Numerical Simulation of Fixed-Bed Biospecific Affinity Chromatography via Lattice-Boltzmann Method

JOSE RABI
Faculty of Animal Science and Food Engineering (FZEA)
University of Sao Paulo (USP)
Av. Duque de Caxias Norte, 225, Pirassununga, SP, 13635-900
BRAZIL
jrabi@usp.br    http://www.usp.br/fzea/

Abstract: Even simplified models for biospecific affinity chromatography (BAC) in fixed bed justify the use of numerical solution so that lattice-Boltzmann method (LBM) appears as a powerful technique. As a first step towards LBM simulation of BAC processes, the present work relies on a time-dependent one-dimensional model evoking sorption-desorption kinetics, uniform flow and species transport by convection and diffusion. Governing equations were then cast into dimensionless form. Proper implementation and functionality of the LBM simulator were checked out by comparing numerical results against experimental data from a classical work on BAC in fixed bed. As simulated breakthrough curves were able to reproduce the general behavior of experimental counterparts, it is believed that such preliminary LBM code can be further adapted or extended in order to numerically simulate other BAC processes of interest.

Key-Words: Lattice-Boltzmann method, Mass transfer, Porous media, Biospecific affinity chromatography.

1 Introduction

The importance of numerical techniques have been recognized for the food industry [1] and simulation of food and/or bioprocess has markedly increased as proper computational tools have been developed [2]. Being a discrete approach for the kinetic theory, LBM has become a powerful and alternative tool in order to simulate food or biosystems related (but not restricted) to emulsions, polymer solutions, colloidal suspensions and flow in porous media [3].

One may distinguish LBM from either molecular dynamics simulation or conventional discretization methods (e.g., finite-differences, finite-elements and finite-volumes). LBM treats the macroscale medium as a large collection of particles occupying lattice sites separated by a discrete set of distances. During discrete time steps, particles travel between adjacent sites along pre-defined lattice links and according to their velocities. When they arrive at sites, particles mutually collide and are rearranged so as to preserve their quantity and momentum [4]-[5]. By assuming that such particle dynamics fulfill basic conservation principles while being isotropic, medium behavior can be properly described and simulated [3]-[5].

The present work applies LBM so as to simulate biospecific affinity chromatography (BAC) in fixed beds. Even when simplifications are evoked, BAC models still justify the use of numerical methods. The main purpose of this work was to check out the proper implementation and functionality of a pilot LBM code by comparing numerically simulated breakthrough curves against experimental data from a classical work on BAC in fixed beds [6].

2 Basic Theoretical Concepts

2.1 Biospecific Affinity Chromatography

Chromatographic columns considered in this work are cylindrical fixed beds of radius $R$ and length $L$, vertically oriented, as shown in Fig. 1(a). Thus, inlet is at $z = 0$ while outlet is at $z = L$. By assuming that porosity $\varepsilon$ is uniform throughout the bed while the volumetric flow rate $V$ of the percolating solution is kept constant during the BAC process, interstitial fluid velocity $v = V / (\varepsilon \pi R^2)$ results uniform as well.

BAC models have evoked species transport by convection and/or diffusion and sorption-desorption kinetics [6]-[12]. Those have been 1st-order models with regard to spatial dependence so that species concentrations have been allowed to vary along a single coordinate $z$ (bed axis), apart from depending on time $t$. As a result, species concentrations in fluid and solid phases have been respectively modeled as $\phi = \phi(z, t)$ and $\theta = \theta(z, t)$, whose governing equations have been usually expressed as:

Fluid phase: $\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial z} = D \frac{\partial^2 \phi}{\partial z^2} - \frac{1 - \varepsilon}{\varepsilon} \frac{\partial \theta}{\partial z} \quad (1)$
Solid phase: \[ \frac{\partial \theta}{\partial t} = \hat{r} \cdot \hat{\mathbf{k}} \left( \theta_{\text{max}} - \theta \right) - k_{1} \theta \]  

(2)

where \( D \) is species diffusivity, \( k_{1} \) and \( k_{2} \) are sorption and desorption coefficients and \( \theta_{\text{max}} \) is the maximum adsorption capacity of the bed. Term \( \hat{r} \) gives the rate at which species are transferred (adsorbed) from fluid to solid phase and it clearly behaves as a sink in Eq. (1) and as a source in Eq. (2).

