Hermite Collocation Method for General Mathematical Modelling for Displacement Washing Of Pulp Fibers

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Abstract

Hermite collocation method has followed for numerical solution of general mathematical model in two dimensional based on particle and fluid phase. Langmuir isotherm has been used to relate fluid-solid interface. Computed results are analyzed by compared with other numerical methods as well as literature data for different values of parameters. The effect of different parameters such as Peclet number, Bed porosity, ψ, displacement ratio has been shown by different graphs. The error of these results is analyzed.

Keywords: Hermite collocation method, Peclet number, Bed porosity, ψ, Displacement ratio

I. INTRODUCTION

The understanding of fluid flow and transport processes in porous medium is very essential for many applications in science and technology. A porous medium may be defined as a structure comprises of pore space from where the fluid is allowed to flow. It is possible for this medium to be filled with one or more fluids. The common examples of porous medium are sponge, cemented sandstone, karstic limestone, soil, sand, foam rubber, bread etc. The concept of porous medium is largely used in the chemical and process industries. Several effective and economical strategies of refinement and improvement of porous medium have been developed. These strategies enjoy wide spread acceptance and recognition. These improvement procedures and strategies primarily involve the separation of gears combination by dissolving one or a lot of them from process mixture. The most common method involve washing the mixture with a solvent, one or additional parts constitute the mixture are soluble while other part are insoluble (Khan et al. 2014, Ramirez et al. 2014).

One of such procedures is known as brownstock washing in which the dissolved inorganic chemical substances and organic material are separated from particle surface. The primary objective of this washing is to extract the residual liquor that might introduce impurities in the paste in the subsequent stages. Simultaneously, the purpose is also to recover the precious dissolved substances. The recovered organic and inorganic substances are used for the regeneration of the weak black liquor. This helps to the carryover of weak black liquor into the bleach plant.

In the washing operation, spray showers spread the washing fluid to displace the liquor present in the cake (Kukreja and Ray (2000)). If the washing is carried out using an excess of wash water, the energy efficiency and the production capacity of the recovery system are reduced (Arora and Potucek (2008), Kukreja and Ray (2009)). In the case of real or ideal washing, the minimum volume of washing water for complete washing is equal to the volume of liquor initially between the particles. The real washing process is far from the ideal conditions of washing due to axial dispersion or back mixing, non uniformity of pores, the structure of the cake is heterogeneous and longitudinal mixing with diffusion takes place. During washing process only 30% to 86% of the preserved filtrate can be removed by displacement washing whereas ideal washing process needs 100% recovery of residual filtrate (Potucek and Skotnicova (2002)).

The purpose of the present study is to develop a mathematical model involving porous particle and to explain the behavior of fluid within the particle phase for finding out the washing behavior of the packed bed of solid particles having different particle geometries through axial dispersion, molecular diffusivity and intraparticle diffusion coefficient.

II. CUBIC HERMITE POLYNOMIALS

Hermite interpolating polynomials was first introduced by Charles Hermite (1822-1905). It is an extension of Lagrange interpolating polynomials as in Hermite interpolating polynomials, both the function and its derivative are to be assigned values at interpolating point. An nth-order Hermite polynomial in x is a polynomial of order 2n+1 and therefore, cubic Hermite interpolating polynomials particular case of general Hermite interpolating polynomials for n=1. It consists of two node points and two tangents in cubic polynomial and defined as

$$H_1(x) = 2x^3 - 3x^2 + 1 \quad H_2(x) = x^3 - 2x^2 + x$$

$$H_3(x) = -2x^3 + 3x^2 \quad H_4(x) = x^3 - x^2$$

III. MATHEMATICAL MODEL

In the present study, axial dispersion model has been proposed that is based on the material balance equation as shown in figure 1. These equations represent mathematical models for a number of physical processes related in the field of fluid dynamics, heat and mass transfer, dispersion – diffusion process, adsorption-desorption process, osmosis and many other areas. The mathematical formulation has been described by one or more of the principle of conservation of mass using Fick's law for diffusion (J = -D ∂C/∂x).

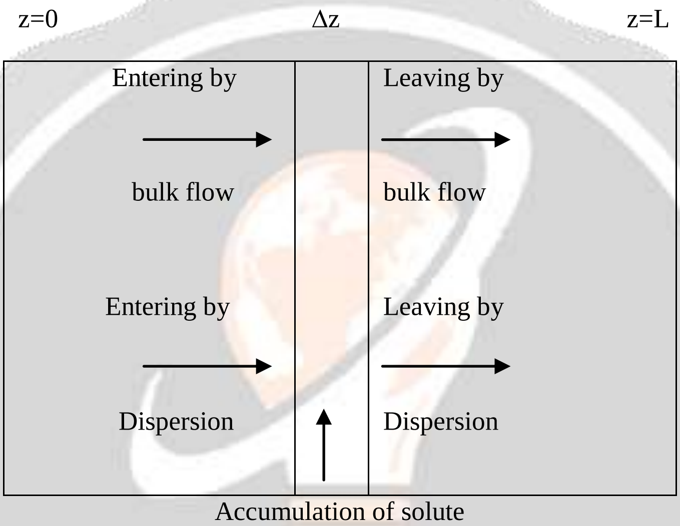

Figure 1: Material balance equation

IV. MATHEMATICAL DEVELOPMENT

Flow of fluid through bed is described by bulk or external fluid concentration $c(z,t)$. Concentration of solute adsorbed on particle surface and intrapore solute concentrations are described by $n(z,t)$ and $q(z,t)$, respectively. Particle and bed porosities are described by β and ε, respectively. The unsteady state transient partial differential equations describing the behavior of fluid flow through the bed are described as:

