

Numerical Simulation of Pulp Washing in Packed Beds of Porous Particles

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Abstract

A theoretical–numerical model has been constructed to interpret the washing response of a packed bed system containing porous particles with spherical geometry. The model equations, dominated by convective–diffusive transport, are numerically resolved using the Cubic Hermite collocation scheme. The approximation space for the trial solution is discretized using $C1$ -continuous cubic Hermite interpolants, ensuring derivative compatibility at the collocation nodes. A parametric impact assessment is performed to theoretically and graphically evaluate the role of the Peclet number (Pe), internal resistance parameter ψ , and bed porosity ε , emphasizing their collective control over washing zone migration and mass transfer impedance.

1. Introduction

In recent decades, mathematics has transitioned into a core enabling science for solving multidimensional real-world and process-intensive industrial problems, with particularly strong adoption in chemical and biochemical engineering sectors. Mathematical models act as conceptual and computational mirrors of industrial units, revealing internal process behavior, transport limitations, and performance trends, thereby steering technological improvements and process design strategies. Due to the vast scale and complexity of industrial phenomena, applied mathematics offers an extensive toolbox of modeling techniques and numerical algorithms to interpret and solve coupled physical–chemical systems.

The pulp and paper industry is a representative domain where mathematical modeling and chemical process engineering coexist as interdependent development drivers. The washing of porous particle networks is largely influenced by reversible molecular attachment and detachment dynamics, commonly interpreted through adsorption equilibrium and desorption flux behavior. Numerous modeling efforts (Kukreja & Ray 2000, Potucek & Pulcer 2004, 2006, Arora *et al.* 2006b, Kumar *et al.* 2009, 2010) have been directed toward understanding impurity removal from porous particles shaped in different geometrical configurations. These geometries—ranging from flat surface-dominant forms to curvature-governed radial structures—introduce distinct internal diffusion resistances and hydrodynamic interactions, which in turn affect washing performance.

The washing process can be defined as an externally assisted impurity removal mechanism in which both soluble and non-soluble contaminants, initially retained on particle surfaces, are detached and transported away by a flowing washing medium. When the washing liquid travels through a packed bed, solute spreading occurs along the flow axis due to velocity variations and structural irregularities inside the bed voids. This flow-aligned mixing and solute redistribution effect is referred to as axial fluid dispersion. In parallel, mass transfer operates across interconnected domains, including diffusion from internal pores to the external surface and convective exchange between particle boundaries and the surrounding fluid stream, forming a bidirectional multi-scale transport process (Arora & Potucek 2008).

The present work focuses on developing and applying a mathematical model to analyze the washing zone of a brown stock washing system, specifically considering porous particles with spherical geometry to evaluate flow-controlled solute displacement and interface-driven mass transfer effects.

2. Mathematical Model

A mathematical model is developed to analyze solute transport in the washing region of a rotary vacuum filtration unit, emphasizing pore-scale diffusion, surface desorption, and vacuum-induced solute displacement in spherical porous particles.

Model Equations:

For Particle Phase

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

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

For Bulk Fluid Phase

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

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

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

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

The dimensionless governing equations (1)–(6) are numerically projected onto a discrete solution space by enforcing pointwise residual satisfaction through the Hermite collocation method.

3. Hermite Collocation Method

In this method, the axial domain is divided into m elements. Zeros of Legendre polynomial has been taken as the interior collocation points. 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

$$\tilde{C}_\lambda = \sum_{i=1}^4 c_i^\lambda(\tau) H_i(\zeta), \quad \tilde{Q}_\lambda = \sum_{i=1}^4 q_i^\lambda(\tau) H_i(\zeta), \quad \tilde{N}_\lambda = \sum_{i=1}^4 n_i^\lambda(\tau) H_i(\zeta) \quad (7)$$

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))

$$\begin{aligned} H_1(\zeta) &= (1 - 3\zeta^2 + 2\zeta^3) \\ H_2(\zeta) &= (\zeta - 2\zeta^2 + \zeta^3) \\ H_3(\zeta) &= (3\zeta^2 - 2\zeta^3) \\ H_4(\zeta) &= (-\zeta^2 + \zeta^3) \end{aligned}$$

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:

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

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

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

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. It reduces the system of differential algebraic equations into a system of ordinary differential equations. The resulting system of equations is convert into a block diagonal structure with each block consists of system of ordinary differential equations defined from (8) to (10) at j^{th} collocation point in λ^{th} element. This system of $(6m+4)$ number of equations is solved using MATLAB with ‘ode15s’ system solver, where m is the total number of elements. The exit solute concentration C_e is calculated at $\xi = 1$.