As far as initial conditions are concerned, one may prescribe the following (at \( t = 0 \)):

\[ \phi = 0 \quad \text{(fluid phase)} \quad \theta = 0 \quad \text{(solid phase)} \]  

(3)

It is worth noting the governing equation for solid-phase concentration \( \theta \), Eq. (2), does not explicitly depend on any spatial coordinate so that boundary conditions are only required for Eq. (1). Being \( \phi_{\text{in}} \neq 0 \) a known fluid-phase concentration at the bed inlet, one may then prescribe the following conditions:

\[ \text{at } z = 0: \quad \phi = \phi_{\text{in}} \quad , \quad \text{at } z = L: \quad \partial \phi / \partial z = 0 \]  

(4)

Fig. 1. (a) Sketch and cylindrical coordinates for chromatographic columns considered in this work; (b) Either D1Q2 or D1Q3 lattice arrangement along with downward and upward lattice velocities.

2.2 Lattice-Boltzmann Method

The basic idea of LBM is to replace the knowledge on each constituent particle (in terms of its position and velocity) by a proper description of their overall effects through a distribution function \( f(\vec{r}, \hat{c}, t) \). At a given time \( t \), such function gives the probability of finding particles about position \( \vec{r} \) with speeds in the range \( \hat{c} \) and \( \hat{c} + \Delta \hat{c} \). As function \( f \) becomes known, one may assess macroscopic properties like species concentration, temperature or flow (drift) velocity.

Boltzmann’s equation is the governing one for function \( f \). In the absence of external forces and under the so-called BGK approach (after Bhatnagar, Gross and Krook), such equation is given as [3],[5]:

\[ \frac{\partial f}{\partial t} + \hat{c} \cdot \nabla f = \frac{1}{\tau} \left( f_{\text{eq}} - f \right) \]  

(5)

where \( \tau \) is known as relaxation time and \( f_{\text{eq}} \) is local equilibrium distribution function.

In LBM, Eq. (5) is discretized along pre-defined directions, i.e., lattice links. Distances \( \Delta z_{k} \) between adjacent lattice sites are discrete (script \( k \) refers to a given link) and so is time so that \( \Delta t \) is a discrete advancing time step. Distinct lattice arrangements are indicated as \( \text{DnQm} \), where \( n \) and \( m \) respectively refer to the lattice dimension and speed model.

In line with axial coordinate \( z \) in Fig. 1(a), Fig. 1(b) depicts a one-dimensional (1-D) lattice known as D1Q3 (which is similar to D1Q2 arrangement), comprising a central site linked to two neighbors. Via those links, particles may “stream” with either downward velocity \( \vec{c}_1 = +\hat{z} \) or upward velocity \( \vec{c}_2 = -\hat{z} \), where \( \hat{z} \) is a unit vector and \( c = \Delta z / \Delta t \) is the lattice speed. Central velocity is null, i.e., \( c_0 = 0 \). Sketches of typical 2-D or 3-D lattice arrangements can be found elsewhere [3],[4],[5].

By writing Eq. (5) for a given lattice link \( k \), one obtains 1-D lattice-Boltzmann equation under BGK approach for the distribution function \( f_k = f_k(z,t) \):

\[ \frac{\partial f_k(z,t)}{\partial t} + c_k \frac{\partial f_k(z,t)}{\partial z} = f_{k,\text{eq}}(z,t) - f_k(z,t) \]  

(6)

where \( c_k = \Delta z / \Delta t \) (with \( \Delta z_k = \pm \Delta z \) depending on the lattice link \( k \)). For D1Q3 lattice, Eq. (6) is written for \( k = 0, 1 \) and 2 (i.e., for \( f_0, f_1 \) and \( f_2 \)) while for D1Q2 it is written only for \( k = 1 \) and 2 as function \( f_0 \) is disregarded (i.e., as introduced ahead, the related weighting factor is null, \( w_0 = 0 \)).