Mathematical formulation for particle phase

$$\frac{\partial q}{\partial t} + \frac{1-\beta}{\beta}\frac{\partial n}{\partial t} = \frac{D_f}{KR^2}(c-q) \tag{1}$$

Adsorption isotherm

Langmuir adsorption isotherm has been followed to relate the intraparticle and interparticle solute concentrations:

$$\frac{\partial n}{\partial t} = \frac{k_1 q}{C_0} - k_2 n \tag{2}$$

Deposition rate constant k_1 is of second order in forward direction and detachment rate constant k_2 is of first order in backward direction. At equilibrium, equation (2) reduces to:

$$n = \frac{qN'}{k^* + \frac{q}{C_0}} \tag{3}$$

Model equations for bulk fluid phase

$$K\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial z} + \frac{a(1-\varepsilon)D_f}{\varepsilon R^2}(c-q) = D_L\frac{\partial^2 c}{\partial z^2} \tag{4}$$

Boundary conditions: $uc - D_L\frac{\partial c}{\partial z} = 0$ at $z = 0$ (5)

$\frac{\partial c}{\partial z} = 0$ at $z = L$ (6)

Initial condition: $c = q = C_0$ and $n = N_0$ at $t = 0$ (7)

The set of equations (1) to (7) is converted into dimensionless form using the non-dimensional variables given in nomenclature:

$$\frac{\partial Q}{\partial \tau} + \frac{1-\beta}{\beta}N'\frac{\partial N}{\partial \tau} = \frac{1}{\psi}(C-Q) \tag{8}$$

$$\frac{\partial N}{\partial \tau} = P^*\left[Q(1-N) - k^*N\right] \tag{9}$$

$$\frac{\partial C}{\partial \tau} = \frac{1}{Pe}\frac{\partial^2 C}{\partial \xi^2} - \frac{\partial C}{\partial \xi} - \frac{a\theta}{\psi}(C-Q) \tag{10}$$

Boundary conditions: $C - \frac{1}{Pe}\frac{\partial C}{\partial \xi} = 0$ at $\xi = 0$ (11)

$\frac{\partial C}{\partial \xi} = 0$ at $\xi = 1$ (12)

Initial condition: $C = Q = N = 1$ at $\tau = 0$ (13)

V. HERMITE COLLOCATION METHOD

Hermite collocation method is a numerical technique for solution of partial differential equations defined over the interval [0, 1]. It is a combination of orthogonal collocation method and cubic Hermite interpolating polynomials. A number of investigators have followed Hermite collocation in different forms to discretize different type of models such as Dyksen & Lynch (2000), Lang & Sloan (2002), Brill (2002), Rocca et al. (2005) & Pierce (2010), etc. In Hermite collocation method, the approximating function is discretized in terms of cubic Hermite polynomials and then orthogonal collocation is applied within each sub-domain of the global domain. Due to the continuity property of Hermite interpolating polynomials there is no need to assume that approximating function and its first derivative should be continuous at node points. Hermite collocation method has the property to transform the mixed collocation method into interior collocation method. Thus there is no need to approximate the function at the boundaries. Hermite collocation is considered for the discretization of second-order boundary value problems, the usual choice of Hermite is either quadratic or cubic at one or two collocation points. In the case of quadratic or cubic, Hermite collocation in second order problems, the computed approximations exhibit up to fourth order convergence (Prenter (1975), Sun (2000), Parand et al. (2010)).

VI. RESULTS AND DISCUSSIONS

To check the validity of the model on washing cell numerical results has been compared with Literature data has given by Arora and Potucek (2012). The numerical technique of HCM is compared with the OCM. The effect of different parameters is checked on solution profiles.

Effect of Peclet number

Peclet number is the ratio of convection to dispersion. In Figure 2, the theoretical effect of Peclet number on exit solute concentration profiles is shown for parameter ψ=0.1 and ε=0.671. It is observed in this case of Pe = 5, 10 the solution profiles are elongated and take large time to converge to zero. It indicates that indefinitely long time is evolved to wash out the impurities adsorbed on the fiber surface. For Pe = 50,100 the solution profiles converge to zero in comparatively less time. However, it is also observed that for *Pe*= 50 and 100 solution profiles converge to steady state condition almost on the similar time. Similarly in Figure 6,10 gives the theoretical behavior of the concentration profiles for small values of Peclet number varying within the range of 5 to 100 for a= 2,3. The only difference converging rate of breakthrough curves for a=1 more rapidly as compared with a=2, 3.

Effect of ψ

Ψ is the ratio of D_f/R^2 and u/L. In Figure 3 the effect of ψ is shown for Pe=20 and ε=0.690. It is observed from this figure that solution profiles converge to steady state condition rapidly for small values of Ψ=0.1 and 0.01 as compared to ψ=1. It is due to reason that for small values of ψ, more diffusion occurs and impurities are removed through the fiber pores having large size of pore radius. It results in better washing operation (Arora et. al. 2006).

Porosity of the Bed

The porosity is the most important and sensitive part of washing process. The porosity (ε) is defined as the ratio of the void volume to the total volume of the bed. The small change in the porosity of the packed bed leads to a big change in the pressure drop required for the fluid flow through the packed bed. Theoretical effect of bed porosity on solution profiles is checked for *Pe* = 15 and parameter ψ =0.5. Numerical values are presented graphically in Figure 4. It can be easily observed from this figure that with the increase in bed porosity ε from 0.5561 to 0.8120, solution profiles converge to steady state condition rapidly. It is due to the reason that with the increase in bed porosity, the volume of black liquor available for displacement also increases. It helps in leaching out the impurities adsorbed on particle surface more rapidly. Consequently, more effective washing operations can be achieved for high bed porosity.

