LATTICE BOLTZMANN SIMULATION OF TRANSPORT PHENOMENA IN FOOD AND BIOPROCESSES: FUNDAMENTALS AND APPLICATIONS

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ABSTRACT
As part of ongoing research on computational modelling of agroindustrial biosystems, lattice Boltzmann method (LBM) have been applied in order to numerically simulate transport phenomena in food and bioprocesses. This paper addresses LBM simulation of two different continuous-flow processes in fixed-bed equipment whose models are quite similar, namely bioaffinity chromatography and extraction of biocompounds. Considering a dynamic one-dimensional model framework for those processes, LBM was implemented in D1Q2 lattice and particle distribution functions were assigned to species (adsorbate or extract) concentrations in both fluid and solid phases. Equilibrium distribution functions were set by considering diffusive-convective transport in the fluid phase whereas the solid phase remains stationary. LBM simulations were carried out in view of existing research work on bioseparation of lysozyme and extraction of essential oil from gorse. As the governing equation for species concentration in the solid phase lacked partial derivatives with respect to the spatial coordinate, the corresponding streaming step was suppressed in the LBM code. No loss of functionality was verified and the expected shapes of breakthrough as well as extraction yield curves were suitably reproduced in all LBM simulations.

KEY WORDS
Computational modelling, chromatography, extraction, porous media, continuous-flow process.

1. Introduction

Comprehensive knowledge of transport phenomena in food and bioprocesses is prone to invoke governing equations whose complexity requires numerical methods [1]. Mathematical hurdles arise due to mutual interference between fluid velocity and scalar quantities (e.g., chemical species) allied to assorted chemical kinetics, composition variability, and moving interfaces typically encountered in multiphase systems. Computational modelling becomes helpful not only when aforementioned difficulties prevent analytical solutions from being deduced but also when obtaining real-operation or experimental data becomes awkward or even unfeasible [2].

Computational modelling has long been a powerful engineering tool in several industrial sectors while other sectors bestow underexplored opportunities. By quoting the editorial of the special issue on “Virtualization of Processes in Food Engineering” in the Journal of Food Engineering: “While a number of manufacturing sectors (e.g., aerospace, defense, automotive) are benefitting for decades from modeling activities and virtualization of processes, the food industry (that represents more than 5% of the global GDP) is still lagging to utilize the wide spectrum potential offered by virtualization as an engineering design tool” [3]. Besides open innovation and social responsibility, modelling and virtualization were identified as new challenges and opportunities for food engineers in the 21st century [4].

Besides aforementioned special issue of the Journal of Engineering, the awareness of the food industry toward computational modelling can also be evidenced by CFD (computational fluid dynamics) simulations in numerous practical applications [5]. While off-the-shelf software has been applied in food manufacturing processes [6], this work is part of ongoing research aiming at developing in-house simulators of food and bioprocesses by the use of lattice Boltzmann method (LBM) [7].

LBM was envisaged in [8] as a spin-off of lattice gas cellular automata (LGCA). More recent than traditional discretization methods such as finite elements or finite volumes, LBM has become an innovative computational technique to simulate food and bioprocesses at different length scales [9]. As it is able to simulate fluid flow and multiphase phenomena without directly solving Navier-Stokes equations [10], LBM leads to relatively simpler computer codes [11]. Such feature is appealing for those who have already programmed their in-house numerical simulators via classic discretization methods.

In view of LBM simulation of food and bioprocesses, there is indeed worldwide research niche to be explored. Among almost 1000 communications in IUFoST 2014 - 17th World Congress of Food Science and Technology, only three directly dealt with LBM simulation [12]-[14]. As an attempt to fill up this research gap, LBM has been applied to simulate transport phenomena in continuous-flow or batch separation processes involving either food or natural products [7],[14]-[17].

While there is no doubt about the efficiency of classic methods to perform similar simulations, this paper aims at presenting LBM as an alternative to simulate transport phenomena in food and bioprocesses. LBM fundamentals will be addressed next and applications will refer to LBM
2. Theory

2.1 Fundamentals of Lattice Boltzmann Method

Lattice Boltzmann method (LBM) treats any macroscopic medium (whether solid or fluid) as comprised by fictitious particles in a fictitious lattice structure (i.e., discrete space) assigned to the medium. During discrete time steps, those constituent particles follow two courses of action, namely streaming and collision.

