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STUDY OF TWO PHASE NON-LINEAR MODEL OF ADVECTION DISPERSION FOR DISPLACEMENT WASHING OF POROUS PARTICLES

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Abstract

Two phase non-linear diffusion dispersion model for cylindrical particle geometry has been presented. Model equations have been divided into two phases namely, bulk fluid phase and particle phase. Particle phase has been characterized by particle geometry. Inter-pore and intra-pore solute concentrations have been related by Langmuir adsorption isotherm. Non-linear set of model equations has been solved using the technique of orthogonal collocation on finite elements with Lagrangian basis. Applicability of the model has also been discussed through industrial parameters.

Introduction

Removal of soluble and insoluble impurities adsorbed on particle surface, with the help of weak wash liquor or clean water is called washing process. It involves a number of complex phenomenon of adsorption-desorption, diffusion and dispersion etc. During this process, the solute present in irregular void channels of bed diffuse out of particle pores. Displacement of solute is associated with dispersion of wash liquid in the direction of flow. Various

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mathematical models have been developed to describe the kinematics of packed bed reactors with the help of breakthrough curves. In general, analytic solution of these model equations is very complicated due to the singularity of convection-diffusion term.

An extended mathematical model is proposed to study the washing of pulp fibers in a packed bed. In displacement washing, the solute present in the irregular voids of the bed is associated with a diffusion-dispersion like phenomenon, referred to as longitudinal dispersion. Due to the porous nature of fibers, the stagnant liquor present in the intrafiber voids diffuse out of the fiber pores in contact with bulk fluid. Since some solute is also adsorbed on the fibrous surface, the internal and external mass transfer occurs through the internal and external fiber surface and from the fiber surface to the bulk fluid.

Model Development

The proposed model is based on the assumptions that the system is isothermal and fibers are porous and of uniform cylindrical size. Particle (fiber) diameter to length are very small as compared to the axial distance of bed. Bed is macroscopically uniform and the movement of solute within the fiber pores is described mathematically by Fick's law. Adsorption equilibrium between interfiber and intrafiber solute concentrations is assumed to be non-linear (Langmuir). The mathematical equations for the particle diffusion and the bulk fluid are presented in the dimensionless form. Details of the model are given in Arora et al. [2].

$$\frac{\partial^2 Q}{\partial \eta^2} + \frac{1}{\eta}\frac{\partial Q}{\partial \eta} = \frac{\partial Q}{\partial \tau} + N_1 \frac{(1-\beta)}{\beta}\frac{\partial N'}{\partial \tau} \tag{1}$$

$$\frac{\partial Q}{\partial \eta} = 0 \text{ at } \eta = 0 \text{ and } \frac{\partial Q}{\partial \eta} = -Bi(Q - C) \text{ at } \eta = 1 \tag{2}$$

$$\frac{\partial N'}{\partial \tau} = \frac{R^2 k_1}{D_F}\left(C_1 Q(1-N') - \frac{N'}{k^*}\right) \tag{3}$$

$$\frac{\partial C}{\partial \tau} = \frac{\psi}{Pe}\frac{\partial^2 C}{\partial \xi^2} - \psi \frac{\partial C}{\partial \xi} - \theta Bi(C - Q|_{\eta=1}) \tag{4}$$

$$C - \frac{1}{Pe}\frac{\partial C}{\partial \xi} = 0 \text{ at } \xi = 0 \text{ and } \frac{\partial C}{\partial \xi} = 0 \text{ at } \xi = 1 \tag{5}$$

$$C = Q = N' = 1 \text{ at } \tau = 0. \tag{6}$$

Orthogonal Collocation on Finite Elements

Orthogonal collocation on finite elements (OCFE) is the combination of orthogonal collocation and finite elements method. In OCFE, the whole domain of interest, i.e., $0 \le \xi \le 1$ is divided into small sub domains, called elements, by placing the dividing points at ξ_ℓ, where $\ell = 1, 2, 3, \ldots, m+1$ with $x_1 = 0$ and $x_{m+1} = 1$ for the two point boundary value problems. Within each element a new variable v is introduced as $v = \frac{\xi - \xi_\ell}{\xi_{\ell+1} - \xi_\ell}$ such that as ξ varies from ξ_ℓ to $\xi_{\ell+1}$, v varies from 0 to 1. By applying the orthogonal collocation directly on v, within each element, one gets the collocation equations in terms of the solutions at the collocation points. To avoid double calculation, the function and its first derivative are assumed to be continuous at the node points. The boundary conditions are applied on the initial and terminal point of first and last element, respectively. The discretization end points are fixed as $v_1 = 0$ and $v_{N+1} = 1$. The zeros of shifted Legendre polynomials have been used as collocation points for the axial domain. The zeros of shifted Chebyshev polynomials have been used as the collocation points in the radial direction. Details of the collocation points are given in Arora et al. [3].