Effect of different parameters (Pe, ψ and ϵ):

In figure 5 solution profiles are plotted for different values of Pe , ψ and ϵ. Peclet number (Pe) and ψ are controlled by the axial dispersion coefficient, which, in turn, depends upon the interstitial velocity. The effective bed porosity is a key factor in determination of the average interstitial velocity (Arora et al.2006). Therefore, the effect of the Peclet number and ψ on exit that better solute concentration is shown through bed porosity. It is found that the area under the curve for Pe= 20.81, ψ=0.55 and ϵ=0.6711, is slightly larger than Pe=12.25, ψ =0.4 and ϵ=0.6898 but both the breakthrough curves approaches to steady state condition within similar time interval. Similarly, values of Pe=16.92, ψ =0.5 and ϵ=0.5561 are higher than Pe=12.96, ψ =0.45 and ϵ=0.812, the bed porosity is very small, which implies that volume available for flow of fluid is very less. Therefore, breakthrough curves take a relatively longer time to converge the steady state condition. On the contrary, the bed porosity is highest and therefore, external fluid has large volume for flow. Solution profiles converge to steady state condition more rapidly. It has been found that better washing operations are achieved for higher bed porosity, if other factor remains the same.

Particle geometry:

Theoretical effect of particle geometry (a) on solution profiles is checked for *Pe* = 15 and parameter ψ =0.5. Numerical values are presented graphically in Figure 14. It is observed from this figure that solution profiles converge to steady state condition rapidly for a=1 as compared to a=2 or 3. Therefore accurate and reasonable results can be achieved for small value of a.

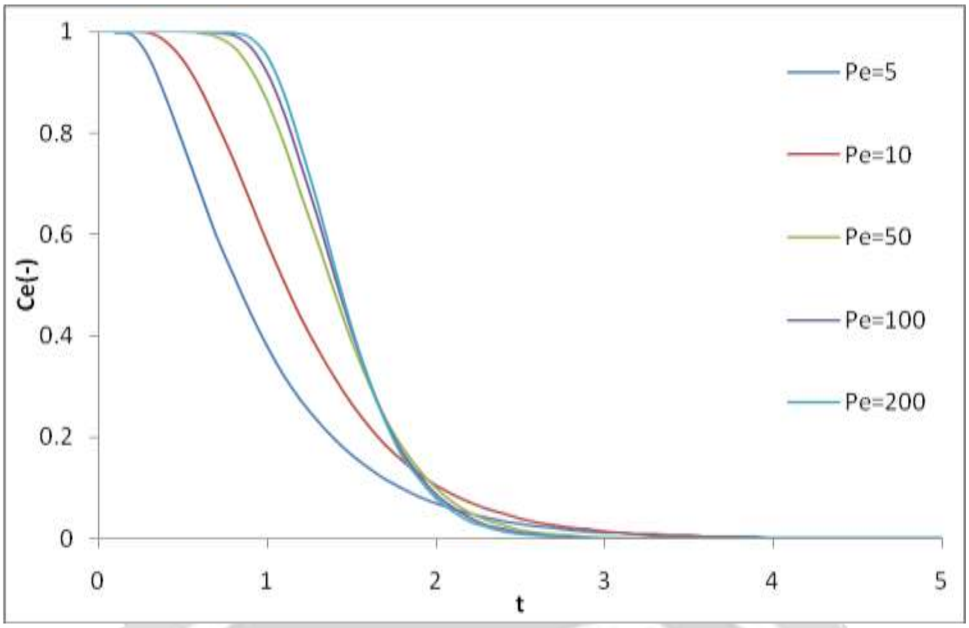

Figure 2: Behavior of solution profiles for varying values of Peclet number for a=1.

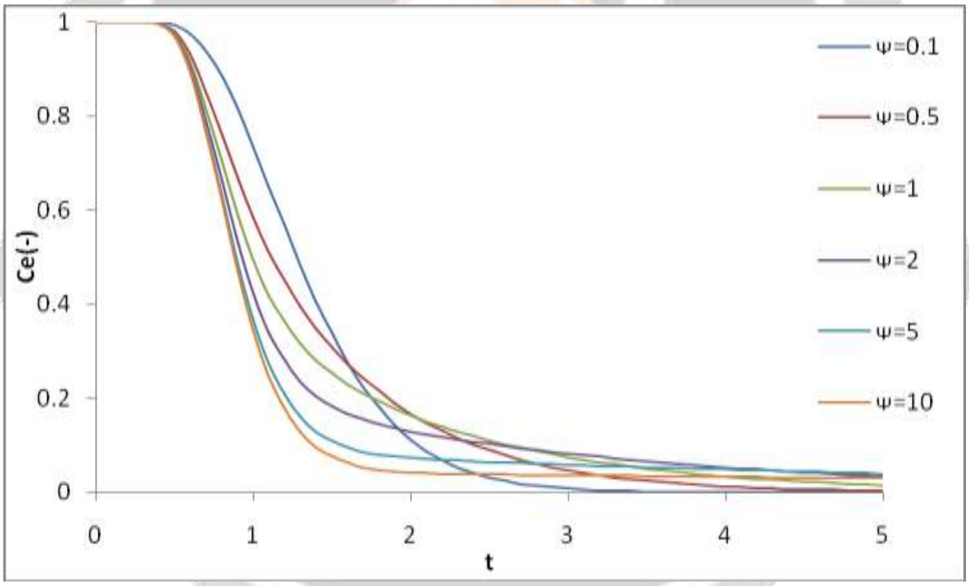

Figure 3: Behavior of solution profiles for varying values of parameter ψ for a=1