During the streaming step particles travel between adjacent lattice sites through different links which are defined by the lattice structure. As they arrive at lattice sites, particles mutually strike during the collision step so that their velocities become rearranged for subsequent streaming-collision processes. By imposing conservation principles to such particle dynamics, the macroscopic behaviour of the medium can be simulated [10].

Inspired by kinetic gas theory, LBM mathematically relies on a particle distribution function \( f(\vec{c}, \vec{r}, t) \) giving the population of particles with velocities between \( \vec{c} \) and \( \vec{c} + d\vec{c} \) about position \( \vec{r} \) at time \( t \). By taking suitable moments of function \( f \), one may assess macroscopic (i.e., observable) properties such as species concentration, bulk flow velocity, and temperature [9]-[11].

Particle distribution function \( f \) is ruled by Boltzmann transport equation. In the absence of any external force, Boltzmann transport equation reads as [9]-[11]:

\[
\frac{\partial f}{\partial t} + \vec{c} \cdot \nabla f = \Omega(f), \quad \text{with} \quad \Omega(f) = \frac{f_{eq} - f}{\Delta t_{relax}}
\]  

(1)

where the collision operator \( \Omega = \Omega(f) \) gives the variation rate of function \( f \) due to collisions between particles. In Eq. (1), BGK approach (after Bhatnagar-Gross-Krook) has been invoked to linearize the collision operator as \( \Omega(f) = \frac{f_{eq} - f}{\Delta t_{relax}} \). This means that particles tend to equilibrium values \( f_{eq} \) of the distribution function at a rate controlled by the relaxation time \( \Delta t_{relax} \) [18].

LBM is implemented to numerically solve Eq. (1) as written in terms of the fictitious lattice structure assigned to the macroscopic medium, when it becomes referred to as lattice Boltzmann equation (LBE). In LBM, lattices are identified as \( DnQm \), where \( n \) is the problem dimension (e.g., \( n = 1 \) = 1-D) whereas \( m \) refers to the speed model (= number of particle distribution functions \( f_k \) to be solved for each observable property). Typical LBM lattices are depicted elsewhere [9]-[11].

As discussed above, model frameworks addressed in this paper are 1-D, without loss of generality. Let LBE-BGK be written for particle distribution function \( f_k(x, t) \) at time \( t \), position \( x \) and a given streaming link \( k \), namely:

\[
\frac{\partial f_k(x, t)}{\partial t} + c_k \frac{\partial f_k(x, t)}{\partial x} = \frac{f_{eq}^k(x, t) - f_k(x, t)}{\Delta t_{relax}}
\]  

(2)

The basic linear structure of lattices D1Q2 and D1Q3 comprises a central site linked to two adjacent sites (one at each side) so that \( k = 1 \) and \( k = 2 \) respectively stand for forward and backward streaming. If \( \Delta t \) is the advancing time step, then \( c_k = \Delta t_0/\Delta t \) refers to each streaming speed, being \( \Delta t_1 = +\Delta t \) (forward) and \( \Delta t_2 = -\Delta t \) (backward). Null speed \( c_0 = 0 \) is allowed in D1Q3 but not in D1Q2 so that Eq. (2) is written for \( k = 0, 1 \) and 2 in D1Q3 while it is written solely for \( k = 1 \) and 2 in D1Q2, i.e., function \( f_0 \) is disregarded (not used) in D1Q2 lattice.

Discretization of Eq. (2) in space and time yields an algebraic equation whose iterative evolution is completed in two steps. In the collision step (time evolution), particle distribution functions \( f_k \) are updated from previous instant \( t \) to subsequent instant \( t + \Delta t \) at all lattice sites. Source or sink terms \( s \) are included at this step so that the following algebraic expression holds:

\[
f_k(x, t + \Delta t) = [1 - \omega] f_k(x, t) + \omega f_{eq}^k(x, t) + w_k s \Delta t
\]  

(3)

where \( \omega = \Delta t_{relax}/\Delta t \) is referred to as relaxation parameter and \( w_k \) are weighting factors whose values (fulfilling the condition \( \sum w_k = 1 \)) depend on the lattice structure as shown in Table 1. During the streaming step (spatial evolution), collision outcomes are propagated to adjacent (i.e., neighbouring) lattice sites as:

\[
f_k(x + \Delta x_k, t + \Delta t) = f_k(x, t + \Delta t)
\]  

(4)

2.2 Physics-Based Models of Transport Phenomena in Food and Bioprocesses Addressed in This Paper

This paper focuses on two continuous-flow processes in fixed-bed equipment, namely, the load step of bioaffinity...
chromatography and the extraction of biocompounds. Although these are distinct processes, their models are similar [19] and common aspects are discussed next.

