,

$$\frac{\partial c}{\partial z} = 0 \tag{5}$$

By making suitable modifications, the present models have been applied to study the mass transfer between solid and liquid phases,[1] the separation of glycerol from biodiesel,[2] tubular flow reactor,[3,4,5] the analysis of the distillation column,[6] the design and development of airlift loop reactors,[7] heat transfer processes in gas-solid turbulent fluidized systems,[8] chromatography,[9] measurement of neutron flux,[10] sorption-desorption,[11,12] enzymatic hydrolysis of racemic ibuprofen ester by lipase,[13] annular flow in a tubular reactor,[14] electrochemical reactors,[15] gas liquid bubble column,[16] solute flow in liquid suspension,[17] cake washing process[18] and mixing flow pattern.[19,20]

A great deal of research is underway to find the exact and numerical solution of these models using Laplace transformation,[15,16,21,22,23] Fourier's method,[17,18,21] moment method,[3] Galerkin finite element method,[24] finite difference method,[7] *FlexPDE* software by means of finite element,[19,20] Euler Maruyama scheme,[14] orthogonal collocation method,[10,25,26] fitted mesh collocation method,[27] Galerkin/Petrov method,[28] orthogonal collocation on finite elements,[29,30] COMSOL Multiphysics finite element package,[2] iterative technique,[4] collocation method,[5] and pdepe-solver.[8]

None of the previous investigators have ever attempted to compare the results of the model for different isotherms, in order to assess their suitability to predict the actual flow pattern in the packed bed. In this work, an attempt is made to compare the linear and nonlinear isotherms using the cubic Hermite collocation method (CHCM) for Gauss Legendre roots as collocation points. The method has the advantage that high-order accuracy can be achieved using a small number of systems of equations and multistep time differencing. In addition, it involves less arithmetic at each time step.

SOLUTION TECHNIQUE

The technique of CHCM, selection of collocation points and differentiation of Hermite interpolation polynomials are explained hereunder.

Cubic Hermite collocation method

In this method, the interval $I=[a,b]$ is subdivided into a partition π by the set of points $\pi : a = x_1 < x_2 < ... < x_{n+1} = b$. The approximating subspace $H_3(\pi)$ will consist of all the functions $f(x)$.

Consider the trial function as proposed by Brill[31] as follows:

$$c(u,t) = \sum_{j=1}^{n+1} \left[a(u_j,t) P_j(u) + a'(u_j,t) Q_j(u) \right] \tag{6}$$

where $a(u_j,t),\ a'(u_j,t)$ are unknown coefficients to be determined. Details about the technique of CHCM are available in Ganaie *et al.*[32]

Selection of collocation points

The Gauss-Legendre quadrature points (Douglas and Dupont[33]) of order 2 are taken as the collocation points for each subinterval $[x_i, x_{i+1}]$, *i.e.*,

$$\eta_{i,\,r} = \left(\frac{x_{i-1} + x_i}{2} \right) + (-1)^r \frac{h_i}{2\sqrt{3}},\ \ 2 \le i \le n+1,\ \ 1 \le r \le 2 \tag{7}$$

By taking $\beta = \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)$ and $\gamma = \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right)$, these points can be written as:

$$\frac{\eta_{j,\,1} - x_j}{h_j} = -\beta,\ \ \frac{\eta_{j,\,2} - x_j}{h_j} = -\gamma,\ \ \frac{\eta_{j,\,1} - x_{j-1}}{h_j} = \beta,\ \ \frac{\eta_{j,\,2} - x_{j-1}}{h_j} = \gamma \tag{8}$$

SOLUTION OF MODEL

Equations (1) to (5) are converted into the dimensionless form by using Péclet number, dimensionless concentration, dimensionless time and dimensionless thickness given below. More details are available elsewhere.[23]

$$C = \frac{c - C_S}{C_i - C_S},\ N = \frac{n - C_S}{C_i - C_S},\ Pe = \frac{uL}{D_L},$$

$$\xi = \frac{z}{L},\ \tau = \frac{ut}{(1+\mu k)L},\ k = \frac{k_1}{k_2},\ \mu = \frac{1-\varepsilon}{\varepsilon}$$