4 Study of Model Equations for Spherical Particle Geometry

This section investigates the combined influence of key parameters—Peclet number, bed porosity, and solute distribution ratio—on exit solute concentrations for spherical particles of radius $a=3$. For discretization, the numerical framework follows the approach of Potucek (1997), where the Peclet number for spherical particles ranges from 33 to 82, significantly higher than the 7–20 range observed for cylindrical geometries. The bed porosity is varied between 0.7 and 0.9, reflecting the greater efficiency of washing in rigid particles such as glass beads and limestone compared to fibrous pulp. Potucek also highlighted that, for the same bed thickness, washing operations are substantially more effective in glass bead beds than in pulp fiber beds.

4.1 Effect of Peclet number (Pe)

Figure 1 depicts the theoretical impact of the Peclet number on exit solute concentration profiles for $\psi=0.1$ and $\epsilon=0.812$. For spherical particles, the Peclet number is relatively high, prompting evaluation over the range 35–100. Consistent with the findings of Al-Jabari et al. (1994), the concentration profiles show negligible variation for Pe values above 30, with only minor differences observed during the initial stages of washing. This indicates that, at constant bed porosity and ψ , the present model reliably captures the behavior reported in previous studies for high- Pe regimes.

4.2 Effect of Distribution ratio (ψ)

In distribution ratio (ψ) plays a crucial role in determining the behavior of solute concentration profiles. At high flow rates, as reported by Neretnieks (1974), the washing

process is primarily controlled by particle pore size and intraparticle diffusion rather than by axial dispersion. The parameter ψ reflects the combined effects of pore radius, internal diffusion, and interstitial velocity on solute transport. Figure 2 shows that, for $Pe = 35$ and $\epsilon=0.812$, smaller values of ψ lead to faster attainment of steady-state profiles. This is attributed to the increase in effective pore radius for lower ψ in spherical particles, which promotes more efficient solute diffusion from the particle interior to the surface, thereby enhancing impurity removal and overall washing efficiency.

4.3 Effect of Bed porosity (ϵ)

Porosity is a key and highly influential parameter in the washing process, significantly affecting both flow resistance and solute removal efficiency. Even slight variations in packed-bed porosity can lead to substantial changes in the pressure drop required for fluid passage. Figure 3 illustrates the effect of bed porosity on exit solute concentration profiles for $Pe = 35$ and $\psi=0.1$. The results show that increasing porosity from 0.6075 to 0.812 accelerates the attainment of steady-state profiles. This occurs because higher porosity provides a greater volume of washing medium, promoting more effective displacement of solutes from particle surfaces and thereby enhancing the overall washing performance of the packed bed.