In Orthogonal collocation on finite elements both the radial and axial domains are first divided into small number of elements and with in each element orthogonal collocation is applied. The detailed description of the method is available in Arora et al. [1]. After discretization following system is obtained:

$$\frac{dQ_\ell^m(k, j)}{d\tau} = \frac{1}{h_m^2}\sum_{i=1}^{p} B_{ji}^* Q_\ell^m(k, i) + \frac{1}{h_m(v_j' h_m + \eta_m)}$$

$$\sum_{i=1}^{p} A_{ji}^{*} Q_{\ell}^{m}(k,\ i) - \left(\frac{1-\beta}{\beta}\right) N_1 \frac{dN'^{m}_{\ell}(k,\ j)}{d\tau} \tag{7}$$

$Q_{\ell}^{m}(k,\ j)$ stands for the collocation solution for j^{th} collocation point in the m^{th} element in radial direction and k^{th} collocation point in the ℓ^{th} element in axial direction, h_m is the length of the m^{th} element in radial direction.

$$\frac{dN'^{m}_{\ell}(k,\ j)}{d\tau} = \frac{R^2 k_1}{D_F}\left(C_1 Q_{\ell}^{m}(k,\ j)(1 - N'^{m}_{\ell}(k,\ j)) - \frac{N'^{m}_{\ell}(k,\ j)}{k^*}\right). \tag{8}$$

Continuity conditions can be defined as:

$$Q_{\ell}^{m}(k,\ p) = Q_{\ell}^{m+1}(k,\ 1) \text{ and } \frac{1}{h_m}\sum_{i=1}^{p} A_{pi}^{*} Q_{\ell}^{m}(k, i) = \frac{1}{h_{m+1}}\sum_{i=1}^{p} A_{1i}^{*} Q_{\ell}^{m+1}(k,\ i). \tag{9}$$

Boundary conditions are:

$$\sum_{i=1}^{p} A_{1i}^{*} Q_{\ell}^{1}(k,\ i) = 0 \text{ and } \frac{1}{h_w}\sum_{i=1}^{p} A_{pi}^{*} Q_{\ell}^{w}(k,\ i) = -Bi(Q_{\ell}^{w}(k,\ p) - C_k^{\ell}) \tag{10}$$

$$\frac{dC_k^{\ell}}{d\tau} = \frac{\psi}{h_{\ell}^2 Pe}\sum_{s=1}^{N+1} B_{ks} C_s^{\ell} - \frac{\psi}{h_{\ell}}\sum_{s=1}^{N+1} A_{ks} C_s^{\ell} - \theta Bi(C_k^{\ell} - Q_{\ell}^{m}(k,\ p)) \tag{11}$$

continuity condition in axial direction are:

$$C_{N+1}^{\ell} = C_1^{\ell+1} \text{ and } \frac{1}{h_{\ell}}\sum_{s=1}^{N+1} A_{1s} C_s^{\ell} = \frac{1}{h_{\ell+1}}\sum_{s=1}^{N+1} A_{N+1s} C_s^{\ell+1} \tag{12}$$

boundary condition are:

$$C_1^1 - \frac{1}{h_{\ell} Pe}\sum_{s=1}^{N+1} A_{1s} C_s^1 = 0 \text{ and } \sum_{s=1}^{N+1} A_{N+1s} C_{N+1}^{ne} = 0. \tag{13}$$

Initially $C = Q = N' = 1$.

The radial domain is divided into w elements and the axial domain is divided into ne elements. A stiff system of $[(w(2p-3)+2)ne \cdot N] + 1$ coupled differential algebraic equations (DAE) appears which is solved using MATLAB with ode15s subroutine.

Results and Discussion

The effect of certain base case parameters such as Péclet number, distribution ratio and bed porosity has been checked. The solute concentration profiles are evaluated with respect to time in the form of breakthrough curves.