The dimensionless form of the model along with initial and boundary conditions is given hereunder:

$$\frac{1}{Pe}\frac{\partial^2 C}{\partial \xi^2} = \frac{\partial C}{\partial \xi} + \frac{\partial C}{\partial \tau} \qquad \text{(linear case)} \tag{9a}$$

$$\frac{1}{Pe}\frac{\partial^2 C}{\partial \xi^2} = \frac{\partial C}{\partial \xi} + \frac{1}{(1+\mu k)}\frac{\partial C}{\partial \tau} + \frac{\mu A_0}{\left[1 + B_0\left\{C\left(C_0 - C_s\right) + C_s\right\}\right]^2}\frac{1}{(1+\mu k)}\frac{\partial C}{\partial \tau}$$

(nonlinear case) (9b)

$$C(\xi,0) = 1 \tag{10}$$

$$Pe\,C(0,\tau) - \frac{\partial C(0,\tau)}{\partial \xi} = 0 \tag{11}$$

$$\frac{\partial C(1,\tau)}{\partial \xi} = 0 \tag{12}$$

The discretized form of the linear case can be written as follows:

$$\sum_{j=1}^{n+1} \left[\dot{a}(\xi_j,\tau) P_j(\xi) + \dot{a}'(\xi_j,\tau) Q_j(\xi) \right]$$

$$= \frac{1}{Pe} \sum_{j=1}^{n+1} \left[\dot{a}(\xi_j,\tau)\, P_j''(\xi) + \dot{a}'(\xi_j,\tau)\, Q_j''(\xi) \right] - \sum_{j=1}^{n+1} \left[a(\xi_j,\tau)\, P_j'(\xi) + a'(\xi_j,\tau)\, Q_j'(\xi) \right]$$

After rearrangement, one gets:

$$\sum_{j=2}^{n} \left[\dot{a}(\xi_j,\tau) P_j(\xi) + \dot{a}'(\xi_j,\tau) Q_j(\xi) \right] + \dot{a}(\xi_1,\tau) P_1(\xi) + \dot{a}'(\xi_1,\tau) Q_1(\xi) + \dot{a}(\xi_{n+1},\tau) P_{n+1}(\xi) + \dot{a}'(\xi_{n+1},\tau) Q_{n+1}(\xi)$$

$$= \sum_{j=1}^{n+1} \left[a(\xi_j,\tau) \phi_j(\xi) + a'(\xi_j,\tau) \psi_j(\xi) \right] \tag{13}$$

where $\phi_j(\xi) = \frac{1}{Pe} P_j''(\xi) - P_j'(\xi)$ and $\psi_j(\xi) = \frac{1}{Pe} Q_j''(\xi) - Q_j'(\xi)$.

Since $P_j(\xi_1) \equiv 0,\ Q_1'(\xi_1) = 1$ and $Q_j'(\xi_1) \equiv 0$ for $j > 1$, boundary condition at $\xi = 0$, gives:

$$a(\xi_1,\tau) - \frac{1}{Pe} a'(\xi_1,\tau) = 0 \tag{14}$$

Differentiating this expression with time, one gets:

$$\dot{a}(\xi_1,\tau) - \frac{1}{Pe} \dot{a}'(\xi_1,\tau) = 0 \tag{15}$$

Similarly, the boundary condition at $\xi = 1$ implies:

$$a'(\xi_{n+1},\tau) = 0 \tag{16}$$

Differentiating this expression with time, one gets:

$$\dot{a}'(\xi_{n+1},\tau) = 0 \tag{17}$$

Now substituting conditions (14) to (17) in (13), one gets:

$$\begin{aligned} &\sum_{j=2}^{n} \left[\dot{a}(\xi_j,\tau)\, P_j(\xi) + \dot{a}'(\xi_j,\tau)\, Q_j(\xi) \right] + \left[Pe Q_1(\xi) + P_1(\xi) \right] \dot{a}(\xi_1,\tau) + \dot{a}(\xi_{n+1},\tau)\, P_{n+1}(\xi) \\ &= \sum_{j=2}^{n} \left[a(\xi_j,\tau)\, \phi_j(\xi) + a'(\xi_j,\tau)\, \psi_j(\xi) \right] + \left[\phi_1(\xi) + \psi_1(\xi) \right] a(\xi_1,\tau) + a(\xi_{n+1},\tau)\, \phi_{n+1}(\xi) \end{aligned} \tag{18}$$

Evaluating Eq. (18) at collocation points $\eta_{i,\,r}$, for $i = 2,3,\ldots,n+1$ and $r = 1,2$. It can be put in the matrix form as follows:

$$A\dot{X} = BX \tag{19}$$

where $X = \left(a(\xi_1,\tau),\ a(\xi_2,\tau),\ a'(\xi_2,\tau),\ a(\xi_3,\tau),\ a'(\xi_3,\tau), \ldots, a(\xi_n,\tau),\ a'(\xi_n,\tau),\ a(\xi_{n+1},\tau) \right)^T$ and

$\dot{X} = \left(\dot{a}(\xi_1,\tau),\ \dot{a}(\xi_2,\tau),\ \dot{a}'(\xi_2,\tau),\ \dot{a}(\xi_3,\tau),\ \dot{a}'(\xi_3,\tau),\ \ldots,\ \dot{a}(\xi_n,\tau),\ \dot{a}'(\xi_n,\tau),\ \dot{a}(\xi_{n+1},\tau) \right)^T$ are dimensional vectors.

The matrix system (19) is solved by MATLAB ode15s solver. Here $2n + 2$ conditions are required at each time to specify the approximate solution. Obviously, two of these conditions are obtained from the boundary conditions and the rest from the differential equation.

Matrices *A* and *B* are given as:

$$A=\begin{bmatrix} P_1(\eta_{2,1})+PeQ_1(\eta_{2,1}) & P_2(\eta_{2,1}) & Q_2(\eta_{2,1}) & 0 & 0 & \ldots & 0 \\ P_1(\eta_{2,2})+PeQ_1(\eta_{2,2}) & P_2(\eta_{2,2}) & Q_2(\eta_{2,2}) & 0 & 0 & \ldots & 0 \\ 0 & P_2(\eta_{3,1}) & Q_2(\eta_{3,1}) & P_3(\eta_{3,1}) & Q_3(\eta_{3,1}) & \ldots & 0 \\ 0 & P_2(\eta_{3,2}) & Q_2(\eta_{3,2}) & P_3(\eta_{3,2}) & Q_3(\eta_{3,2}) & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 0 & P_n(\eta_{n+1,1}) & Q_n(\eta_{n+1,1}) & P_{n+1}(\eta_{n+1,1}) \\ 0 & 0 & \ldots & 0 & P_n(\eta_{n+1,2}) & Q_n(\eta_{n+1,2}) & P_{n+1}(\eta_{n+1,2}) \end{bmatrix}$$

and

$$B=\begin{bmatrix} \phi_1(\eta_{2,1})+\psi_1(\eta_{2,1}) & \phi_2(\eta_{2,1}) & \psi_2(\eta_{2,1}) & 0 & 0 & \ldots & 0 \\ \phi_1(\eta_{2,2})+\psi_1(\eta_{2,1}) & \phi_2(\eta_{2,2}) & \psi_2(\eta_{2,2}) & 0 & 0 & \ldots & 0 \\ 0 & \phi_2(\eta_{3,1}) & \psi_2(\eta_{3,1}) & \phi_3(\eta_{3,1}) & \psi_3(\eta_{3,1}) & \ldots & 0 \\ 0 & \phi_2(\eta_{3,2}) & \psi_2(\eta_{3,2}) & \phi_3(\eta_{3,2}) & \psi_3(\eta_{3,2}) & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 0 & \phi_n(\eta_{n+1,1}) & \psi_n(\eta_{n+1,1}) & \phi_{n+1}(\eta_{n+1,1}) \\ 0 & 0 & \ldots & 0 & \phi_n(\eta_{n+1,2}) & \psi_n(\eta_{n+1,2}) & \phi_{n+1}(\eta_{n+1,2}) \end{bmatrix}.$$