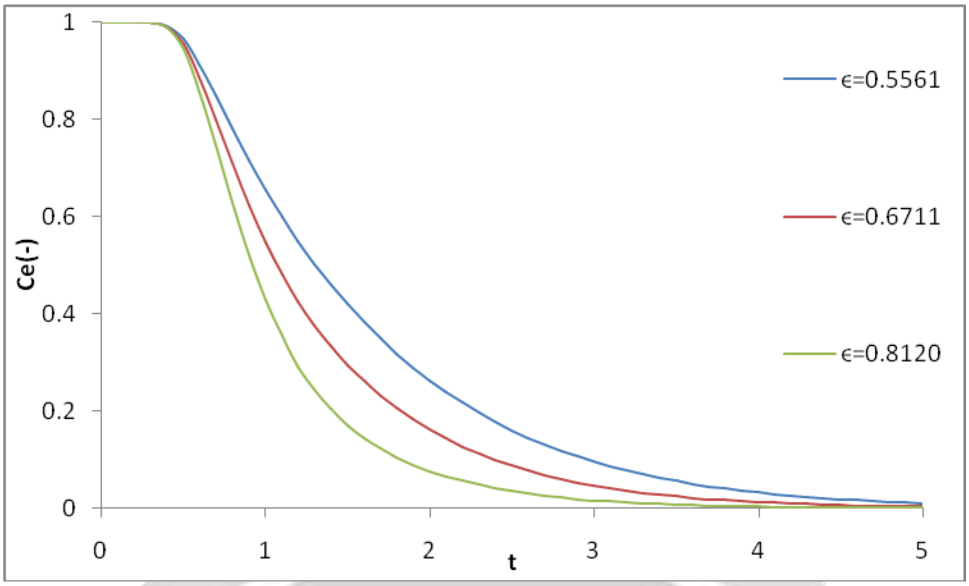

Figure 4: Behavior of solution profiles for varying values of bed porosity for a=1.

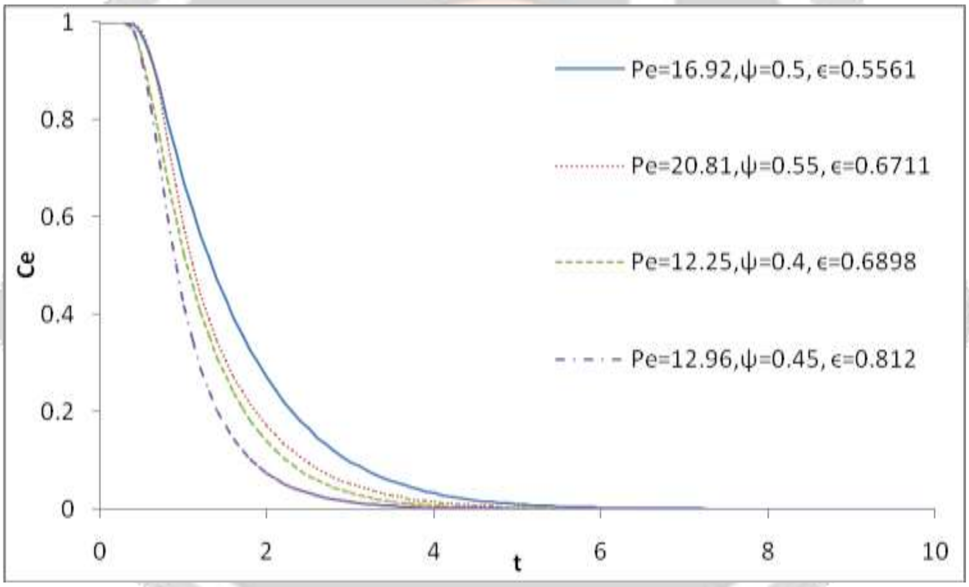

Figure 5: Behavior of solution profiles for varying values of P , ψ, ϵ for a=1.

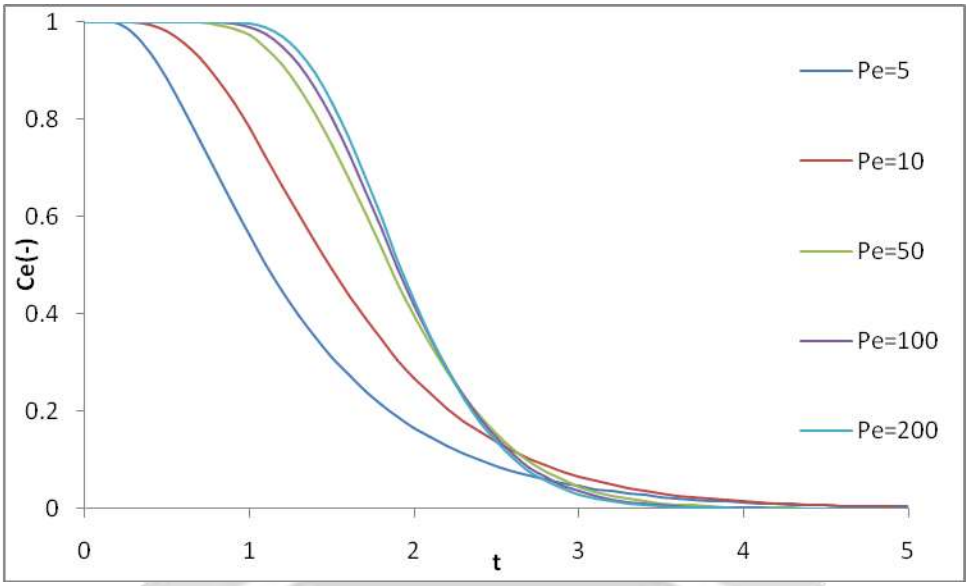

Figure 6: Behavior of solution profiles for varying values of Peclet number for a=2.