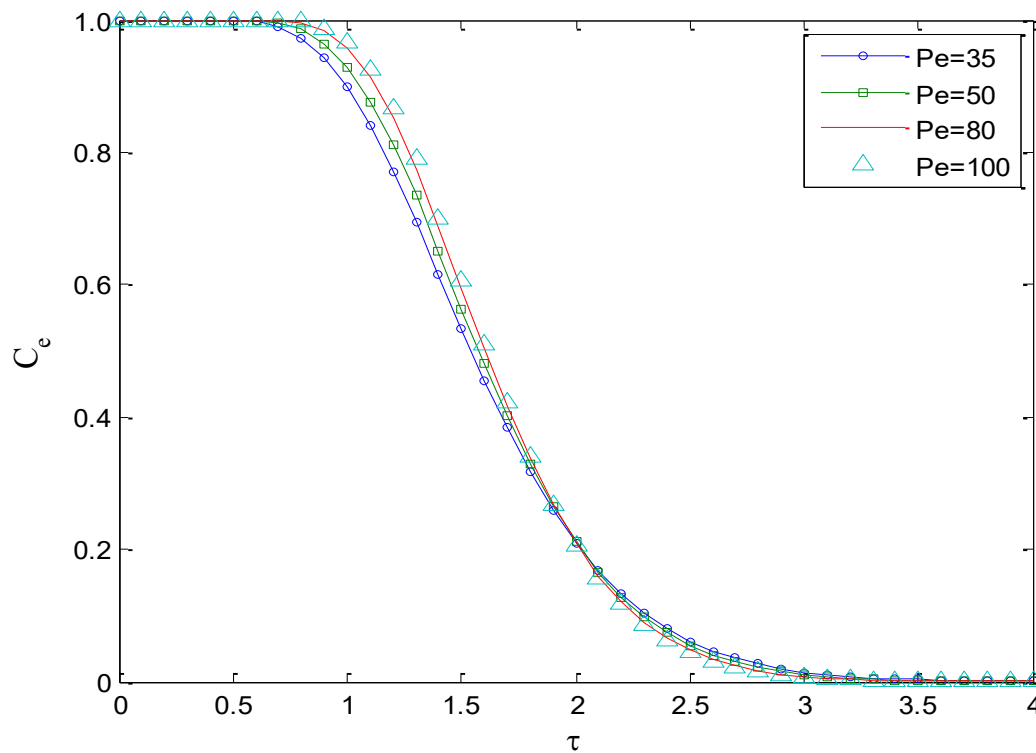


Figure 1: Behavior of solution profiles for varying values of Peclet number.

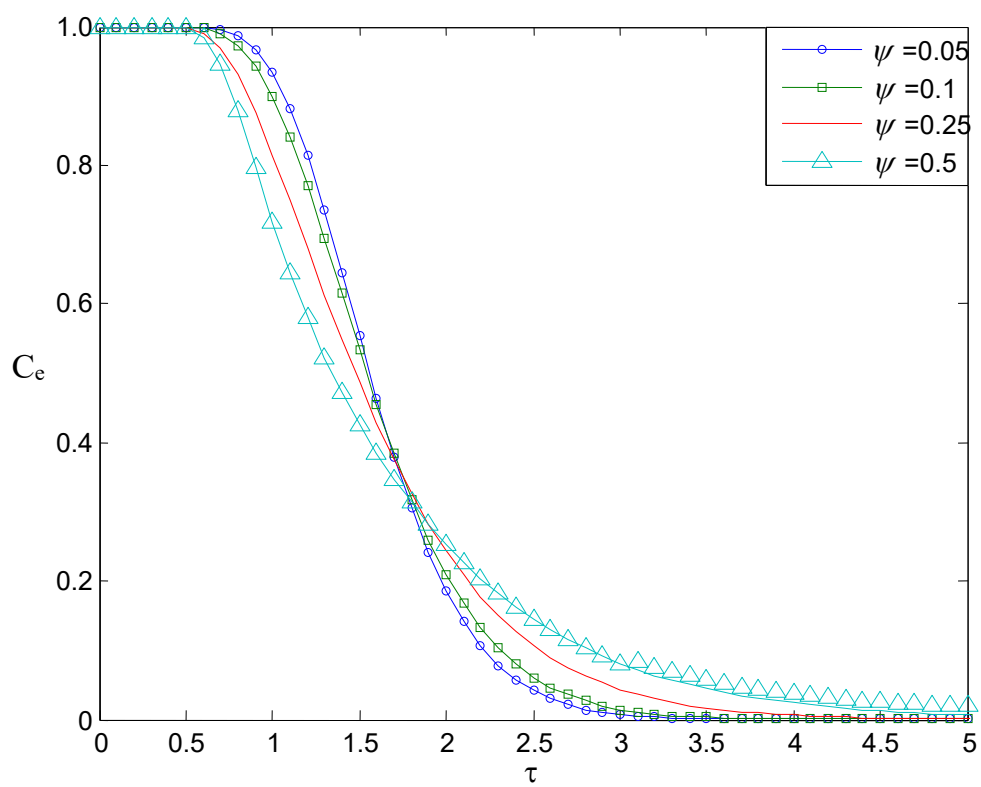


Figure 2: Behavior of solution profiles for varying values of ψ .

