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Mathematical modeling of pulp washing on rotary drums and their numerical solution for various adsorption isotherms

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Abstract. The mechanism of the displacement washing of the bed of pulp fibers is mathematically modeled by the basic material balance equation. Linear as well as non-linear adsorption isotherms are used to describe the relationship between the concentration of the solute in the liquor and concentration of the solute on the fibers. In the present study, the numerical solutions are obtained of pulp washing model with different adsorption isotherms. For the numerical solution "pdepe" solver in MATLAB is applied on the axial domain of the system of partial differential equations. Numerical results thus obtained are compared with earlier workers analytically and numerically. The comparison shows that results are in good agreement with both analytically as well as numerically and also show the suitability of the isotherm coupling with the washing model. The technique used in the present investigation is simple, elegant and convenient for solving two point boundary value problems with varying range of parameters.

Keywords: MATLAB: "pdepe" solver, pulp washing model, Peclet number, adsorption isotherm, brown stock washer

1 Introduction

Modeling of pulp washing is done mainly using three approaches namely (a) Process modeling (b) Physical modeling (c) Statistical modeling. In process modeling approach, each stage in pulp washing operation is treated as black box. Using material balances, process models express the efficiency of an individual washing stage in terms of some performance parameters such as Displacement Ratio, Norden Efficiency Factor, and Equivalent Displacement Ratio. Although these models are useful for routine process design calculations, but provide little information as to how the design or operation of a washer improves its efficiency. A complete review of the various process models used so far describing the pulp washing process has been presented by [13]. Physical models describe the washing operation in terms of fundamental fluid flow and mass transfer principles, occurring at microscopic level during displacement washing of a fibrous bed. These models involve parameters such as longitudinal dispersion coefficient and mass transfer coefficients. Physical models proposed by various investigators such as [2, 3, 9, 10, 14–16] has been classified based on mass transfer principles of two types (1) Differential contact models (macroscopic). (2) Dispersion models (macroscopic). [10] have studied the effect of longitudinal diffusion in ion exchange and chromatographic columns and obtained differential equation for the wash liquor. [2] studied the washing of filter cake by neglecting the accumulation capacity of fibers and assumed that the phenomena of longitudinal mixing and obtained model in terms of the differential equation.

[16] has described the overall movement of solute in the bed of non porous granular material with the diffusion like differential equation by replacing molecular diffusion coefficient with longitudinal dispersion coefficient as molecular diffusion coefficient was found very small as compared to longitudinal dispersion coefficient. An additional term was used to account for the accumulation (or depletion) capacity of material

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sorbed by the solids. [14] has studied the longitudinal dispersion of solute, intra particle diffusion of solute and liquid phase mass transfer for the particles of cylindrical and spherical geometry by using a modified step function input. [9] neglected the longitudinal dispersion coefficient to study Sodium Chloride washing and obtained differential equation for the wash liquor. [3] has divided the packed bed of cellulose fibers into three different zones namely zone of flowing liquor, stagnant liquor and fibers. Longitudinal dispersion and mass transfer in the flowing liquor zone is characterized by the differential equation. [15] had taken the model equation without considering the effect of longitudinal dispersion coefficient.

Most of the researcher described the washing model by coupling the transport equation with various adsorption isotherms to describe the relationship between the concentration of the solute in the liquor and concentration of the solute on the fibers. [3, 11, 14, 16, 18] have considered the linear or non linear adsorption isotherm equations along with the dispersion diffusion based transport equations.

In the present study dispersion diffusion based transport equations of pulp washing are developed based on the assumptions of [14, 16] coupled with the equation of mass transfer i.e. Fick's second law of diffusion. The equations are coupled with many other fluid mechanical parameters and finally eight set of models differing in various adsorption isotherms given by [10, 15, 16] and Langmuir isotherm along with varying boundary and initial conditions applicable to rotary vacuum brown stock washer are obtained. The above mentioned mathematical models of two simultaneous partial differential equations with various boundary conditions are extremely intricate in nature and practically appear to be unsolvable even by using sophisticated numerical techniques. It is important to mention that the problem with its simplified version has been solved analytically by [2, 7] using Laplace transform and numerically using Orthogonal Collocation by [1, 3]. [8] attempted to solve the washing model using Finite difference method. All these methods are very complex and time consuming.