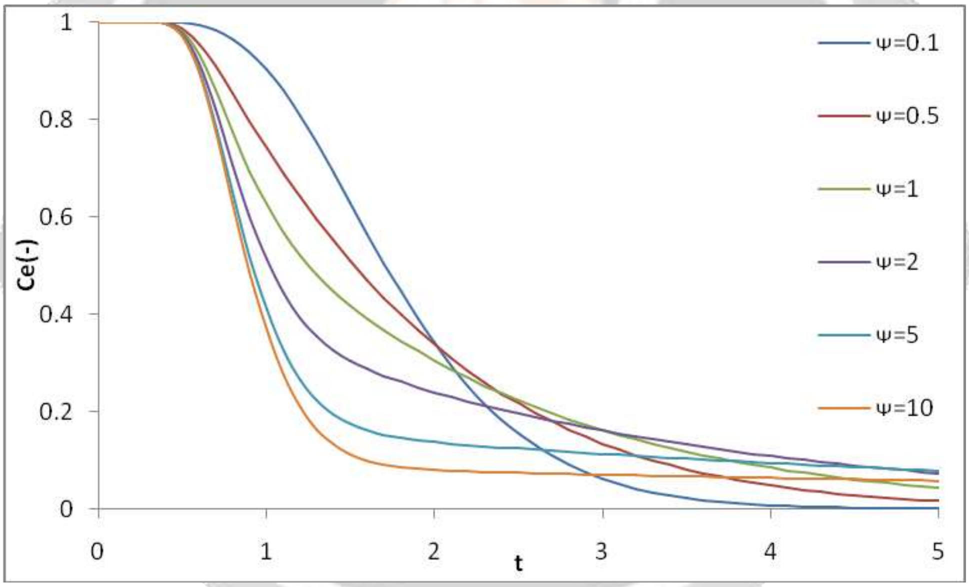

Figure 7: Behavior of solution profiles for varying values of parameter ψ for a=2.

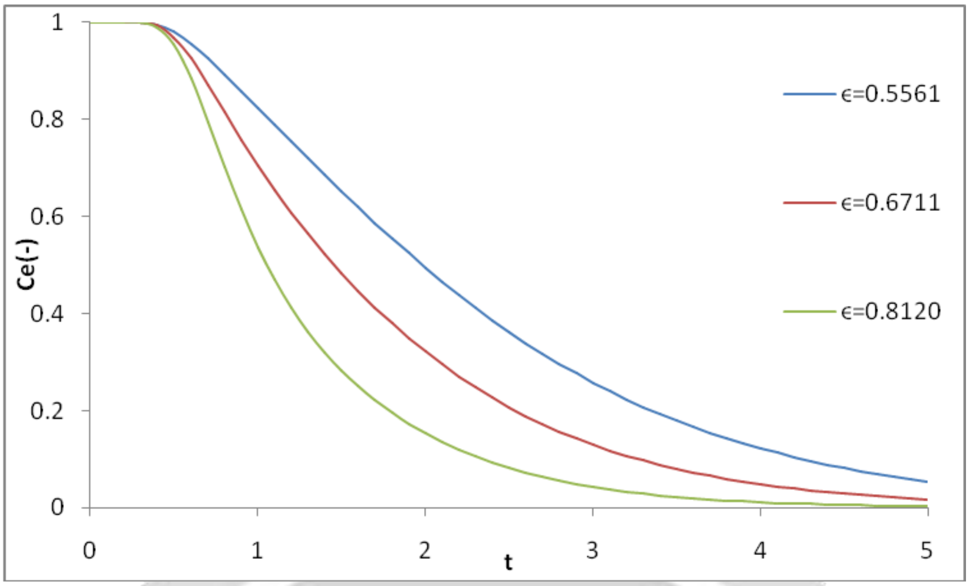

Figure 8: Behavior of solution profiles for varying values of bed porosity for a=2.

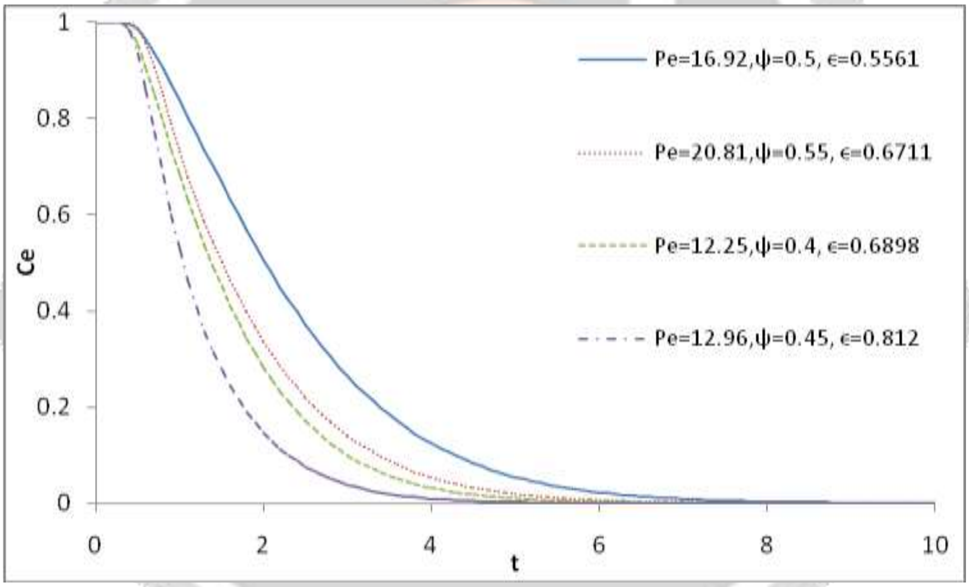

Figure 9: Behavior of solution profiles for varying values of P , ψ, ϵ for a=2.