Space-time discretization of Eq. (6) renders an algebraic equation whose evolution is numerically accomplished in two steps [5]. During the collision step (= time evolution), distribution functions \( f_k \) for each direction \( k \) and at each lattice site are updated from \( t \) to \( t + \Delta t \) according to:

\[ f_k(z,t+\Delta t) = [1 - \omega] f_k(z,t) + \omega f_{k,\text{eq}}(z,t) \]  

(7)

where \( \omega = \Delta t / \tau \) is known as relaxation parameter. In the streaming step (= spatial evolution), collision results are propagated to adjacent sites simply as:

\[ f_k(z + \Delta z_k,t + \Delta t) = f_k(z,t + \Delta t) \]  

(8)

System physics is determined by the equilibrium distribution function \( f_{k,\text{eq}} \) and the relaxation parameter \( \omega \). While the former sets the transport phenomenon nature (i.e., heat, momentum or mass transfer), the later dictates the corresponding transport coefficient (i.e., thermal diffusivity, kinematic viscosity or mass diffusivity). For mass transfer problems (e.g., BAC), mass diffusivity \( D \) depends on \( \omega \) as well as on the so-called lattice sound speed \( c_s \) as follow [3],[5]:

\[ f_{k,\text{eq}}(z,t) = \frac{1}{\tau} \left( f_{k,\text{eq}} - f_k \right) \]  

(5)
\[ D = c_s \left( \frac{1}{\omega} - \frac{1}{2} \right) \Delta t \quad \Leftrightarrow \quad \frac{1}{\omega} = \frac{D}{c_s^2 \Delta t} + \frac{1}{2} \] (9)

For both D1Q2 and D1Q3, lattice sound speed is \( c_s = c = \Delta c/\Delta t \). As far as the equilibrium distribution function is concerned, the following expression can be used for advection-diffusion problems [3],[5]:

\[ f_k^{eq} = w_k \phi \left[ 1 + \frac{\tilde{c}_1 \cdot v}{c_s^2} \right] \] (10)

where \( \phi \) is the transported property whereas \( w_k \) are weighting factors obeying the normalizing condition \( \sum w_k = 1 \). For D1Q2 arrangement, \( w_0 = 0 \) refers to the central site while \( w_1 = w_2 = 1/2 \) refer to each streaming direction, which in line with Fig. 1(b) are related to lattice velocities \( \tilde{c}_1 = +c \tilde{z} \) and \( \tilde{c}_2 = -c \tilde{z} \).

For D1Q3, weighting factors are \( w_0 = 4/6 \) (central site) and \( w_1 = w_2 = 1/6 \) (each streaming direction).

Last but not least, at any instant \( t \) and position \( z \) one may retrieve the transported quantity \( \phi = \phi(z,t) \) from the distribution functions simply as [3],[5]:

\[ \phi(z,t) = \sum_k f_k(z,t) \] (11)

### 3 Numerical Method

#### 3.1 Dimensionless Method

Aiming at a dimensionless formulation of the BAC model considered in the present work, the following dimensionless variables are introduced:

\[ Z = \frac{z}{\Delta z}, \quad T = \frac{t}{\Delta t}, \quad \Phi = \frac{\phi}{\phi_{\text{in}}}, \quad \Theta = \frac{\theta}{\theta_{\text{max}}}, \quad \tilde{R} = \frac{\tilde{r}}{\tilde{r}_{\text{ref}}} \] (12)

being \( \tilde{r}_{\text{ref}} \neq 0 \) a reference value for species transfer rate (which is defined ahead) while the remaining parameters have been already introduced. In view of that, one may rewrite Eqs. (1) and (2) respectively in the following dimensionless form:

\[ \frac{\partial \Phi}{\partial T} + \text{Ma} \frac{\partial \Phi}{\partial Z} = \frac{1}{\text{Pe}_{\text{m}}} \frac{\partial^2 \Phi}{\partial Z^2} - \frac{1 - \varepsilon}{\varepsilon} P_0 \tilde{R} \] (13)

\[ \frac{\partial \Theta}{\partial T} = \tilde{R} = P_1 \Phi (1 - \Theta) - P_2 \Theta \] (14)