Effect of Péclet number: The effect of Péclet number on exit solute concentration is shown in Figure (1). With the increase in the axial dispersion coefficient, Péclet number decreases, as a result more back mixing occurs, leading to less removal of the black liquor solids from the solute. Figure (1) indicates that for large values of the Péclet number, the breakthrough becomes broadens as a result less time is evolved in the recovery of black liquor solids and hence better washing can be achieved. For efficient washing operations higher Péclet number is preferred.

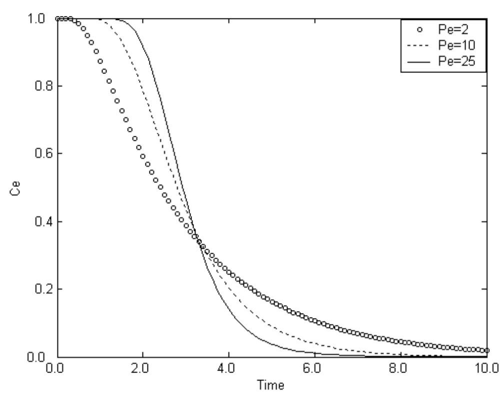

Figure 1. Effect of Péclet number on exit solute concentration.

Effect of bed porosity: Porosity of the packed bed (ε) is most important and sensitive physical factor which effects the concentration profiles very significantly. Higher the particle porosity, higher will be the permeability of the solute, smaller will be the flow rates and better will be the washing. In Figure (2) it is evident that with the increase in the bed porosity, the breakthrough curves rapidly converge to zero and efficient washing operations can be performed. Hence it is also in agreement with the study of Lee [4] and Trinh [5].

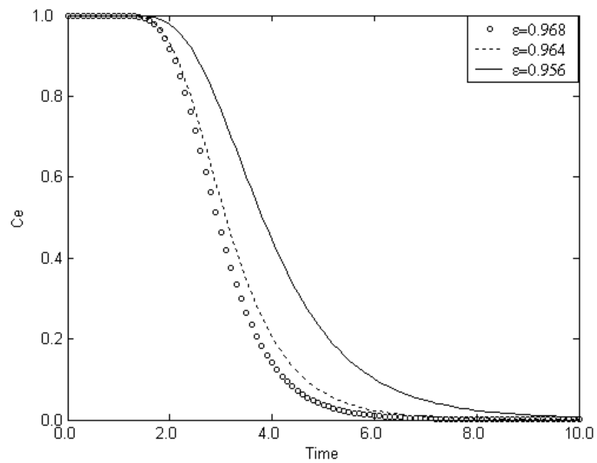

Figure 2. Effect of bed porosity on exit solute concentration.

Effect of distribution ratio: The effect of distribution ratio D_F/R^2 on breakthrough curves can be seen from Figure (3). The solution profiles converge to zero more rapidly as the value of ψ increases with the decrease in the value of D_F/R^2. It is due to the fact that both the ψ and τ are effected by distribution ratio. With the increase in the value of D_F/R^2, ψ decreases whereas τ increases, resulting in the increase in the retention time. Due to this fact concentration profiles are elongated and take large time to converge to the steady state condition.

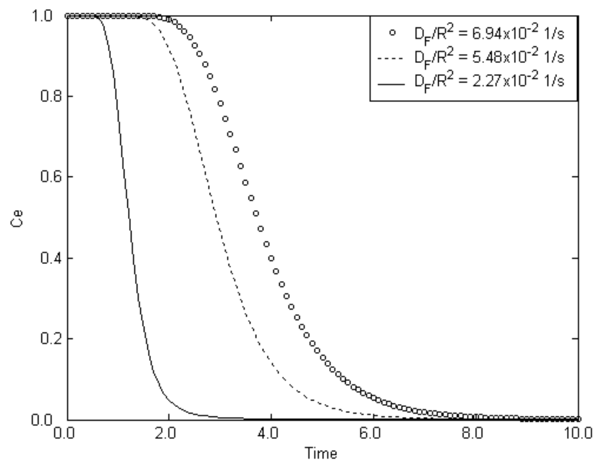

Figure 3. Effect of distribution ratio D_F/R^2 on exit solute concentration.

Conclusions

An extended mathematical model giving detailed description of the washing behavior of porous semi solid cylindrical particles is presented. A robust and convenient numerical technique of OCFE is applied to solve the model equations. It is found that washing operation is highly sensitive for axial dispersion coefficient, bed porosity and distribution ratio.

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