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Mathematical model-based analysis of washing dynamics in porous pulp beds

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Abstract

This study presents a mathematical model for analyzing the washing process in a packed bed of spherical porous particles. The governing equations are solved using the Hermite collocation method with cubic Hermite basis functions. The effects of Peclet number (Pe), parameter ψ , and bed porosity (ϵ) on washing efficiency are examined through numerical and graphical analysis.

Keywords: Packed bed washing, spherical porous particles, mathematical modeling

1. Introduction

Mathematical modeling has become an important tool for analyzing and improving industrial processes, especially in chemical engineering. In the pulp and paper industry, washing of porous particles involves complex mass transfer and adsorption-desorption mechanisms. Mathematical models help in understanding these processes and optimizing washer performance (Kukreja & Ray 2000, Potucek & Pulcer 2004, 2006, Arora *et al.* 2006b, Arora & Potucek 2008, Kumar *et al.* 2009, 2010) [1, 2, 3, 5, 8, 6, 7]. This study focuses on the washing zone of a brown stock washer containing spherical porous particles and develops a model to describe the transport of impurities during the washing operation.

2. Mathematical Model

A mathematical framework is proposed to simulate the washing process occurring in the washing zone of a rotary vacuum washer, considering particles of spherical shape.

3. Model Equations

3.1 For Particle Phase

$$\frac{\partial Q}{\partial \tau} + \frac{1-\beta}{\beta} N' \frac{\partial N}{\partial \tau} = \frac{1}{\psi} (C - Q), (\xi, \tau) \in (0, 1) \times (0, T) \quad (1)$$

$$\frac{\partial N}{\partial \tau} = P^* [Q(1 - N) - k^* N], (\xi, \tau) \in (0, 1) \times (0, T) \quad (2)$$

For Bulk Fluid Phase

$$\frac{\partial C}{\partial \tau} = \frac{1}{Pe} \frac{\partial^2 C}{\partial \xi^2} - \frac{\partial C}{\partial \xi} - \frac{a\theta}{\psi} (C - Q) (\xi, \tau) \in (0, 1) \times (0, T) \quad (3)$$

$$\text{Boundary conditions: } C - \frac{1}{Pe} \frac{\partial C}{\partial \xi} = 0 \text{ at } \xi = 0 \quad (4)$$

$$\frac{\partial C}{\partial \xi} = 0 \text{ at } \xi = 1 \quad (5)$$

$$\text{Initially: } C = Q = N = 1 \quad (6)$$

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A Hermite collocation-based discretization procedure was employed to numerically evaluate the dimensionless governing equations presented in Eqs. (1)-(6).

3.2 Hermite Collocation Method

To carry out the numerical procedure, the axial domain is divided into smaller m elements. The interior nodes required for collocation are obtained from the zeros of the Legendre polynomial. The collocation variable for ℓ^{th} element is $\zeta = \frac{\xi - \xi_\ell}{h}$, where h is the length of the ℓ^{th} element.

Consider an approximation $\tilde{C}_\lambda$ of C , $\tilde{Q}_\lambda$ of Q and $\tilde{N}_\lambda$ of N such that $\tilde{C}_\lambda = \sum_{i=1}^4 c_i^\lambda(\tau) H_i(\zeta)$, $\tilde{Q}_\lambda = \sum_{i=1}^4 q_i^\lambda(\tau) H_i(\zeta)$, $\tilde{N}_\lambda = \sum_{i=1}^4 n_i^\lambda(\tau) H_i(\zeta)$ (7)

where c_i^λ, q_i^λ and n_i^λ are undetermined functions of ' τ ' and $H_i(\zeta)$ defined as (Dyksen and Lynch (2000), Brill (2002))

$$H_1(\zeta) = (1 - 3\zeta^2 + 2\zeta^3)$$

$$H_2(\zeta) = (\zeta - 2\zeta^2 + \zeta^3)$$

$$H_3(\zeta) = (3\zeta^2 - 2\zeta^3)$$

$$H_4(\zeta) = (-\zeta^2 + \zeta^3)$$

After substituting $\tilde{C}_\lambda$, $\tilde{Q}_\lambda$ and $\tilde{N}_\lambda$ in equations (1) to (3) at j^{th} collocation point, one gets the following system of equations:

$$\sum_{i=1}^4 \frac{dq_i^\lambda}{d\tau} H_i(\zeta_j) + \frac{1-\beta}{\beta} N' \sum_{i=1}^4 \frac{dn_i^\lambda}{d\tau} H_i(\zeta_j) = \psi^{-1} \sum_{i=1}^4 (c_i^\lambda - q_i^\lambda) H_i(\zeta_j); j = 2, 3; \lambda = 1, 2, \dots, m \quad (8)$$

$$\sum_{i=1}^4 \frac{dn_i^\lambda}{d\tau} H_i(\zeta_j) = P^* (((\sum_{i=1}^4 q_i^\lambda(\tau) H_i(\zeta_j)) (1 - \sum_{i=1}^4 n_i^\lambda(\tau) H_i(\zeta_j))) - k^* \sum_{i=1}^4 n_i^\lambda(\tau) H_i(\zeta_j)); j = 2, 3; \lambda = 1, 2, \dots, m \quad (9)$$

$$\sum_{i=1}^4 \frac{dc_i^\lambda}{d\tau} H_i(\zeta_j) = \frac{1}{Pe h_\lambda^2} \sum_{i=1}^4 c_i^\lambda B_{ji} - \frac{1}{h_\lambda} \sum_{i=1}^4 c_i^\lambda A_{ji} = \alpha \theta \psi^{-1} \sum_{i=1}^4 (c_i^\lambda - q_i^\lambda) H_i(\zeta_j); j = 2, 3; \lambda = 1, 2, \dots, m \quad (10)$$

Using boundary condition, one gets $c_1^1(\tau) = \frac{1}{Pe} c_2^1(\tau)$ in the first element and $c_4^m(\tau) = 0$ in m^{th} element. Consequently, the differential-algebraic equations are reduced to an equivalent system of ordinary differential equations. These equations are organized into a block-diagonal matrix structure, with each block representing the governing equations at the j^{th} collocation node of the λ^{th} element, as given in Eqs. (8)-(10). The resulting $(6m+4)$ equation system is integrated numerically using MATLAB's ode15s solver, where m represents the total number of discretized elements. The exit concentration of the solute, C_e , is determined at $\xi = 1$.

4. Study of Model Equations for Spherical Particle Geometry

This section analyzes the impact of Peclet number, bed porosity, and distribution ratio (ψ) on the outlet solute concentration of spherical porous particles. The results show that higher porosity materials, such as glass beads, provide more efficient washing than pulp fibers.

4.1 Effect of Peclet number (Pe)

Figure 1 shows that increasing the Peclet number has little influence for parameter $\psi = 0.1$ and $\varepsilon = 0.812$ on the exit solute concentration when Pe is above 35 (Al-Jabari *et al.* (1994))^[11]. Only slight variations appear at the initial stage, indicating that the concentration profile remains nearly unchanged at higher Peclet numbers. Therefore, for fixed value of bed porosity and parameter ψ , the model agrees well with the study of Al-Jabari *et al.* (1994)^[11].

4.2 Effect of Distribution ratio (ψ)

Figure 2 presents the influence of the distribution ratio (ψ) on exit solute concentration for $Pe = 35$ and $\varepsilon = 0.812$. Lower ψ values promote faster attainment of steady state and enhance washing efficiency. The larger effective pore size associated with smaller ψ increases solute diffusion, leading to greater impurity removal from spherical particles.

4.3 Effect of Bed porosity (ε)

Figure 3 shows the effect of bed porosity (ε) on exit solute concentration for $Pe = 35$ and $\psi = 0.1$. Increasing bed porosity from 0.6075 to 0.812 accelerates the attainment of steady state and improves washing efficiency. Higher porosity provides more space for liquid flow, enhancing impurity removal from the packed bed.

