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ORIGINAL ARTICLE

A robust technique of cubic hermite collocation for solution of two phase non linear model

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Abstract A non-linear advection dispersion model involving Peclet number (*Pe*) and intraparticle diffusion coefficient is proposed for displacement washing process of porous particles. Non-linear model equations are solved using cubic Hermite collocation method (HCM) to compute exit and average solute concentrations. Effect of different parameters such as Peclet number, intraparticle diffusion coefficient and bed porosity (ε) has been discussed theoretically as well as graphically. Industrial parameter such as displacement ratio (DR) is calculated by using model predicted values. Effect of different parameters on displacement ratio, exit and average solute concentrations is discussed through surface plots.

1. Introduction

Washing of porous structure of solid and semi-solid particles having cylindrical or spherical geometries such as pulp fibers or glass beads is of great interest for mathematicians, as well as for chemical engineers. In washing process, the solute or contaminants adsorbed on particle surface are washed out using an external aid. During this process, the solute lying within particle pores is coerced to pull out due to diffusion–dispersion phenomenon in the direction of wash liquor. Therefore, the mechanism involved is the sum of displacement of liquor by movement of water plug controlled by fluid mechanics, dispersion due to back mixing, diffusion due to concentration gradients and adsorption–desorption due to relative affinity of various solutes toward the particle surface. The mass transfer takes place from particle pores to particle surface and from particle surface to external fluid as long as driving force exists and vice versa (Arora et al., 2006).

The purpose of pulp washing is not only to remove soluble impurities adsorbed on particle surface such as sodium compounds and alkali lignin in black liquor or the byproducts after each processing step, but at the same time to achieve it with as little wash liquor as possible. Regardless of the type of washing equipment used, separation involves a combination of

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Nomenclature

c	concentration of solute in liquor, kg/m^3
c_{av}	average solute concentration in packed bed, kg/m^3
c_e	exit solute concentration, kg/m^3
C	dimensionless concentration, $(=c/C_0)$
C_0	initial solute concentration, kg/m^3
C_e	dimensionless exit solute concentration, $(=c/C_0)$
C_s	solute concentration in wash liquor, kg/m^3
D_L	axial dispersion coefficient, m^2/s
D_f	intraparticle diffusion coefficient, m^2/s
DR	displacement ratio, $\frac{C_0-c_{av}}{C_0-C_s}$
k_1	mass transfer coefficient for solute adsorption, 1/s
k_2	mass transfer coefficient for solute desorption, 1/s
k^*	dimensionless parameter, $(=k_2/k_1)$
K	equilibrium constant, dimensionless
L	thickness of the bed, m
n	concentration of solute adsorbed on the fibers, kg/m^3
N	dimensionless concentration of solute adsorbed on fibers, $(=n/N_0)$
N_0	initial concentration of solute adsorbed on the fibers, kg/m^3
N'	dimensionless parameter, $(=N_0/C_0)$
P^*	dimensionless parameter, $(=k_1KL/u)$
Pe	Peclet number, $(=uL/D_L)$, dimensionless
q	intrapore solute concentration, kg/m^3
Q	dimensionless intrapore solute concentration, $(=q/C_0)$
R	pore radius of fibers, m
t	time, s
u	interstitial wash liquid velocity through bed, m/s
z	distance from point of introduction of solvent, m

Greek symbols

θ	dimensionless parameter, $=2(1-\varepsilon)/\varepsilon$, dimensionless
ξ	dimensionless axial distance, $=z/L$, dimensionless
τ	dimensionless time, $=tu/KL$, dimensionless
ψ	$=$dimensionless parameter, R^2u/LD_f

displacement and diffusion processes. In an ideal displacement washing process, plug flow action of wash liquor moving through the stationary pulp bed, completely removes the adsorbed solute.

2. Description of mathematical model

Over the last fifty-two years from Brenner (1962) to Arora et al. (2014) a plethora of literature has been documented to study the displacement washing behavior of porous particles. The axial dispersion model proposed in the present study is based on the following material balance equation:

$$\begin{bmatrix}\text{Entering by}\\ \text{bulk flow}\end{bmatrix}+\begin{bmatrix}\text{Entering by}\\ \text{dispersion}\end{bmatrix}=\begin{bmatrix}\text{Leaving by}\\ \text{bulk flow}\end{bmatrix}+\begin{bmatrix}\text{Leaving by}\\ \text{dispersion}\end{bmatrix}+\begin{bmatrix}\text{Accumulation}\\ \text{of solute}\end{bmatrix}.$$

The mechanism related to fluid concentration in packed bed of porous particles is based on the transfer rate of material between fluid and fibers and is given explicitly by the equation:

$$\frac{\partial \overset{\Delta}{q}}{\partial t}=f(n,q).$$

The objective of the present study is to develop a mathematical model involving geometry of particles, axial dispersion coefficient (D_L), intraparticle diffusion coefficient (D_f), pore radius of particles (R), particle and bed porosity to describe the washing process. The packed bed is assumed to be composed of porous compressible particles uniformly distributed in the bed. The behavior of exit and average solute concentrations flowing through the bed, as well as the concentration of solute adsorbed on the particle surface will be discussed in the subsequent sections.

The present model has been developed keeping in view, that system is isothermal and bed is macroscopically uniform. Particles are porous and are of uniform cylindrical size with pore radius as well as particle length to be very small as compared to axial distance. Langmuir adsorption isotherm is assumed between interparticle and intraparticle solute concentration. The movement of solute within the particle pores is described by Fick's law. The intraparticle diffusion coefficient and axial dispersion coefficient are independent of axial distance and particle radius. Average solute concentration is defined over the bed cross section.

3. Models for particle and fluid phase

Flow of fluid through bed is described by 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 partial differential equations describing the behavior of fluid flow through the bed are described below.

3.1. Mathematical formulation for particle phase

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

3.2. Adsorption isotherm

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

$$\frac{\partial n}{\partial t}=\frac{k_1 q}{C_0}(N_0-n)-k_2 n. \quad (2)$$

The deposition and detachment rate constants k_1 and k_2 are of second order in forward direction and first order in backward direction, respectively.