In Eqs. (13) and (14), lattice-based Mach number (Ma) and mass-transfer Peclet number (Pe_{m}) are:

\[ \text{Ma} = \frac{v}{c_s}, \quad \text{Pe}_{\text{m}} = \frac{c \Delta z}{D} = \frac{c^2 \Delta t}{D} = \frac{(\Delta c)^2}{\Delta t D} \] (15)

while the remaining dimensionless parameters are:

\[ P_0 = \tilde{r}_{\text{ref}} \Delta t \frac{\theta_{\text{max}}}{\phi_{\text{in}}}, \quad P_1 = k_1 \phi_{\text{in}} \Delta t, \quad P_2 = k_2 \Delta t \] (16)

It is worth noting that the reference value for species transfer rate results as \( \tilde{r}_{\text{ref}} = \theta_{\text{max}}/\Delta t \).

Being \( N_z = L/\Delta z \) so that \( N_z + 1 \) gives the number of lattice sites along the axial direction (end points included), the initial conditions as given by Eq. (3) assume the following dimensionless form (at \( T = 0 \)):

\[ \Phi = 0 \ (\text{fluid phase}) \quad , \quad \Theta = 0 \ (\text{solid phase}) \] (17)

while the boundary conditions expressed by Eq. (4) are cast in dimensionless form as:

\[ \text{at } z = 0: \quad \Phi = 1 \ , \quad \text{at } z = L: \frac{\partial \Phi}{\partial Z} = 0 \] (18)

#### 3.2 Implementation of LBM to numerically simulate BAC processes in fixed bed

Simulation of BAC processes needs two distribution functions. While \( f_k = f_k(Z,T) \) refers to the fluid-phase species concentration, \( s_k = s_k(Z,T) \) refers to the solid-phase species concentration. LBM was implemented on a D1Q2 lattice, according to the dimensionless formulation previously presented. In view of Eq. (11), dimensionless species concentrations in each phase are assessed as:

\[ \Phi(Z,T) = \sum_k f_k(Z,T) = f_1(Z,T) + f_2(Z,T) \]

\[ \Theta(Z,T) = \sum_k s_k(Z,T) = s_1(Z,T) + s_2(Z,T) \] (19)

In relation to equilibrium distribution functions \( f_k^{eq} \) and \( s_k^{eq} \), one must recall that Eqs. (13) and (14) refer respectively to an advective-diffusive transfer and a stationary medium. Using the same weighting factors \( w_k \) (\( w_0 = 0, w_1 = w_2 = 1/2 \)), one may adopt:

\[ f_k^{eq}(Z,T) = w_k \Phi(Z,T) [1 \pm \text{Ma}] \]

\[ s_k^{eq}(Z,T) = w_k \Theta(Z,T) \] (20)

Mach number sign in fluid-phase function depends on the streaming direction, namely +Ma for \( k = 1 \) (downward) and –Ma for \( k = 2 \) (upward).

In LBM, source or sink terms are introduced on the right-hand side of Eq. (5) and, thus, on the right-hand side of the related discrete approximation, Eq. (6). In line with the dimensionless formulation here introduced, the collision step with reference to the fluid phase is extended to include a sink term as:

\[ f_1(Z,T + \Delta T) = [1 - \omega_1] f_1(Z,T) + \omega_1 f_1^{eq}(Z,T) \]

\[ -w_k \left( \frac{1 - \varepsilon}{\varepsilon} \right) P_0 \tilde{R} \Delta T \] (21)
being \( R = P \Phi (1 - \Theta) - P \Theta \). A similar expression for the solid phase incorporates a source term as:

\[
s_z(Z,T + \Delta T) = [1 - \omega_s] s_z(Z,T) + \omega_s \Theta s_{eq}(Z,T)
\]

\[+ w_z \tilde{R} \Delta T \tag{22}\]

Distinct relaxation factors \( \omega_f \) and \( \omega_s \) are obtained as one adapts Eq. (9) to the physics of each phase, i.e.:

\[
\omega_f = (1/\text{Pe}_m + 1/2)^{-1}, \quad \omega_s = 2 \tag{23}\]

As far as the solid-phase species concentration is concerned, it is worth noting that there is no explicit dependence on the axial coordinate \( Z \) in Eq. (14). As suggested in [13], streaming in such phase can be implemented by either imposing periodic boundary conditions or by suppressing such LBM step itself. In this work, the later alternative has been adopted.