RESULTS AND DISCUSSION

Comparison for linear case

The analytic solution for a packed bed of finite length is derived by Brenner[34] using Laplace transform. The exact solution for exit solute concentration reported by Brenner[34] is given hereunder:

For small values of Pe:

$$C_e=\exp\left\{\frac{Pe}{4}(2-T)\right\}\sum_{k=1}^{\infty}\left(\frac{\lambda_k\sin(2\lambda_k)}{\lambda_k^2+\left(\frac{Pe}{4}\right)^2+\left(\frac{Pe}{4}\right)}\right)\exp\left(-\frac{4\lambda_k^2T}{Pe}\right) \qquad (20a)$$

For large values of Pe:

$$\begin{aligned}C_e={}&1-\frac{1}{2}\,erfc\left\{(1-T)\sqrt{\frac{Pe}{4T}}\right\}-\left[\left\{3+\frac{Pe}{2}(1+T)\right\}\exp\left\{-\frac{Pe(1-T)^2}{4T}\right\}\sqrt{\frac{PeT}{\pi}}\right]\\&+\left[\frac{1}{2}+\frac{Pe}{2}(3+4T)+\left(\frac{Pe}{4}\right)^2(1+T)^2\right]\exp(Pe)\;erfc\left\{(1+T)\sqrt{\frac{Pe}{4T}}\right\}\end{aligned} \qquad (20b)$$

Numerical results for the linear case from Eq. (9a), obtained using the cubic Hermite collocation method, are compared with the exact ones, in Tables 1, 2 and 3 for Péclet numbers 10, 40 and 80, respectively. The numerical computation is performed using shifted Gauss Legendre roots of order 2. A close match is found between the results for small values of *N*, but the results become accurate to a greater number of decimal places as *N* increases. Here *N* stands for the number of elements introduced within the interval 0 to 1.

For Péclet numbers 10, 40 and 80, the exact and numerical results of exit solute concentration for linear and nonlinear isotherms are compared in Figs. 2 to 4. The exact and linear isotherm results are overlapping each other. For these cases, the solute removal process starts later than the nonlinear isotherm. It is found that the exit solute concentration for the linear case is of the order 10^{-20} (almost negligible), whereas for the nonlinear case it is of the order 10^{-4}. This indicates that a very small amount of leaching continues for some time.

Table 1
Comparison at *Pe* = 10 for linear case

Time	Exact solution[34]	Numerical solution using CHCM		
		N = 25	*N* = 50	*N* = 100
0.0	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.2	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.4	9.99987E-01	1.00000E+00	9.99987E-01	9.99987E-01
0.6	9.87554E-01	9.87600E-01	9.87600E-01	9.87557E-01
0.8	8.18514E-01	8.18500E-01	8.18520E-01	8.18519E-01
1.0	4.57337E-01	4.56500E-01	4.56525E-01	4.56991E-01
1.2	1.73343E-01	1.73300E-01	1.73303E-01	1.73340E-01
1.4	4.95553E-02	4.95600E-02	4.95587E-02	4.95585E-02
1.6	1.16114E-02	1.16200E-02	1.16240E-02	1.16230E-02
1.8	2.37146E-03	2.37200E-03	2.37201E-03	2.37198E-03
2.0	4.38032E-04	4.38200E-04	4.38128E-04	4.38123E-04
2.2	7.52085E-05	7.51900E-05	7.52171E-05	7.52166E-05
2.4	1.22255E-05	1.22200E-05	1.22243E-05	1.22244E-05
2.6	1.90602E-06	1.90500E-06	1.90524E-06	1.90529E-06
2.8	2.87684E-07	2.87400E-07	2.87446E-07	2.87460E-07
3.0	4.23275E-08	4.22600E-08	4.22706E-08	4.22736E-08