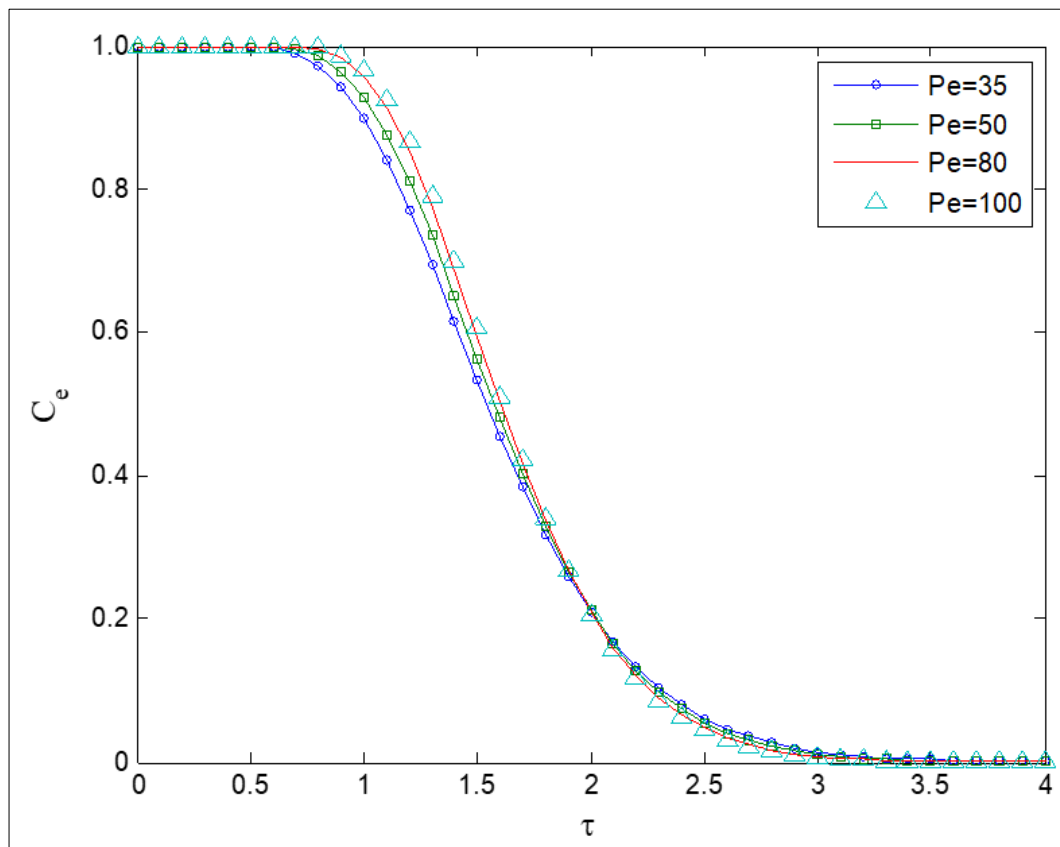


Fig 1: Influence of the Peclet Number on the Evolution of Solution Profiles

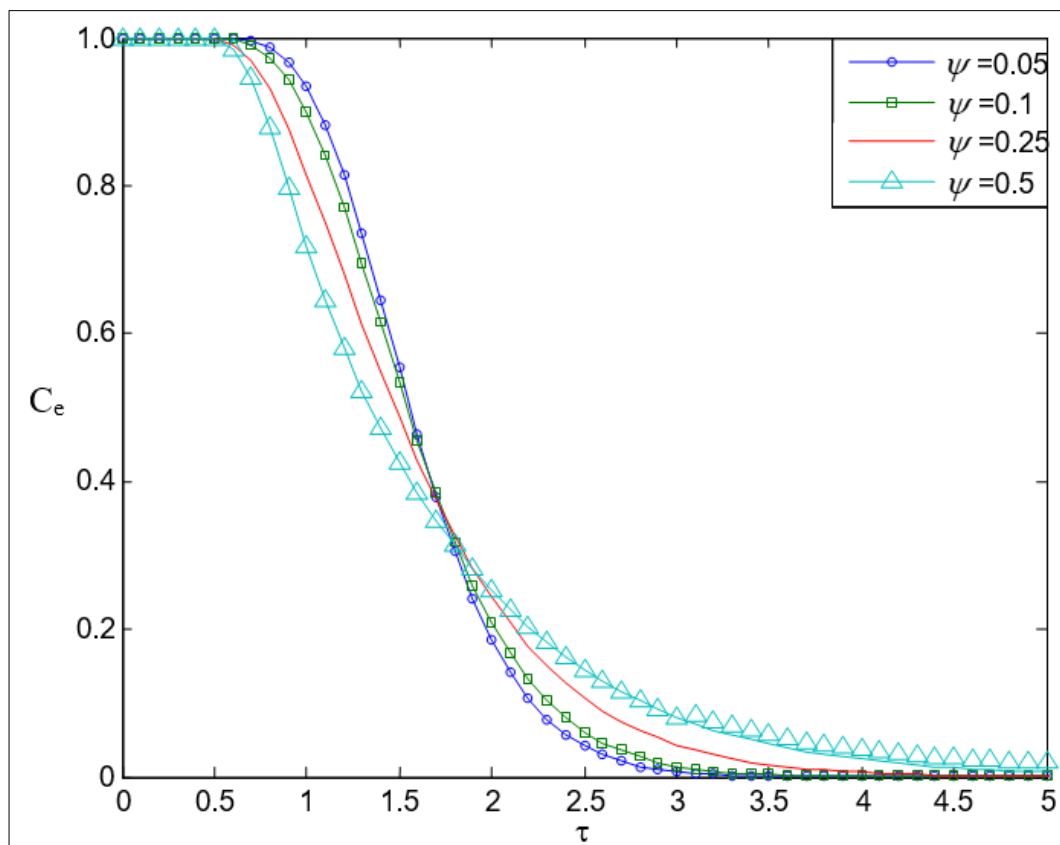


Fig 2: Influence of the parameter ψ on the evolution of the solution profile

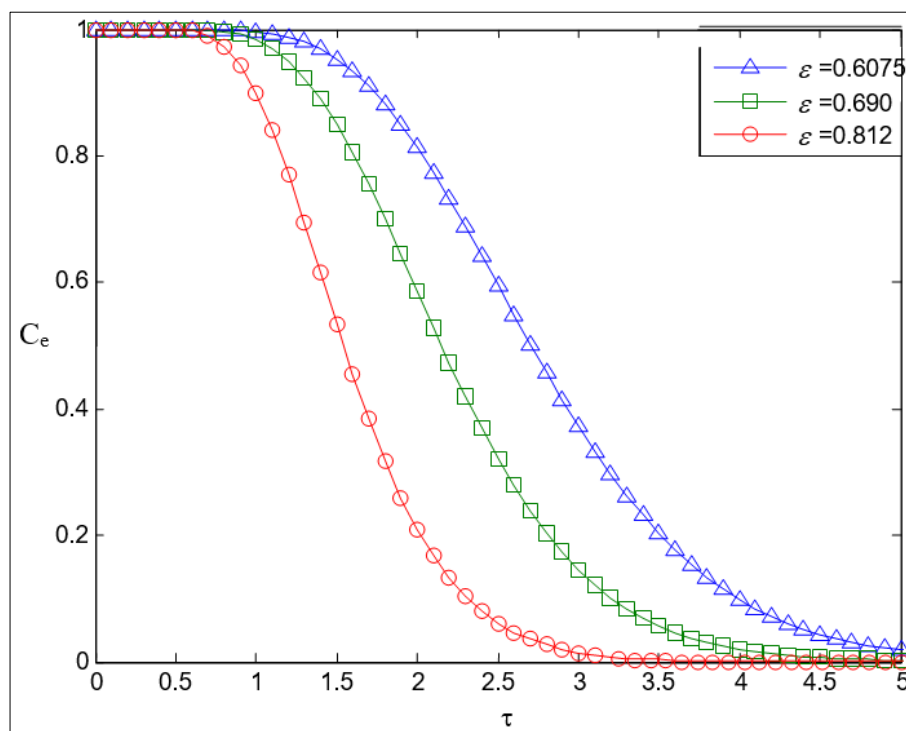


Fig 3: Influence of the parameter ε on the evolution of the solution profiles

5. Conclusion

The nonlinear two-phase model for spherical particles was numerically analysed to study the washing process in a rotary vacuum washer. The Hermite collocation method was employed to solve the governing equations. The effects of the Peclet number (Pe), Bed Porosity (ε), Distribution ratio (ψ) were evaluated through time-dependent breakthrough curves. The numerical findings suggest that higher values of these parameters enhance the washing efficiency and lead to improved process performance.

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