Bearing in mind Eq. (17), initial conditions for the fluid-phase functions are imposed as:

\[
f_1(Z,0) = w_1 \Phi(Z,0), \quad f_2(Z,0) = w_2 \Phi(Z,0) \tag{24}\]

with a similar rationale applied for the solid phase:

\[
s_1(Z,0) = w_1 \Theta(Z,0), \quad s_2(Z,0) = w_2 \Theta(Z,0) \tag{25}\]

At bed inlet \((Z = 0)\), the boundary condition for \( f_2(0,T) \) is obtained by streaming from adjacent site \( f_2(1,T) \), thus \( f_1(0,T) \) is the only unknown. Imposing \( \Phi(0,T) = 1 \) as given by Eq. (18), Eq. (19) provides:

\[
f_1(0,T) = 1 - f_2(0,T) \tag{26}\]

At bed outlet \((Z = N_z)\), the null Neumann condition imposed by Eq. (18) can be approximated by first-order finite differences, as described in [5], in order to arrive at the following conditions:

\[
f_1(N_z,T) = f_1(N_z - 1,T), \quad f_2(N_z,T) = f_2(N_z - 1,T) \tag{27}\]

4 Results and Discussion

LBM simulations were performed bearing in mind a classical work on bioaffinity separation in fixed bed [6], referenced in [7],[14] to test BAC simulators. Together with lattice parameters \( \Delta z \) and \( \Delta t \), Table 1 shows data regarding a chromatographic column studied in [6] as used in simulations in [7], together with values for lattice parameters \( \Delta z \) and \( \Delta t \).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column (bed) length</td>
<td>( L = 0.014 ) m</td>
</tr>
<tr>
<td>Column (bed) radius</td>
<td>( R = 0.005 ) m</td>
</tr>
<tr>
<td>Column (bed) porosity</td>
<td>( \varepsilon = 0.5 )</td>
</tr>
<tr>
<td>Inlet fluid-phase concentration</td>
<td>( \phi_{in} = 0.0071 ) mol/m(^3)</td>
</tr>
<tr>
<td>Maximum adsorption capacity</td>
<td>( \theta_{max} = 0.875 ) mol/m(^3)</td>
</tr>
<tr>
<td>Sorption coefficient</td>
<td>( k_1 = 0.286 ) m(^3/(mol-s))</td>
</tr>
<tr>
<td>Desorption coefficient</td>
<td>( k_2 = 0.0005 ) s(^{-1})</td>
</tr>
<tr>
<td>Interstitial fluid velocity</td>
<td>( v = 2.24 \times 10^{-4} ) m/s</td>
</tr>
<tr>
<td>Distance between sites</td>
<td>( \Delta z = 0.0001 ) m</td>
</tr>
<tr>
<td>Advancing time step</td>
<td>( \Delta t = 0.05 ) s</td>
</tr>
</tbody>
</table>

Table 2. Resulting dimensionless parameters used to perform LBM simulations in the present work.

\[
N_z = L/\Delta z = 140 \tag{28}\]

\[
P_0 = \theta_{max}/\phi_{in} = 123.24 \tag{29}\]

\[
P_1 = k_1 \phi_{in} \Delta t = 1.0153 \times 10^{-2} \tag{30}\]

\[
P_2 = k_2 \Delta t = 2.5 \times 10^{-5} \tag{31}\]

\[
Ma = v/c_a = v/(\Delta z/\Delta t) = 0.112 \tag{32}\]

\[
\Delta Z = \Delta T = 1 \tag{33}\]

Breakthrough curves simulated through LBM are compared to experimental results from [6] in Fig. 2, for the pre-defined testing \( \text{Pe}_m \) values. The aforesaid curves refer to the fluid-phase species concentration at bed outlet, i.e., \( \Phi_{out}(T) = \Phi(N_z,T) \). On qualitative basis, the breakthrough curve pertaining to \( \text{Pe}_m = 1 \) seems to better reproduce the experimental data.