Fixed beds have been modelled as cylindrical porous media with diameter \(d\), length \(L\), and uniform porosity \(\varepsilon\) throughout the bed. Coordinate axis \(x\) is aligned with the flowing direction of the percolating fluid so that bed inlet is at \(x = 0\) while bed exit is at \(x = L\). Volumetric flow rate \(V\) has been supposed constant so that the interstitial fluid velocity \(v = 4V/(\pi d^2)\) results constant and uniform.

Stratification has been assumed with respect to axis \(x\) so that species concentrations (or any physical quantity) are functions of time \(t\) and coordinate \(x\), i.e. models are dynamic with first-order dependence in space. Therefore, concentrations in solid and fluid phases are respectively identified as \(q(x,t)\) and \(c(x,t)\) in the present work.

Some models have neglected species diffusion in the fluid phase [20]-[27] as convective-dominant differential equations remain parabolic, therefore dismissing an extra boundary condition (at bed exit) while enabling the use of marching numerical methods (e.g. Runge-Kutta). In view of comprehensiveness towards long equipment [28]-[29], diffusive transport has been taken into account in the fluid phase since early versions of LBM simulators [7].

### 2.2.1 Load Step of Bioaffinity Chromatography

Bioaffinity chromatography models have invoked 2nd-order adsorption and 1st-order desorption kinetics (i.e. Langmuir kinetics) during the load step [20],[30]-[35]. If \(k_{ads}\) and \(k_{des}\) are respectively adsorption and desorption kinetic coefficients while concentration \(q_{max}\) refers to the maximum adsorption capacity of the chromatographic column, the governing differential equation for adsorbate concentration \(q\) in solid phase has been proposed as:

\[
\frac{dq}{dt} = \dot{r} \quad \text{with} \quad \dot{r} = k_{ads}c(q_{max} - q) - k_{des}q
\]

where \(\dot{r} > 0\) (source term in this equation) is the net rate at which adsorbate is transferred from fluid to solid phase.

Let adsorbate be transported in the fluid phase via diffusion and convection. By accounting for the above net transfer rate \(\dot{r}\) behaving as sink term (as the fluid phase depletes adsorbate), the governing equation for adsorbate concentration \(c\) in the fluid phase has been put forward as:

\[
\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} - \frac{1 - \varepsilon}{\varepsilon} \dot{r}
\]

where \(D\) is adsorbate diffusivity in the fluid phase.

The initial conditions for Eqs. (6) and (7) have been imposed as:

\[
q(x,0) = 0 \quad \text{and} \quad c(x,0) = 0 \quad , \quad \text{for} \quad 0 \leq x \leq L
\]  

While Eq. (6) does not require boundary conditions (as it lacks partial derivatives with respect to coordinate \(x\)), Eq. (7) needs two boundary conditions. If \(c_0\neq 0\) is adsorbate concentration in feeding solution, at column inlet (\(x = 0\)) one may impose either Dirichlet condition [20],[25],[34]:

\[
c(0,t) = c_0 \quad , \quad \text{for} \quad t > 0
\]

or Danckwerts condition [32],[33],[35]:

\[
v c_0 = v c(0,t) - D \frac{\partial q}{\partial x} \bigg |_{x=0} \quad , \quad \text{for} \quad t > 0
\]

which simplifies to Dirichlet condition for \(D = 0\). At exit (\(x = L\)), null Neumann condition has been imposed:

\[
\frac{\partial c}{\partial x} \bigg |_{x=L} = 0 \quad , \quad \text{for} \quad t > 0
\]

### 2.2.2 Extraction of Biocompounds

Some extraction models have assumed that extract (i.e. biocompound) is released from solid phase at a rate \(\dot{r}\) set by an intra-particle diffusion time \(\Delta_{intra}\) together with a concentration difference \(q - q_{s-f}\), where \(q_{s-f}\) is extract concentration at the solid-fluid interface [26]. Aiming at similarity with Eq. (6), the following equation is written:

\[
\frac{dq}{dt} = \dot{r} \quad , \quad \text{with} \quad \dot{r} = \frac{q - q_{s-f}}{\Delta_{intra}} \quad \text{and} \quad \Delta_{intra} = \frac{\mu_s l_s^2}{D_{intra}}
\]