Similar problem for a single stage advection-dispersion washing has been solved recently by [17] by pdepe solver easily by using much less time and give the similar results as analytical solution given by [2]. The present work focuses on the mathematical model for pulp washing and describing the washing theory based on linear as well as non linear adsorption isotherm. Further an attempt has been made for obtaining the solution of such types of models in dimensionless form through 'pdepe' solver in MATLAB source code by using the data of [3] for sodium specie Na+ in brown stock pulp.

2 Description of mathematical models

To develop the model for this zone is rather complex. In fact most of the investigators such as [1–3, 5–7, 9–15, 18] differ in their proposed model for this zone. In the present investigation an attempt has been made to describe the detailed model for washing zone of a rotary drum washer compatible with the practical system.

The mat of pulp fibers can be assumed to be stationary packed bed of homogeneous symmetrical cylindrical fibers. Instantaneous behavior of any system of this type can only be expressed by an equation involving the variables and their partial derivatives. Using simple material balance for setting up a differential equation, consider a thin slice of a filter cake (pulp mat) as shown in Fig. 1, through which filtrate or wash water flows.

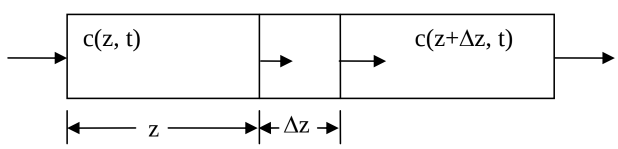

Fig. 1. A simple shell balance

Material balance across the simple shell given in Fig. 1, in the z direction can be written as:

Rate of Mass of solute in + Rate of Mass production by chemical reaction = Rate of Mass out + Rate of Mass Accumulation in the liquid phase + Rate of Mass Accumulation in the solid phase due to Adsorption-Desorption.

If A' is the area of the bed, ε_t, the total average porosity (sum of porosities in the displaceable liquid ε_d and in the immobile phase ε_s), μ, the velocity of the liquor in the mat, c, the concentration in the liquid phase, the equation in one dimension can be written as:

$$(uc\varepsilon_t A')_{z,t} - (uc\varepsilon_t A')_{z+\Delta z,t} = \left[\frac{\partial}{\partial t}\{c\varepsilon_t A'\Delta z + n(1-\varepsilon_t)A'\Delta z\}\right]_{\overline{z},t}, \tag{1}$$

where $z < \overline{z} < z + \Delta z$. Taking εt and A' as constant and taking the limit as $\Delta z \to 0$, one can obtain the following expression,

$$-\varepsilon_t c\left(\frac{\partial u}{\partial z}\right) = \varepsilon_t u\left(\frac{\partial c}{\partial z}\right) + \varepsilon_t\left(\frac{\partial c}{\partial t}\right) + (1-\varepsilon_t)\left(\frac{\partial n}{\partial t}\right). \tag{2}$$

The above equation contains principally two accumulation terms, one related to dispersion-diffusion and another related to adsorption-desorption. Other terms are velocity gradient and convective flow terms. Using Fick's second law of diffusion, i.e.

$$-c\left(\frac{\partial u}{\partial z}\right) = (D_L + D_V)\left(\frac{\partial^2 c}{\partial z^2}\right), \tag{3}$$

the following equation is obtained,

$$(D_L + D_V)\left(\frac{\partial^2 c}{\partial z^2}\right) = u\left(\frac{\partial c}{\partial z}\right) + \left(\frac{\partial c}{\partial t}\right) + \frac{(1-\varepsilon_t)}{\varepsilon_t}\left(\frac{\partial n}{\partial t}\right). \tag{4}$$