In [7], simulations were also accomplished for a lower value for the maximum adsorption capacity of the column, namely \( \theta'_{max} = 0.845 \) mol/m\(^3\), for which

![Fig. 2. Experimental data [6] and LBM-simulated breakthrough curves for distinct \( \text{Pe}_m \), using process parameters as adopted in [7].](image-url)
Eq. (16) yields \( P'_0 = 119.01 \). The corresponding new breakthrough curves simulated via LBM are shown in Fig. 3. The curve concerning \( \text{Pe}_m = 1 \) seems now to better reproduce the experimental data, though at the expenses of larger deviations at the final portion of the curve (i.e., near column saturation).

![Fig. 3. Experimental data [6] and LBM-simulated breakthrough curves for distinct \( \text{Pe}_m \), using a lower maximum adsorption capacity as suggested in [7].](image1)

A slightly higher value for maximum adsorption capacity is here tested so as to yield \( P'_0 = 125 \). The corresponding LBM-simulated breakthrough curves are shown in Fig. 4. Again, the breakthrough curve related to \( \text{Pe}_m = 1 \) reproduce closer the experimental data but with better performance than that in Fig. 2.

![Fig. 4. Experimental data [6] and LBM-simulated breakthrough curves for distinct \( \text{Pe}_m \), using a lower maximum adsorption capacity as suggested in [7].](image2)

Regardless of the testing \( \text{Pe}_m \) (and \( P_0 \)) values, it is worth noting that LBM-simulated breakthrough curves reasonably reproduce the overall behavior of experimental data. As far as noted discrepancies are concerned, the following points should be pondered.

Firstly, bed porosity was arbitrarily set as \( \varepsilon = 0.5 \) to yield \( (1 - \varepsilon)/\varepsilon = 1 \) so that Eq. (1) could become equivalent to the governing equation adopted in [7]. In such later work, bed porosity influence is already accounted in values for \( \theta_{\text{max}}, k_1 \) and \( k_2 \) as shown in Table 1, which are those used in LBM simulations.

Secondly (and as already cited), mass diffusivity is neglected in [7] so that species transport becomes advection-dominant. On the contrary, this work tests some distinct values for \( \text{Pe}_m \) (and thus for \( D \)) as an attempt to simulate an advection-diffusion problem. Respectively via Eq. (9) and (23), \( D \) and \( \text{Pe}_m \) dictate the relaxation factor \( \omega_f \) in LBM simulations.

From Eq. (15) one clearly notes that \( D = 0 \) leads to \( \text{Pe}_m \to \infty \). Yet, as Fig. 2 shows, greater deviations are verified for larger \( \text{Pe}_m \), which may suggest a re-evaluation of some (if not all) process parameters in Table 1. As the main purpose here is to check out proper implementation and functionality of the pilot LBM code, such comprehensive investigation falls beyond the scope of this work.

### 5 Concluding Remarks

Even for simplified models for biospecific affinity chromatography (BAC), mathematical hurdles still justify the use of numerical methods. As a first step towards simulation of BAC processes in fixed beds through lattice-Boltzmann method (LBM), this work applied LBM by relying on a time-dependent one-dimensional model evoking uniform flow, sorption-desorption kinetics and mass (species) transport by convection and diffusion. As governing equations were cast into dimensionless formulation, additional dimensionless parameters emerged besides lattice-based Mach and mass-transfer Peclet numbers.

It was noticed that the governing equation for the solid-phase species concentration lacked explicit dependence on the spatial coordinate (bed axis). For that reason, the related streaming step was simply suppressed with no loss functionality as far as the implementation of LBM code is concerned.