Extract release rate \(\dot{r}\) is inherently negative (sink term) consistent with \(\dot{q} < 0\) (because extract concentration decreases within the solid phase). Intra-particle diffusion time \(\Delta_{intra}\) is assessed from particle features including a dimensionless shape coefficient \(\mu_s\), a characteristic length \(l_s\), and intraparticle diffusivity \(D_{intra}\) [36].

At any time \(t\) and position \(x\), a direct proportion has been assumed between concentration \(c\) in fluid phase and concentration \(q_{s-f}\) at solid-fluid interface, namely:

\[
c(x,t) = k_p q_{s-f}(x,t)
\]

where \(k_p\) is known as partition coefficient [26]. Together with intraparticle diffusivity, partition coefficient has been typically invoked in extraction models [37]. By inserting Eq. (13) in Eq. (12) one obtains the following governing equation for the extract concentration \(q\) in the solid phase:

\[
\frac{dq}{dt} = \dot{r} \quad , \quad \text{with} \quad \dot{r} = -\frac{1}{\Delta_{intra}} \left( q - \frac{c}{k_p} \right)
\]

Diffusive-convective transport has been considered in the fluid phase. By recalling that extract release rate \(\dot{r}\) is
negative, the governing equation for extract concentration \( c \) in the fluid phase has been put forward as follows:

\[
\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} - \frac{1 - \varepsilon}{\varepsilon} \dot{r} \tag{15}
\]

which is similar to Eq. (7) to the point that symbols have the same meaning. The difference is that \(-\dot{r}(1-\varepsilon)/\varepsilon > 0\) now behaves as a source term (as \( \dot{r} < 0 \)), in line with the fact that extract is released from solid to fluid phase.

If \( q_{\text{max}} \) now refers to maximum extraction capacity of raw products (i.e. solid phase), initial conditions for Eqs. (14) and (15) are:

\[
q(x,0) = q_{\text{max}} \quad \text{and} \quad c(x,0) = 0 \quad \text{for} \quad 0 \leq x \leq L \tag{16}
\]

As Eq. (14) lacks derivatives with respect to coordinate \( x \), boundary conditions are only imposed to Eq. (15). Null Dirichlet condition has been invoked at extractor inlet:

\[
c(0,t) = c_m = 0 \quad \text{for} \quad t > 0 \tag{17}
\]

and null Neumann condition has been imposed at the exit:

\[
\frac{\partial c}{\partial x}\bigg|_{x=L} = 0 \quad \text{for} \quad t > 0 \tag{18}
\]

3. Numerical Method

With codes lines following those in [11], LBM has been programmed in FORTRAN 90/95 to simulate bioaffinity chromatography and biocompounds extraction as based on 1-D dynamic models described in the previous section. At their current development stage, those LBM simulators have used D1Q2 lattice to computationally model species concentrations in both fluid and solid phases.

Accordingly, two particle distribution functions are needed. Specifically, functions \( s_k \) and \( f_k \) refer to species concentrations \( q \) and \( c \) respectively in solid and fluid phases. In view of Eq. (5) written for D1Q2 lattice (being \( k = 1 \) for forward streaming and \( k = 2 \) for backward streaming), at any axial position \( x \) and time \( t \) those species concentrations can be assessed as:

\[
q(x,t) = s_1(x,t) + s_2(x,t) \quad \text{and} \quad c(x,t) = f_1(x,t) + f_2(x,t) \tag{19}
\]

In line with Eq. (3), collision steps were numerically implemented as:

\[
s_k(x,t + \Delta t) = [1 - \omega_k] s_k(x,t) + \omega_k s_k^\text{eq}(x,t) + w_k \dot{s}_k \Delta t \tag{20} \]

\[
f_k(x,t + \Delta t) = [1 - \omega_k] f_k(x,t) + \omega_k f_k^\text{eq}(x,t) + w_k \dot{s}_k \Delta t
\]

with \( \dot{s}_k = \dot{r} \) and \( \dot{s}_k = -\dot{r}(1-\varepsilon)/\varepsilon \) behaving as either sink or source according to the governing equations, i.e. Eqs. (6) and (7) for bioaffinity chromatography and Eqs. (14) and (15) for biocompounds extraction. Weighting factors \( w_k \) are those in Table 1 for D1Q2 lattice.