According to [16] the longitudinal dispersion coefficient DL is a function of flow pattern within the bed (unless very low flow rates are used). The molecular diffusion coefficient DV is very small compared to DL and so may be neglected. Writing $(1-\varepsilon_t)/\varepsilon_t$ as μ for convenience, the equation (iv) may be written as:

$$D_L\left(\frac{\partial^2 c}{\partial z^2}\right) = u\left(\frac{\partial c}{\partial z}\right) + \left(\frac{\partial c}{\partial t}\right) + \mu\left(\frac{\partial n}{\partial t}\right). \tag{5}$$

This is a non homogeneous, non linear, first degree, second order, parabolic, partial differential equation. Here μ, ε_t and D_L are functions of z while c and n are functions of both z and t. As the lumen of the fiber is porous and the same is true with the wall of the fiber, the porosity values for these cases are different from the porosity of the interfiber mass. Therefore three porosity values are required to represent the pulp mat system. It is extremely difficult to distinguish precisely between the values of porosity at the lumen and at the wall. Therefore, for practical calculations these are assumed to be the same. Hence, to describe the system two porosity values are assumed, one for the interfibers εd and another for intrafibers ε_s, so that $\varepsilon_d + \varepsilon_s = \varepsilon_t$, the total porosity for the entire system. The model Eq. (5) is same as dispersion model for pulp washing given by [14, 16].

2.1 Adsorption isotherms

The details of the adsorption isotherms which are used in the present investigation are as follows. [10] used the adsorption isotherm given by:

$$\frac{\partial n}{\partial t} = k_1 c - k_2 n \tag{6}$$

and assumed that the rate of adsorption is finite and plotted the effect of longitudinal diffusion for an infinite column in which equilibrium is established locally. Initial adsorbate concentration was assumed to be zero.

[16] used the adsorption of diacetyl solution by porous viscous fibers with simple isotherm equation i.e.

$$n = kc \quad \text{or} \quad \frac{\partial n}{\partial t} = k\frac{\partial c}{\partial t} \tag{7}$$

and assumed the liquid solid concentration inside the fibers and surrounding the fibers to be identical at any time and at any position within the bed, implying that diffusion, both within the fiber and between the fiber and the surrounding fluid is sufficiently rapid which does not affect the rate of the overall transport process.

[15] used the isotherm equation i.e.

$$\frac{\partial n}{\partial t} = k(c - n), \tag{8}$$

the diffusion of the solute within the fibers towards the washing liquor is described by a partial differential Eq. (8), which is solved assuming that the mass transfer rate through the stagnant film is finite.

Langmuir adsorption isotherm is assumed to describe the relationship between the concentration of the solute in the liquor and concentration of the solute on the fibers as:

$$N = \frac{Ac}{1 + Bc}, \tag{9}$$

where A and B are Langmuir constants.

2.2 Initial and boundary conditions

Initial and boundary conditions are used in the present investigation are given below. Initial condition is: $c(z,t) = C_0$, $n(z,t) = N_0$ at $t = 0$, $z \in (0, L)$. Boundary condition at the inlet of the bed is:

$$uc - D_L \frac{\partial c}{\partial z} = uC_s, \quad \text{at} \quad z = 0 \quad \text{for all} \quad t > 0. \tag{10}$$

[15] give the boundary condition at the inlet of the bed:

$$c = C_s, \quad \text{at} \quad z = 0 \quad \text{and} \quad t > 0. \tag{11}$$

Boundary condition at bed exit is given by:

$$\frac{\partial c}{\partial z} = 0, \quad \text{at} \quad z = L \quad \text{and} \quad t > 0. \tag{12}$$

Thus in the present investigation two cases arise for two different boundary conditions at inlet of the bed given by (10) and (11) together with bed exit (6). Thus the set of eight models is obtained for the solution with two different boundary conditions as depicted in Tab. 1.

