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Lattice-Boltzmann simulation of lipase separation via bioaffinity chromatography: imposing Dirichlet or Danckwerts inlet condition

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Abstract

Lipase bioseparation can be achieved via biospecific affinity chromatography (BAC), whose governing equations need numerical methods. BAC load step has been simulated via lattice Boltzmann method (LBM) by imposing Dirichlet condition to fluid-phase adsorbate concentration at column inlet. One may instead impose Danckwerts condition and the goal of this work was to compare breakthrough curves simulated via LBM under each condition above. A dynamic 1-D model was adopted comprising Langmuir adsorption-desorption kinetics and convective-diffusive transport. D1Q2 lattice was used and particle distribution functions were assigned to adsorbate concentrations in fluid and solid phases. Numerical breakthrough curves were compared with experimental data and the expected "S" shape was reproduced in LBM simulations. In convective-dominant scenarios no clear effect was noted when one condition type was replaced by the other. Differences became evident in diffusion-dominant scenarios and Danckwerts inlet condition should be imposed in diffusion-dominant scenarios as experimental data were simulated better.

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Keywords: Computational modeling; lattice Boltzmann method; mass transfer; porous medium; bioseparation

1. Introduction

Much attention has been paid to lipases (i.e. enzymes that catalyze the hydrolysis of lipids) in view of their industrial and medical applications [1]. High-degree purification of lipases can be achieved via biospecific affinity chromatography (BAC), whose mathematical models are complex enough to justify numerical solution methods [2-5]. Modeling and simulation of bioprocesses have augmented not only because their importance has been recognized

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but also as suitable techniques have been developed and applied [6].

Lattice-Boltzmann method (LBM) was envisaged by McNamara and Zanetti [7] as a spin-off of lattice gas cellular automata (LGCA) [8] and it has become a promising numerical technique to simulate food and bioprocesses [9] such as chromatography [10,11]. By means of LBM one is able to simulate fluid flow and transport phenomena without directly solving Navier-Stokes equations, which leads to relatively simpler computational codes [12].

As part of ongoing research on LBM simulation of bioprocesses, BAC load step has been investigated by relying on a dynamic 1-D model framework [13]. Besides Langmuir adsorption-desorption kinetics, the model has also comprised differential equations for species (adsorbate) concentrations in fluid and solid phases [14]. As diffusive mass transport is considered in the fluid phase, two boundary conditions are necessary and Dirichlet condition has been imposed at column inlet [13,14]. In previous numerical tests against a classic BAC work on lysozyme [15], the imposition of Danckwerts condition [16] was also imposed and the effects on breakthrough curves were examined by means of LBM simulations of convective-dominant and diffusive-dominant transport scenarios [17].

The goal of this work was to extend aforesaid initial numerical tests towards lipase bioseparation studied in [18]. Accordingly, LBM simulations were performed by imposing either Danckwerts or Dirichlet condition at the column inlet. Effects on breakthrough curves were examined via LBM simulations with different adsorbate diffusivities in the fluid phase and two disputable values of the maximum adsorption capacity of the chromatographic column.

Nomenclature

Latin symbols, units

f	particle distribution function related to fluid-phase concentration, dimensionless
k_{ads}	adsorption kinetic coefficient, $m^3/(U \cdot s)$
k_{des}	desorption kinetic coefficient, s^{-1}
Pe_m	mass-transfer Péclet number, dimensionless
$\dot{r}$	adsorbate transfer rate, $mol/(m^3 \cdot s)$
s	particle distribution function related to solid-phase concentration, dimensionless
v	interstitial fluid velocity, m/s
w	weighting factors, dimensionless

Greek symbols, units

ε	bed porosity, dimensionless
ϕ	adsorbate concentration in fluid phase, U/m^3
θ	adsorbate concentration in solid phase, U/m^3
ω	relaxation parameter, dimensionless

Subscripts and superscripts

eq	equilibrium distribution function
f	fluid phase
k	lattice link (for streaming)
max	maximum adsorption capacity of the column
relax	relaxation time
s	solid phase
1	forward (downward) streaming direction
2	backward (upward) streaming direction

2. Mathematical model

BAC models have invoked Langmuir kinetics (i.e. 2^{nd}-order adsorption and 1^{st}-order desorption kinetics), species (i.e. adsorbate) transport by convection and/or diffusion, and constant volumetric flow rate $\dot{V}$ of the downward percolating solution [19]. Moreover, chromatographic columns have been modeled as cylindrical stratified fixed