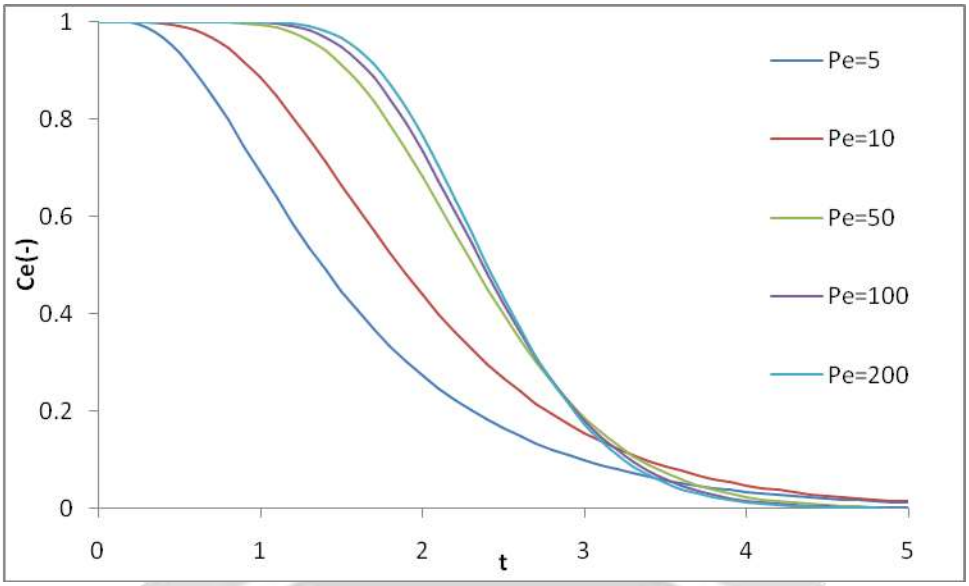

Figure 10: Behavior of solution profiles for varying values of Peclet number for a=3.

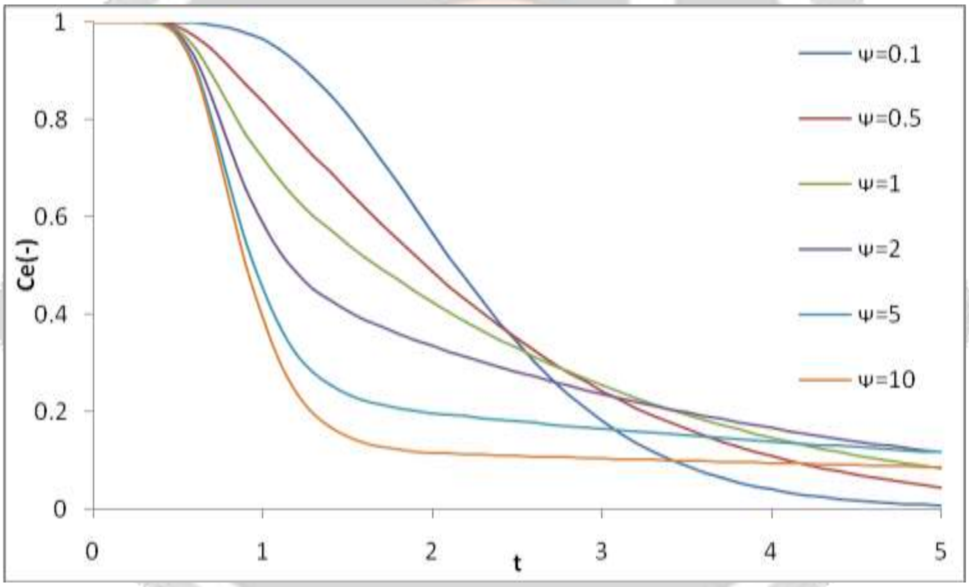

Figure 11: Behavior of solution profiles for varying values of parameter ψ for a=3.

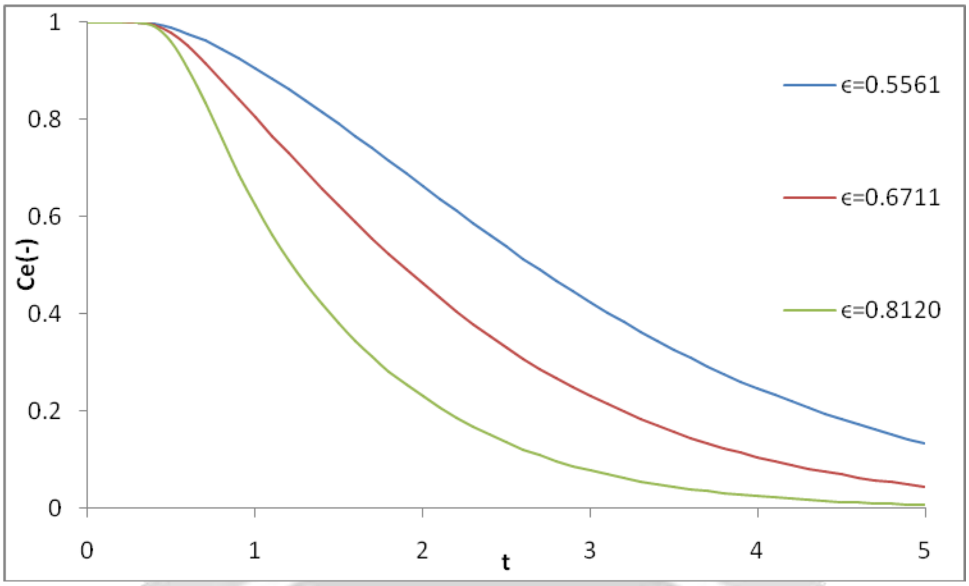

Figure 12: Behavior of solution profiles for varying values of bed porosity for a=3.