2.3 Dimensionless models

Before solution, models are converted into dimensionless form by using certain dimensionless parameters like Peclet number (or Bodenstein number), dimensionless time, dimensionless thickness and dimensionless concentration given below. All models with respective boundary and initial conditions in dimensionless form are given in Tab. 1. For all models, $\mathrm{Pe} = \frac{uL}{D_L}$ & $Z = \frac{z}{L}$.

Dimensionless Time, for all models except 5 & 6, $T = \frac{ut}{L}$;

For models 5 & 6, $T = \frac{ut}{(1+\mu k)L}$;

Dimensionless concentrations of solute in liquor, for first six models $C = \frac{c-C_s}{C_0-C_s}$;

Dimensionless concentrations of solute in fiber, for first four models $N = \frac{n-C_s}{C_0-C_s}$;

For models 1 & 3, $K = \frac{k_1}{k_2}$, $G = \frac{k_2 L}{u}$ and $H = \frac{(K-1)C_s}{C_0-C_s}$;

For models 2 & 4, $K = 1$, $G = \frac{kL}{u}$ and $H = 0$;

For models 7 & 8 (Langmuir adsorption isotherm);

$$C = \frac{c}{C_0}, N = \frac{n}{N_0}, \quad \text{and} \quad \mu' = \frac{\mu N_0}{C_0}.$$

Table 1. Existing mathematical models for washing zone used in present investigation (dimensionless form)

S. No.	Transport Equation	Adsorption Isotherm (dimensionless form)	Boundary Conditions (dimensionless form)
1	$\partial^2 C/\partial^2 Z = \mathrm{Pe}(\partial C/\partial Z + \partial C/\partial T + \mu\partial N/\partial T)$	$\partial N/\partial T = G(H + KC - N)$	$C(0,T) = 0$ for $T > 0$, & $\partial C/\partial Z = 0 (Z = 1)$
2	$\partial^2 C/\partial^2 Z = \mathrm{Pe}(\partial C/\partial Z + \partial C/\partial T + \mu\partial N/\partial T)$	$\partial N/\partial T = G(C - N)$	$C(0,T) = 0$ for $T > 0$, & $\partial C/\partial Z = 0 (Z = 1)$
3	$\partial^2 C/\partial^2 Z = \mathrm{Pe}(\partial C/\partial Z + \partial C/\partial T + \mu\partial N/\partial T)$	$\partial N/\partial T = G(H + KC - N)$	$\partial C/\partial Z = \mathrm{Pe}\, C$ for $(Z = 0, T > 0)$ & $\partial C/\partial Z = 0 (Z = 1)$
4.	$\partial^2 C/\partial^2 Z = \mathrm{Pe}(\partial C/\partial Z + \partial C/\partial T + \mu\partial N/\partial T)$	$\partial N/\partial T = G(C - N)$	$\partial C/\partial Z = \mathrm{Pe}\, C$ for $(Z = 0, T > 0)$ & $\partial C/\partial Z = 0 (Z = 1)$
5.	$\partial^2 C/\partial^2 Z = \mathrm{Pe}(\partial C/\partial Z + \partial C/\partial T + \mu\partial N/\partial T)$	$\partial N/\partial T = K\partial C/\partial T$	$C(0,T) = 0$ for $T > 0$, & $\partial C/\partial Z = 0 (Z = 1)$
6.	$\partial^2 C/\partial^2 Z = \mathrm{Pe}(\partial C/\partial Z + \partial C/\partial T + \mu\partial N/\partial T)$	$\partial N/\partial T = K\partial C/\partial T$	$\partial C/\partial Z = \mathrm{Pe}\, C$ for $(Z = 0, T > 0)$ & $\partial C/\partial Z = 0 (Z = 1)$
7	$\partial^2 C/\partial^2 Z = \mathrm{Pe}(\partial C/\partial Z + \partial C/\partial T + \mu\partial N/\partial T)$	$NN_0 = AC_0C/(1 + BC_0C)$	$C(0,T) = 0$ for $T > 0$, & $\partial C/\partial Z = 0 (Z = 1)$
8	$\partial^2 C/\partial^2 Z = \mathrm{Pe}(\partial C/\partial Z + \partial C/\partial T + \mu\partial N/\partial T)$	$NN_0 = AC_0C/(1 + BC_0C)$	$\partial C/\partial Z = \mathrm{Pe}\, C$ for $(Z = 0, T > 0)$ & $\partial C/\partial Z = 0 (Z = 1)$