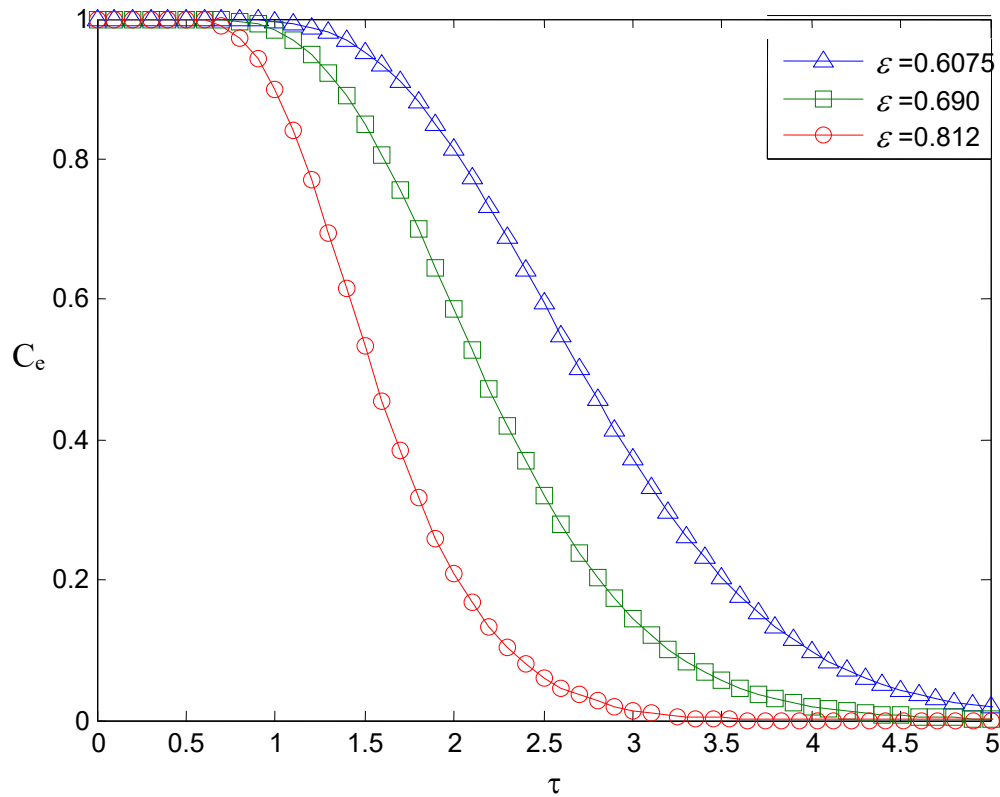


Figure 3: Behavior of solution profiles for varying values of ϵ .

CONCLUSIONS

An in-depth analysis of the two-phase nonlinear model has been performed for spherical particle geometries. The model equations are numerically addressed using the Hermite collocation technique. Breakthrough curves are presented for different Peclet numbers (Pe), bed porosity (ϵ), and distribution ratios (ψ) to examine their influence on the washing process over time. The results suggest that maintaining higher values of Pe, ϵ , and ψ significantly enhances washing efficiency, emphasizing their importance in effective solute removal from the packed bed.

REFERENCE

- [1]. Kukreja V.K. & Ray A.K. (2000). Solving pulp washing problems through mathematical models. American Institute of Chemical Engineering; 96, 276-280.

- [2]. Potucek F. & Pulcer M. (2004). Displacement of black liquor from pulp bed. 31st International conference of the Slovak Society of Chemical Engineering; 58(6), 377-381.
- [3]. Potucek F. & Pulcer M. (2006). Displacement washing of pulp with urea solution. 33rd International conference of the Slovak society of Chemical Engineering, Tatranske Matliare; 60(5), 365-370.
- [4]. Arora S., Dhaliwal S. S. & Kukreja V.K. (2006a). A computationally efficient technique for solving two point boundary value problems in porous media. Applied Mathematics and Computation; 183(2), 1170-1180.
- [5]. Arora S., Dhaliwal S. S. & Kukreja V.K. (2006b). Simulation of washing of packed bed of porous particles by orthogonal collocation on finite element. Computers and Chemical Engineering; 30, 1054-1060.
- [6]. Kumar D., Kumar V. & Singh V.P. (2009). To study the parameter effects on the performance of brown stock washer in paper industry using Matlab. World Journal of Modelling and Simulation; 5, 30-37.
- [7]. Kumar D., Kumar V. & Singh V. (2010). Mathematical modeling of pulp washing on rotary drums and their numerical solution for various adsorption isotherms. World Journal of Modelling and Simulation; 6 (3), 214-222.
- [8]. Arora S., Dhaliwal S.S. & Kukreja V.K. (2008). Mathematical modelling of the washing zone of an industrial rotary vacuum washer. Indian Journal of Chemical Technology; 15, 332-340.
- [9]. Dyksen W. R. & Lynch R. E. (2000). A new decoupling technique for the Hermite cubic collocation equations arising from boundary value problems. Mathematics and Computers in Simulation; 54, 359–372.
- [10]. Brill S. H. (2002). Analytic solution of Hermite collocation discretization of the steady state convection- diffusion equation. International Journal of Differential Equations and Application; 4, 141-155.

- [11]. Al-Jabari M., VanHeiningen A.R.P. & Van De Ven T.G.M. (1994). Modeling the flow and the deposition of fillers in packed bed of pulp fibers. *Journal of Pulp and Paper Science*; 20(9), J249-J253.
- [12]. Neretnieks I. (1974). A mathematical model for continuous counter current adsorption. *Svens Papperstidning-Nordisk Cellulosa*; 11, 407–411.