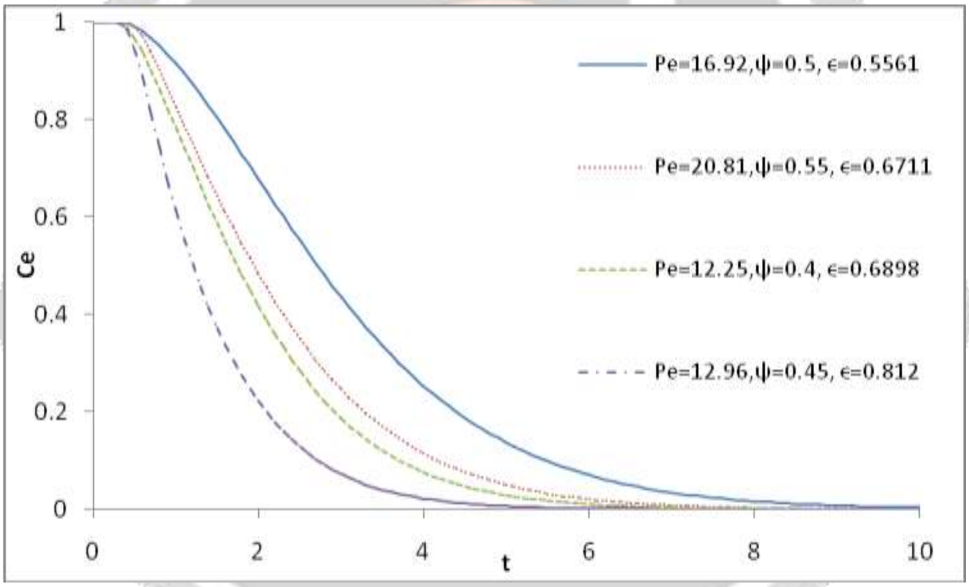

Figure 13: Behavior of solution profiles for varying values of P , ψ, ϵ for a=3.

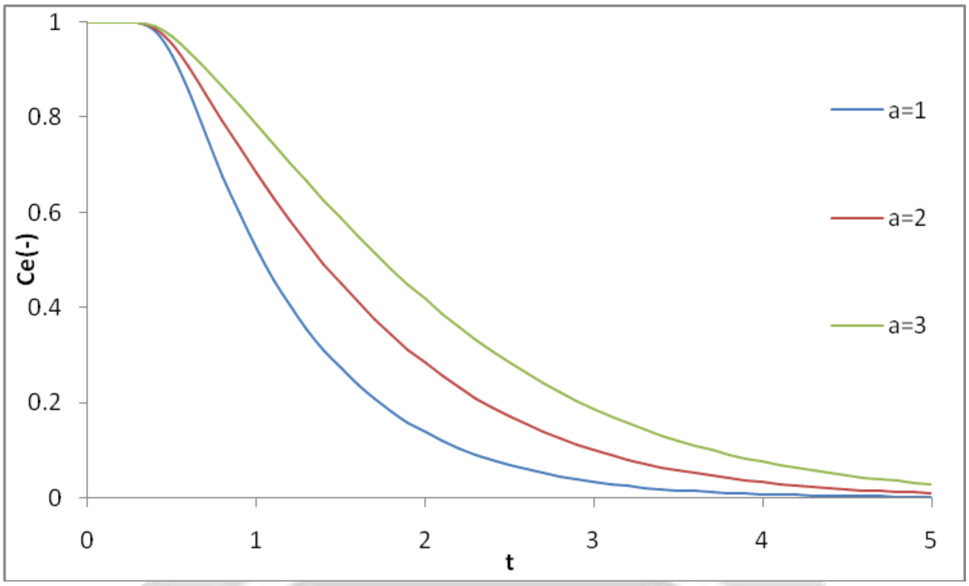

Figure 14: Behavior of solution profiles for varying values of particle geometry (a)

Effect on Displacement Ratio (DR)

During displacement washing process some part of the mother liquor which remains in the pulp, while the displaced liquor will always be diluted partly by the wash water. Thus displacement can never be performed ideally. Displacement washing is measured in terms of displacement ratio, which may be defined as the concentration of actually displaced liquor (V_d) divided by the concentration of the original liquor which is the same as the liquor on the pulp out of the washer (V_o) *i.e.* DR = V_d/V_o. In Figure 15, the behavior of displacement ratio (DR) is shown for different values of *Pe*, parameter ψ andε. It is obvious from Figure 15 that for *Pe* = 20.81 which is higher than the *Pe* = 12.25, *DR* profiles are almost similar and converge to steady state at almost same time period due to the bed porosity of the two runs which are 0.6711 and 0.6898, respectively, having very small difference. Similarly, the *DR* profiles converge rapidly for *Pe*= 12.96 as compared to other values of *Pe*. Also, the solution profiles at ε = 0.8120 converges to maximum possible reduction of solids rapidly than at ε = 0.5561 for *Pe*= 16.92, where lesser amount of solute is available for displacement, while relatively large amount of a solute is removed by leaching, based on the diffusive mechanism taking place slowly, and depending on the driving force. Therefore, along with Peclet number and parameter ψ, the porosity level also effects the solution profiles significantly. It results in removal of more impurities adsorbed on fiber surface within less time interval. Hence, greater effectiveness of washing operations can be achieved.