As numerical breakthrough curves were able to reproduce the general behavior of experimental data from a standard work on BAC in fixed beds, it is believed that one may adapt and/or extend such pilot LBM code so as to simulate other BAC processes of interest. In particular, the goal is to use it to support on-going experimental BAC research at FZEa/USP (Pirassununga campus, Brazil).

**Acknowledgement**

The author thanks FAPESP (São Paulo Research Foundation, Brazil) for their financial support to the research project (No. 05/02538-1) from which the present work derives.
**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$c$</td>
<td>lattice speed (m·s$^{-1}$)</td>
</tr>
<tr>
<td>$D$</td>
<td>species diffusivity (m$^2$·s$^{-1}$)</td>
</tr>
<tr>
<td>$f$</td>
<td>distribution function (dimensionless)</td>
</tr>
<tr>
<td>$k_1$</td>
<td>sorption constant (m$^3$·mol$^{-1}$·s$^{-1}$)</td>
</tr>
<tr>
<td>$k_2$</td>
<td>desorption constant (s$^{-1}$)</td>
</tr>
<tr>
<td>$L$</td>
<td>fixed-bed length (m)</td>
</tr>
<tr>
<td>$Ma$</td>
<td>Mach number (dimensionless)</td>
</tr>
<tr>
<td>$N_c$</td>
<td>index of last lattice site (dimensionless)</td>
</tr>
<tr>
<td>$Pe_m$</td>
<td>mass-transfer Peclet number (dimensionless)</td>
</tr>
<tr>
<td>$P_i$</td>
<td>dimensionless parameters ($i = 0, 1, 2$)</td>
</tr>
<tr>
<td>$R$</td>
<td>fixed-bed inner radius (m)</td>
</tr>
<tr>
<td>$R_d$</td>
<td>dimensionless source or sink term</td>
</tr>
<tr>
<td>$r$</td>
<td>source or sink term (mol·m$^{-3}$·s$^{-1}$)</td>
</tr>
<tr>
<td>$s$</td>
<td>distribution function (dimensionless)</td>
</tr>
<tr>
<td>$T$</td>
<td>dimensionless time</td>
</tr>
<tr>
<td>$t$</td>
<td>time (s)</td>
</tr>
<tr>
<td>$v$</td>
<td>interstitial fluid velocity (m·s$^{-1}$)</td>
</tr>
<tr>
<td>$w$</td>
<td>weighting factors (dimensionless)</td>
</tr>
<tr>
<td>$Z$</td>
<td>dimensionless fixed-bed axial coordinate</td>
</tr>
<tr>
<td>$z$</td>
<td>fixed-bed axial coordinate (m)</td>
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**Greek symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$\varepsilon$</td>
<td>fixed-bed porosity (dimensionless)</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>dimensionless fluid-phase concentration</td>
</tr>
<tr>
<td>$\phi$</td>
<td>fluid-phase concentration (mol·m$^{-3}$)</td>
</tr>
<tr>
<td>$\Theta$</td>
<td>dimensionless solid-phase concentration</td>
</tr>
<tr>
<td>$\theta$</td>
<td>solid-phase concentration (mol·m$^{-3}$)</td>
</tr>
<tr>
<td>$\tau$</td>
<td>relaxation time (s)</td>
</tr>
<tr>
<td>$\omega$</td>
<td>relaxation parameter (dimensionless)</td>
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**Subscripts and superscripts**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>eq</td>
<td>equilibrium distribution function</td>
</tr>
<tr>
<td>f</td>
<td>fluid phase</td>
</tr>
<tr>
<td>in</td>
<td>fixed-bed inlet</td>
</tr>
<tr>
<td>k</td>
<td>lattice direction / lattice link</td>
</tr>
<tr>
<td>max</td>
<td>maximum adsorption capacity of the column</td>
</tr>
<tr>
<td>ref</td>
<td>reference value</td>
</tr>
<tr>
<td>s</td>
<td>solid phase or lattice sound speed</td>
</tr>
<tr>
<td>z</td>
<td>fixed-bed axial coordinate</td>
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<td>central lattice site</td>
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<tr>
<td>$^\wedge$</td>
<td>unit vector</td>
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**References:**