Since both Eqs. (6) and (14) lack partial derivatives with respect to coordinate \( x \), it was possible to suppress the streaming step relating to distribution functions \( s_k(x,t) \) from the LBM code [38]. In opposition, streaming was implemented for functions \( f_k(x,t) \) according to Eq. (4).

By recalling that the solid phase remains stationary while diffusive-convective transport occurs in fluid phase, equilibrium distribution functions were set as [11]:

\[
s_k^\text{eq}(x,t) = w_k q(x,t) \quad f_k^\text{eq}(x,t) = w_k c(x,t)(1 + \text{Ma}) \tag{21}
\]

where \( \text{Ma} = v \cdot \Delta t/\Delta x \) is lattice-based Mach number with \( \Delta x_1 = +\Delta x \) (forward) and \( \Delta x_2 = -\Delta x \) (backward) in D1Q2 lattice. In view of the underlying physics of the governing equations, relaxation factors \( \omega_s \) and \( \omega_f \) referring to solid and fluid phases were defined as [11]:

\[
\omega_s = 2 \quad \text{and} \quad \omega_f = \left[ \frac{D \Delta t}{(\Delta x)^2} + \frac{1}{2} \right]^{-1} = \left[ \frac{\text{Ma}}{\text{Pe}_s} + \frac{1}{2} \right]^{-1} \tag{22}
\]

where \( \text{Pe}_s = v \cdot \Delta x/D \) is lattice-based Péclet number for mass (species) transfer whereas \( \omega_f = 2 \) was obtained by imposing null diffusivity for the solid phase.

With initial concentrations \( q(x,0) \) and \( c(x,0) \) given by Eqs. (8) and (16), the initial conditions for corresponding particle distribution functions were set as [11]:

\[
s_k(x,0) = w_k q(x,0) \quad \text{and} \quad f_k(x,0) = w_k c(x,0) \tag{23}
\]

At bed inlet \((x = 0)\), \( f_2(0,t) \) is obtained through backward streaming from the adjacent lattice site so that \( f_2(0,t) \) is the unknown. By invoking flux conservation [11] together with Eq. (9) or (17), Dirichlet condition was implemented in the LBM simulation code as:

\[
f_1(0,t) = c(0,t) - f_2(0,t) \Rightarrow f_1(0,t) = c_m - f_2(0,t) \tag{24}
\]

For brevity, Danckwerts condition will not be considered in this work. At bed exit \((x = L)\), \( f_2(L,t) \) is obtained via forward streaming and \( f_1(L,t) \) is the unknown. By relying on 1st-order finite-differences approximation of \( \partial c/\partial x \), the null Neumann condition, either Eq. (11) or (18), leads to:

\[
f_2(L,t) = f_2(L - \Delta x,t) \tag{25}
\]

4. Results and Discussion

4.1 Load Step of Bioaffinity Chromatography

As far as the load step of bioaffinity chromatography is concerned, the LBM simulator can supply breakthrough curves at column exit \((x = L)\), which are time-dependent
dimensionless curves mathematically defined as \( c(L,t) / c_{in} \). In order to exemplify aforesaid curves, the present work performed LBM simulations in view of a classic work on lysozyme bioseparation [39], whose process parameters are shown in Table 2.

### Table 2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concentration in feed solution</td>
<td>( c_{in} = 0.0071 \text{ mol/m}^3 )</td>
</tr>
<tr>
<td>Maximum adsorption capacity ( q_{\text{max}} )</td>
<td>( 0.875 \text{ mol/m}^3 )</td>
</tr>
<tr>
<td>Adsorption kinetic coefficient ( k_{\text{ads}} )</td>
<td>( 0.286 \text{ m}^3/(\text{mol-s}) )</td>
</tr>
<tr>
<td>Desorption kinetic coefficient ( k_{\text{des}} )</td>
<td>( 5 \times 10^{-4} \text{ s}^{-1} )</td>
</tr>
<tr>
<td>Interstitial velocity of solution ( v )</td>
<td>( 2.24 \times 10^{-4} \text{ m/s} )</td>
</tr>
</tbody>
</table>

![Figure 1](image1.png)

Figure 1. LBM simulations for each trial \( D \) value: experimental breakthrough curves [39] compared with LBM-simulated counterparts by using (a) \( q_{\text{max}} = 0.875 \text{ mol/m}^3 \) as in [39] and (b) \( q_{\text{max}} = 0.845 \text{ mol/m}^3 \) as in [20].