Table 2
Comparison at *Pe* = 40 for linear case

Time	Exact solution [34]	Numerical solution using CHCM		
		N = 40	*N* = 80	*N* = 160
0.0	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.2	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.4	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.6	1.00000E+00	9.99998E-01	9.99998E-01	1.00000E+00
0.8	9.74640E-01	9.74616E-01	9.74640E-01	9.74640E-01
1.0	4.77840E-01	4.77902E-01	4.77843E-01	4.77840E-01
1.2	4.49280E-02	4.49056E-02	4.49265E-02	4.49278E-02
1.4	9.90370E-04	9.89062E-04	9.90306E-04	9.90364E-04
1.6	7.90010E-06	7.93846E-06	7.90259E-06	7.90028E-06
1.8	3.11080E-08	3.19352E-08	3.11537E-08	3.11106E-08
2.0	7.40610E-11	7.93789E-11	7.43584E-11	7.40884E-11

Table 3
Comparison at *Pe* = 80 for linear case

Time	Exact solution [34]	Numerical solution using CHCM		
		N = 100	*N* = 200	*N* = 400
0.0	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.2	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.4	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.6	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.8	9.97410E-01	9.97410E-01	9.97411E-01	9.97411E-01

1.0	4.84280E-01	4.84289E-01	4.84280E-01	4.84280E-01
1.2	9.28220E-03	9.28058E-03	9.28206E-03	9.28215E-03
1.4	7.61530E-06	7.62324E-06	7.61583E-06	7.61535E-06
1.6	7.11770E-10	7.18406E-10	7.12188E-10	7.11804E-10
1.8	1.50320E-14	1.86514E-14	1.61947E-14	1.60089E-14
2.0	-7.71670E-20	-8.07200E-18	-1.03347E-16	-1.46734E-16