3 Solution of mathematical models using-matlab source code

The mathematical model of pulp washing given by Eq. (5) together with the corresponding equations of linear as well as non-linear isotherms given in Tab. 1 (Dimensionless form) with various boundary conditions is extremely intricate in nature and practically appears to be unsolvable even by using sophisticated numerical techniques. It is important to mention that the problem with its simplified version has been solved analytically by [2, 7] using Laplace transform and numerically using Orthogonal Collocation by [1, 3]. [8] attempted to solve the washing model using Finite difference method. All these methods are very complex and time consuming. Models based on two simultaneous partial differential equations make the solution procedure more complex. Application of such solution techniques in control systems is not possible due to the more processing time and involvement of high mathematical skills at operator level.

Table 2. Dimensionless concentration for all Models for corresponding value of dimensionless time

Dimensionless Time	Model-1	Model-2	Model-3	Model-4	Model-5	Model-6	Model-7	Model-8
0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.1	0.9999	1.0000	0.9999	1.0000	1.0000	1.0000	1.0000	1.0000
0.2	0.9998	1.0000	0.9998	1.0000	1.0000	1.0000	1.0000	1.0000
0.3	0.9997	1.0000	0.9997	1.0000	1.0000	1.0000	1.0000	1.0000
0.4	0.9996	1.0000	0.9996	1.0000	1.0000	1.0000	1.0000	1.0000
0.5	0.9991	0.9996	0.9991	0.9996	1.0000	1.0000	0.9992	0.9992
0.6	0.9947	0.9953	0.9948	0.9954	0.9998	0.9998	0.9921	0.9922
0.7	0.9713	0.9719	0.9714	0.9720	0.9984	0.9985	0.9566	0.9568
0.8	0.8941	0.8948	0.8943	0.8950	0.9915	0.9916	0.8533	0.8535
0.9	0.7294	0.7300	0.7297	0.7303	0.9680	0.9681	0.6602	0.6605
1.0	0.4894	0.4899	0.4897	0.4901	0.9089	0.9091	0.4154	0.4155
1.1	0.2462	0.2465	0.2464	0.2467	0.7963	0.7965	0.1964	0.1965
1.2	0.0775	0.0776	0.0775	0.0776	0.6283	0.6285	0.0581	0.0581

For control purpose the transient behavior of the solute concentration in the black liquor is of more interest, rather than solute concentration in fiber, so that the value of $\partial N/\partial T$ from adsorption isotherm, substituted in the equation of flow (Transport equation) both are given in Tab. 1 and an attempt has been made to solve these equations directly by using "pdepe" solver in MATLAB source code. This technique is simple, elegant