Among columns of different lengths studied in [39], the present work carried out LBM simulations for column with \( L = 0.041 \text{ m} \). LBM parameters were set as \( \Delta x = 1.0 \times 10^{-4} \text{ m} \) and \( \Delta t = 0.05 \text{ s} \) in order to ensure low lattice-based Mach number [11]. LBM simulations were performed by adopting some trial (i.e. non-fitted) values of adsorbate diffusivities in fluid phase, namely \( D \text{ (m}^2/\text{s}) = 1.0 \times 10^{-7}, 2.0 \times 10^{-7} \) and \( 4.0 \times 10^{-7} \). In Figure 1(a), experimental data from [39] are compared with breakthrough curves simulated via LBM by adopting aforesaid trial \( D \) values together with process parameters in Table 2. Bed porosity was set as \( \varepsilon = 0.5 \) to render \( (1 - \varepsilon) / \varepsilon = 1 \) so that Eq. (7) could exactly match its counterpart as proposed in [39]. It is worth recalling that diffusive transport spreads species (i.e. adsorbate) in forward as well as backward directions in 1-D transport. Hence, the slope of numerical breakthrough curves becomes reduced as \( D \) increases so that curves deviate from experimental data. Yet, the “S” shape of breakthrough curves was suitably reproduced in all LBM simulations.

Additional LBM simulations were carried out by adopting \( q_{\text{max}} = 0.845 \text{ mol/m}^3 \), which is a lower value also tested in [20]. By using the same trial diffusivities \( D \) as in preceding simulations, Figure 1(b) compares experimental data [39] with those additional numerical breakthrough curves. When compared with counterparts in Figure 1(a), one verifies that curve slopes remain basically unchanged while curve saturation is anticipated, i.e. the instant when \( c(L,t) / c_{in} = 1 \) becomes shifted to the left. Such anticipation is expected as the maximum adsorption capacity \( q_{\text{max}} \) of the column was reduced, i.e. column saturates faster.

### 4.2 Biocompounds Extraction

Simulations were performed in view of the extraction of essential oil from gorse by the use of supercritical \( \text{CO}_2 \) as investigated in [26]. Table 3 shows the process parameters concerning the extraction carried out at 70°C. Based on such parameters, Eq. (12) then renders \( \Delta t_{\text{intra}} = 305.25 \text{ s} \) as intraparticle diffusion time.

### Table 3

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bed length and diameter ( L )</td>
<td>( 0.045 \text{ m}, d = 0.011 \text{ m} )</td>
</tr>
<tr>
<td>Bed porosity ( \varepsilon )</td>
<td>0.669</td>
</tr>
<tr>
<td>Maximum extraction capacity ( q_{\text{max}} )</td>
<td>( 27.0 \text{ kg/m}^3 )</td>
</tr>
<tr>
<td>Shape coefficient ( \mu )</td>
<td>( 1/3 )</td>
</tr>
<tr>
<td>Characteristic length ( l_c )</td>
<td>( 5 \times 10^{-4} \text{ m} )</td>
</tr>
<tr>
<td>Intraparticle diffusivity ( D_{\text{intra}} )</td>
<td>( 2.73 \times 10^{-10} \text{ m}^2/\text{s} )</td>
</tr>
<tr>
<td>Partition coefficient ( k_p )</td>
<td>0.0667</td>
</tr>
<tr>
<td>Interstitial velocity of ( \text{CO}_2 )</td>
<td>( 5.243 \times 10^{-4} \text{ m/s} )</td>
</tr>
<tr>
<td>Total mass of raw material ( m_{\text{total}} )</td>
<td>( 0.0015 \text{ kg} )</td>
</tr>
</tbody>
</table>

LBM parameters were set as \( \Delta x = 2.0 \times 10^{-4} \text{ m} \) and \( \Delta t = 0.1 \text{ s} \). Analogous to prior section, LBM simulations were performed for the following trial values of species (i.e. extract) diffusivities in fluid phase: \( D \text{ (m}^2/\text{s}) = 1.0 \times 10^{-6}, 2.0 \times 10^{-6} \) and \( 4.0 \times 10^{-6} \). For each testing \( D \) value, Figure 2(a) shows the simulated curves for \( c_{\text{out}}(t) = c(L,t) \), i.e. time evolution of extract concentration in the fluid phase at bed exit, while Figure 2(b) shows the simulated
curves for $q_0(t) = q(0,t)$, i.e. time evolution of the extract concentration in the solid phase at bed inlet.