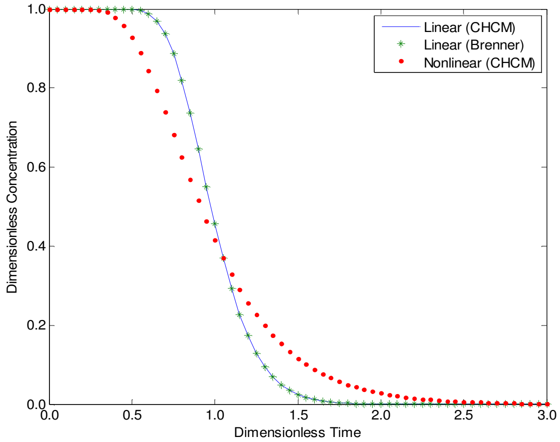

Figure 2: Comparison of linear and nonlinear cases for *Pe* =10

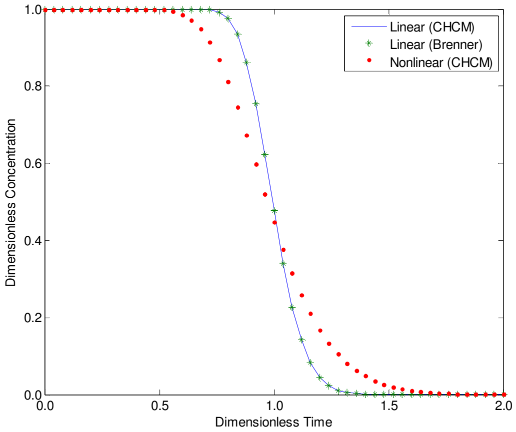

Figure 3: Comparison of linear and nonlinear cases for *Pe* = 40

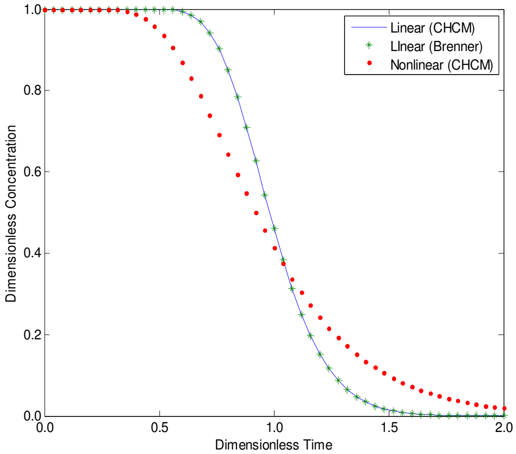

Figure 4: Comparison of linear and nonlinear cases for *Pe* = 80

Linear *vs* nonlinear case

The model for the packed bed of porous particles is simulated using the experimental data of a rotary vacuum washer.[35] The mill was using wheat straw as raw material. The inlet and outlet consistencies were in the range of 1-2% and 10-12%, respectively. The concentration of the black liquor solids inside the vat was 8-9 kg/m^3 and fresh water was sprayed to wash the pulp.

Using the experimental data listed in Table 4, the exit solute concentration profiles for the linear and nonlinear isotherms are plotted for axial dispersion coefficient, cake thickness and interstitial velocity in Figs. 5 to 7, respectively. During the actual washing process in a plant, the displacement of black liquor solids from the packed bed starts instantaneously, as soon as the wash liquor comes in contact with the bed. These figures indicate that, for the same set of parameters, mathematically, such type of behaviour is better described by the nonlinear isotherm than by the linear one. A similar behaviour has been observed practically, during laboratory experiments by Crotogino *et al.*,[36] i.e. the leaching of solute continues even after 72 hours. The present study verifies the experimental results of Crotogino *et al*.[36] for the nonlinear isotherm. It can be concluded that the solute removal process can be simulated more accurately using the nonlinear isotherm.

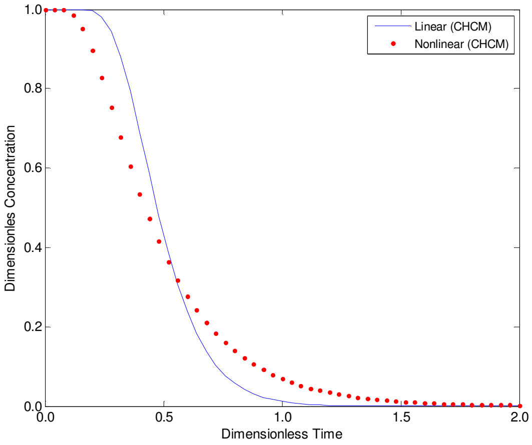

Figure 5: Comparison of linear and nonlinear case at $D_L = 5 \times 10^{-5}$ m^2/s