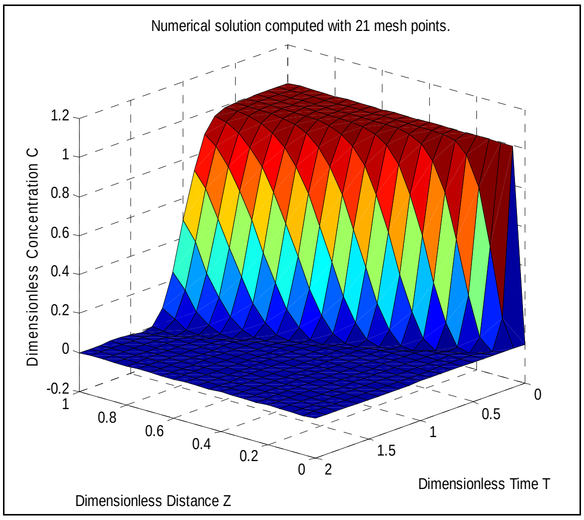

Fig. 2. Solution of Model-1

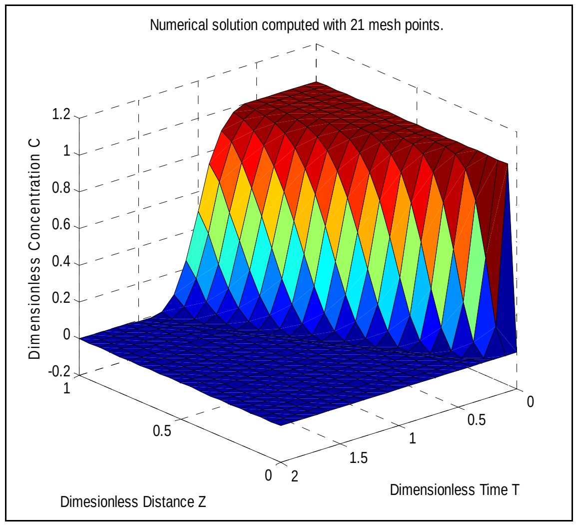

Fig. 3. Solution of Model-2

and convenient for solving to a non-mathematician also. For simulation, data of [4] for the specie sodium (Na^+) is used. The solutions of each equation are obtained by taking 21 mesh points which are shown in the figures for corresponding values of Z and T and also find out the solutions at dimensionless distance $Z = 1$ and so the value of $C(1, T)$ are shown in Tab. 2 for corresponding values of dimensionless time T.

4 Results and discussion

As mentioned earlier in our previous work [17], we compare the solution of simple advection-dispersion washing problem (without adsorption isotherm) with the analytical results of [2]. The results are similar to the analytical results. In the present work linear as well as non-linear isotherm are coupled with the transport equation and then an attempt has been made to solve these washing models. The results at dimensionless distance at $Z = 1$ for different values of dimensionless time, are obtained and given in Tab. 2. The results are in good agreement with the earlier workers. In the present investigation transportation equations of all models

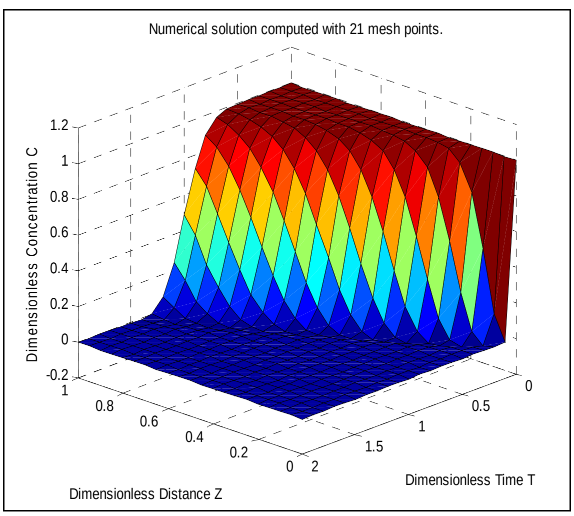

Fig. 4. Solution of Model-3

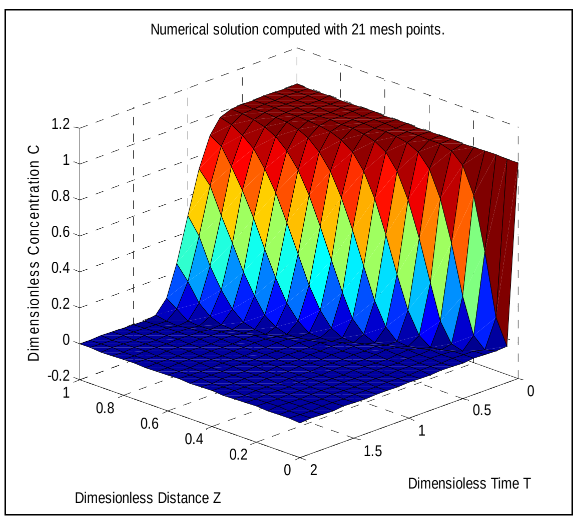

Fig. 5. Solution of Model-4

are same and also the behavior of the dimensionless concentration with respect to the dimensionless time and dimensionless distance of all models are similar which are depicted by the Fig. 2 to Fig. 9 respectively. For