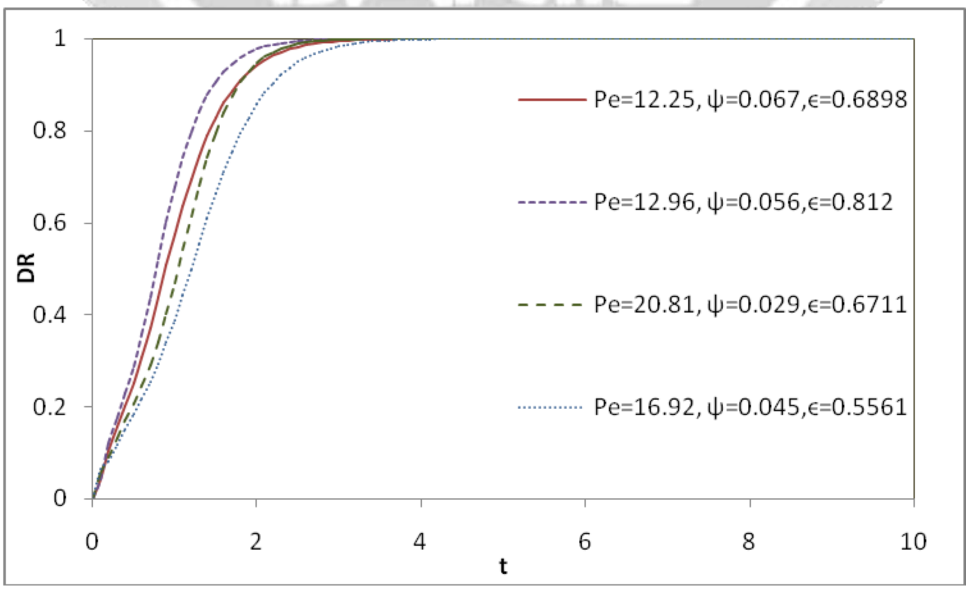

Figure 15: Behavior of solution profiles for varying values of DR for a=1.

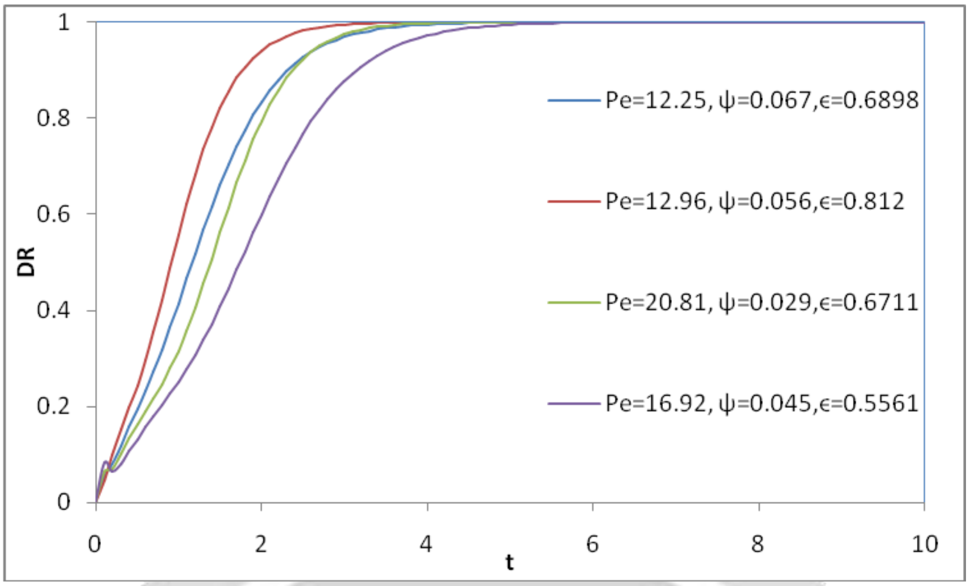

Figure 16: Behavior of solution profiles for varying values of DR for a=2.

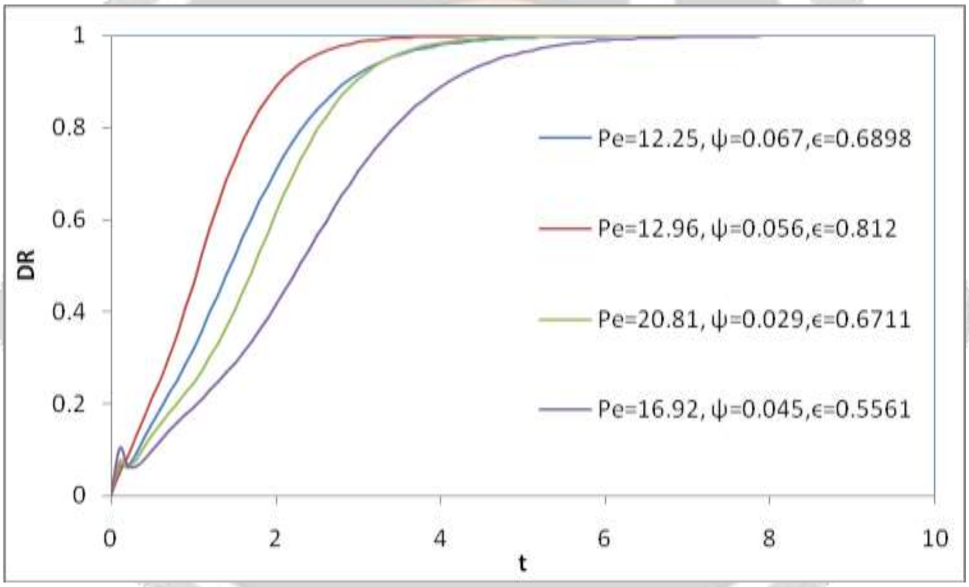

Figure 17: Behavior of solution profiles for varying values of DR for a=3.

VII. CONCLUSION

In the present model, the particle diffusion equation has presented to represent the intraparticle diffusion and the solute adsorbed on the particle surface. The adsorption isotherm has been taken to be Langmuir to link the interparticle and intrapore solute concentrations in a dynamic approach. The Hermite collocation method has been used to solve model equations. HCM has been compared with OCM and it is found that HCM gives better and accurate results for different range of parameters.

VIII CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests regarding the publication of this paper.

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