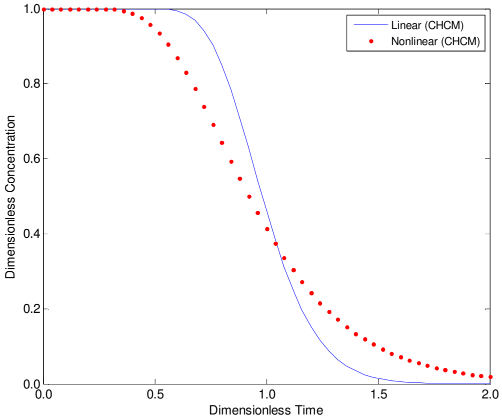

Figure 6: Comparison of linear and nonlinear case at $L = 0.05$ m

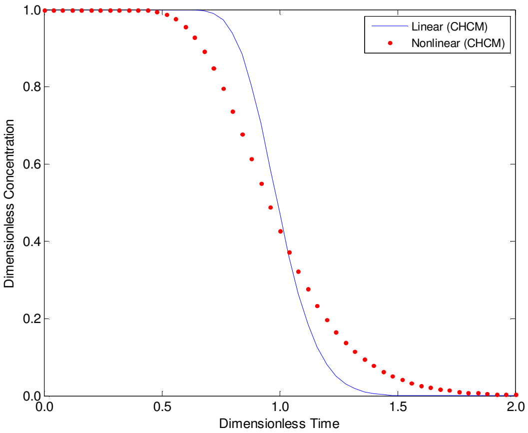

Figure 7: Comparison of linear and nonlinear case at $u = 0.019$ m/s

Table 4

Results from the experimental study

Parameter	Range	Unit
C_0	$(8.3341\text{-}8.3782) \times 10^{0}$	kg/ m^3
C_F	$(4.7059\text{-}6.6176) \times 10^{1}$	kg/ m^3
u	$(1.9321\text{-}1.9584) \times 10^{-3}$	m/s
L	$(0.6960\text{-}1.0531) \times\times 10^{-1}$	m
k_1/k_2	$(2.9389\text{-}4.1104) \times 10^{-3}$	-
ε	$(9.5500\text{-}9.6800) \times 10^{-1}$	-
D_L/u	3.99×10^{-3}	m

Table 5

Exit concentration values for nonlinear case

Time	$N = 50$	$N = 100$	$N = 200$	$N = 300$
0.0	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.2	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
0.4	9.99980E-01	9.99980E-01	9.99990E-01	9.99990E-01
0.6	9.85000E-01	9.86290E-01	9.86930E-01	9.87140E-01
0.8	8.03380E-01	8.10980E-01	8.14760E-01	8.16020E-01
1.0	4.38510E-01	4.47520E-01	4.52040E-01	4.53540E-01
1.2	1.63630E-01	1.68480E-01	1.70920E-01	1.71730E-01
1.4	4.62050E-02	4.78800E-02	4.87230E-02	4.90040E-02
1.6	1.07430E-02	1.11820E-02	1.14040E-02	1.14780E-02
1.8	2.17880E-03	2.27520E-03	2.32390E-03	2.34010E-03
2.0	4.00620E-04	4.19350E-04	4.28790E-04	4.31950E-04

Table 5 contains numerical results for the nonlinear isotherm, for the data (Arora *et al.*[35]) for $Pe = 40$, $A_0 = 5.20E-4$ 1/s, $B_0 = 6.25E-5$ m^3/kg-s, $\mu = 3.31E-2$, $C_0 = 8.33$ kg/m^3, $k = 2.94E-3$. Since no exact solution is available in the literature for the nonlinear isotherm, in Table 5 it is shown that the numerical results remain consistent and stable, even by increasing the number of elements.

CONCLUSION

A diffusion-dispersion model is solved for two isotherms, using the cubic Hermite collocation method. The technique is found to be simple, elegant and stable even for a large number of collocation points. The leaching of the solute from the fibers into the bulk liquor accompanies the displacement and the sorption phenomena continue for some time. Simulations are carried out using industrial data and it is found that for a more realistic investigation, the nonlinear isotherm should be preferred over the linear one.

NOMENCLATURE

A_0 :Langmuir constant (1/s)
B_0 :Langmuir constant (m^3/kg s)
c : Concentration of the solute in the liquor (kg/m^3)
C_i : Concentration of the solute in the vat (kg/m^3)
C_S : Concentration of the solute in the wash liquor (kg/m^3)
C_F : Fiber consistency (kg/m^3)
D_L : Longitudinal dispersion coefficient (m^2/s)
K : Mass transfer coefficient (dimensionless)
k_1, k_2 : Mass transfer coefficients (1/s)
L : Cake thickness (m)
n : Concentration of solute on the fibers (kg/m^3)
N_i : Initial concentration of solute on the fibers (kg/m^3)
t : Time (s)
u : Velocity of liquor in the mat (m/s)
z : Variable cake thickness (m)

Greek symbols:

ε : Total average porosity (dimensionless)
μ : Ratio of porosities (dimensionless)
ξ : Dimensionless distance (dimensionless)
τ : Dimensionless time (dimensionless)

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