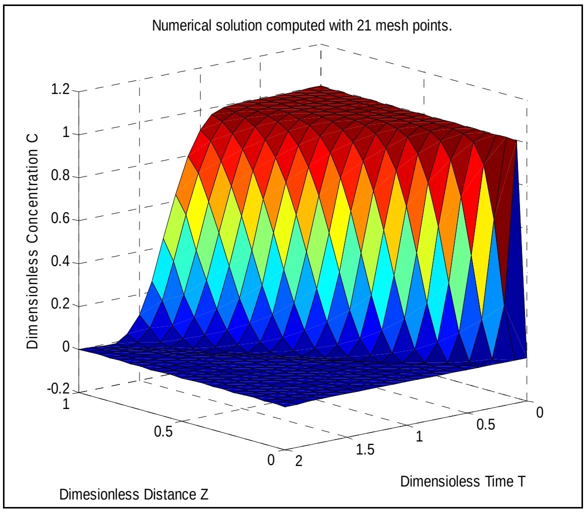

Fig. 6. Solution of Model-5

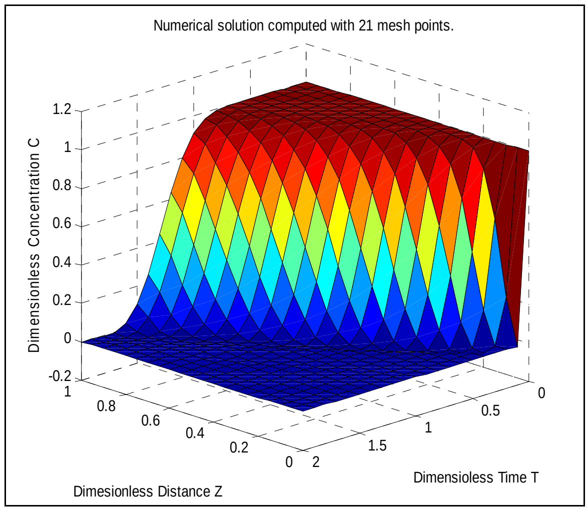

Fig. 7. Solution of Model-6

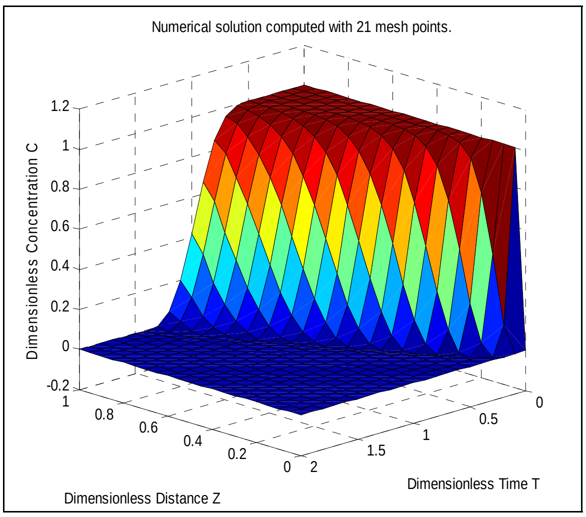

Fig. 8. Solution of Model-7

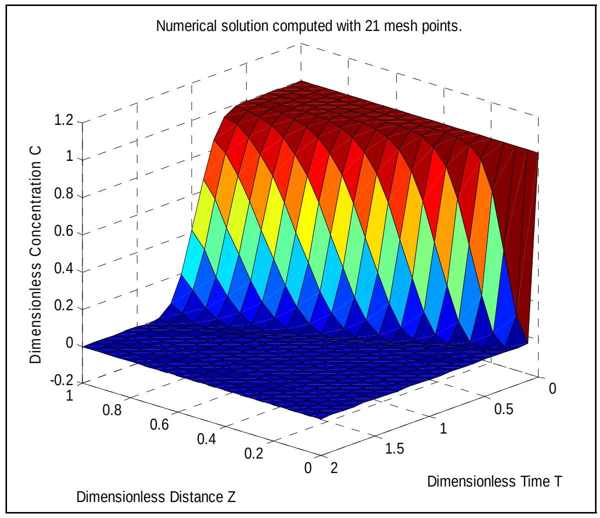

Fig. 9. Solution of Model-8

obtaining much accurate solution of the above mentioned washing models, dimensionless bed depth as well as dimensionless time is divided into 21 equal parts and then the influence of these parameters (Z and T) on C is estimated. The behaviors of exit solute concentration with respect to time as well as variable cake thickness are shown by 3-D graphs. It is clear from figures that the dimensionless concentration of the solute in the liquor decreases with the increase of the dimensionless time, whereas increases with the increase in the dimensionless distance, which is same as obtained by earlier workers[1–3, 8]. Thus it is observed that with change in the cake thickness & time significant changes occur in the concentration profiles.

It is also important to mention that the models 5 & 6 with same transport equation and adsorption isotherm given by [16] are differ with boundary conditions give slightly different results up to dimensionless time $T = 0.8$ but when dimensionless time goes up to $T = 0.9$ to 1.2 results are different from other models and this range is not valid as mentioned by some earlier workers such as [2, 3]. This concludes that the adsorption isotherm given by [16] is not suitable for the development of pulp washing model.

5 Conclusions

These investigations are based on mathematical models derived for washing zone of a rotary vacuum washer in Paper Industry. Linear as well as non-linear (Langmuir isotherm) adsorption isotherms are used to describe the relationship between the concentration of the solute in the liquor and concentration of the solute on the fibers. The numerical results are obtained for the solution of the above mathematical model by using "pdepe" solver in MATLAB source code. For simulation, data of [4] for the specie sodium (Na^+) is used. The following conclusions may be drawn from the present study.

(1) Rate of Mass Accumulation in the solid phase due to Adsorption-Desorption is taken into consideration for evaluation of the solute concentration in the fiber the isotherm given by [10, 15] and non linear Langmuir are best suitable for the satisfactory performance;

(2) If we consider the adsorption isotherm given by [16] then the solution gives erratic values of solute concentration, which are not acceptable, so it may be concluded that the development of pulp washing model is not possible with this isotherm;

(3) Pdepe solver can be used successfully for the solution of pulp washing model;

(4) The pdepe solver used in the present investigation is simple, elegant and convenient for solving two point boundary value problems with varying range of parameters and show a comparable performance with QUICK method in terms of CPU time and average numerical errors;

(5) The algorithms in this solver are easy to set up, and so the method represents an advantage and good alternative to the available techniques for such type problems.

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Appendix

A'	: Surface area of bed, m^2;	D_v	: Molecular diffusion coefficient, m^2/s;
c	: Concentration of the solute in the liquor, kg/m^3;	A, B	: Langmuir constants;
C_0	: Concentration of solute inside the vat, kg/m^3;	L	: Cake thickness, m;
N_0	: Amount of solute accumulated on the fiber suface;	Z	: Dimensionless Distance;
C_s	: Concentration of solute in the wash liquor, kg/m^3;	t	: Time, s;
D_L	: Longitudinal dispersion coefficient, m^2/s;	T	: Dimensionless Time;
n	: Concentration of solute on fibers, kg/m^3;	z	: Variable cake thickness, m;
C	: Dimensionless Concentration of solute in the liquor;	u	: Liquor speed in cake pores, m/s;
N	: Dimensionless Concentration of solute in the fiber;	Δz	: Small increment in cake thickness, m.