As one may observe in Figure 2(a), large amounts of essential oil are extracted at initial instants of the process. As the solid phase becomes depleted, as exemplified by Figure 2(b), the extract concentration in the fluid phase at bed exit $c_{\text{out}}(t)$ gradually decreases as expected. As Figure 2(b) shows, it is worth noting that extract concentration in solid phase (at bed inlet) are rather insensitive to species diffusivity $D$ in the fluid phase. Conversely, as diffusion spreads species in both forward and backward directions in 1-D transport, this spreading effect could be evidenced in extract concentration in the fluid phase, Figure 2(a).

Figure 2. LBM simulations for each trial $D$ value: (a) time evolution of extract concentration in the fluid phase at the bed outlet and (b) in the solid phase at bed inlet.

As Figure 2 illustrates, the LBM simulator deals with extract concentrations in either fluid or solid phase. Yet, experimental results have been habitually presented and compared in terms of the time evolution of extract yield $Y(t)$. On mass basis, one may express $Y(t)$ as the mass of species extracted up to instant $t$ divided by the total mass $m_{\text{total}}$ of raw material in the extractor. Based on total mass $m_{\text{total}}$, exiting concentration $c_{\text{out}}(t)$ and volumetric flow rate $\dot{V} = \frac{\pi d^2}{4} \varepsilon$, one may assess extraction yield $Y(t)$ as:

$$Y(t) = \frac{1}{m_{\text{total}}} \int_0^t \dot{V} c_{\text{out}}(t') \, dt' \quad (26)$$

The integration in Eq. (26) is numerically evaluated in the simulation code.

For each extract diffusivity $D$ examined in Figure 2, Figure 3 compares extract yields numerically simulated via LBM against experimental counterparts obtained at $70^\circ C$ [26]. While LBM simulations were able to replicate the overall trend of extraction yield curve $Y(t)$, observed discrepancies with respect to experimental data [26] are addressed next.

Figure 3. LBM simulations for each trial $D$ value: comparison between experimental extract yield curves [26] and LBM-simulated counterparts.

It is worth bearing in mind that process parameters in Table 3 were originally obtained via fine-tuning as based on a convective-dominant model framework [26]. In other words, diffusive transport in the fluid phase was neglected ($D = 0$) in [26] so that adsorbate transport was convective dominant. However, numerical schemes for convective transport (e.g. upwind scheme) are prone to render false (numerical) diffusion [40], which is not the case of LBM [9],[11]. For instance, with respect to numerical simulation of species transport via finite differences method, false diffusion becomes noticeable as convection prevails over diffusion, i.e. as $D \rightarrow 0$ [19]. Accordingly, re-evaluation of either some or all process (model) parameters in Table 3 might be claimed.

5. Conclusion and Future Work

Even in relatively simple models, transport phenomena in food and bioprocesses are keen to involve different phases (i.e. solid and fluid phases) so that governing differential equations require numerical methods. Lattice Boltzmann method (LBM) has become an interesting technique and, as part of ongoing research on computational modelling of agroindustrial biosystems, LBM have been applied to simulate transport phenomena in food and bioprocesses. This paper addressed the LBM simulation of two different continuous-flow processes in fixed-bed equipment whose models are similar, namely bioaffinity chromatography and biocompounds extraction.

As the governing equation for species concentration in the solid phase lacked partial derivatives with respect to the spatial coordinate (in the present case, the bed axis), it was possible to suppress the related streaming step from
the LBM simulation code. No loss of functionality was verified as the LBM simulator was able to numerically reproduce the expected shapes of both breakthrough and extraction yield curves.

Bearing in mind the comprehensiveness towards long equipment, species transport via diffusion was accounted in the fluid phase (although it has been neglected in some modes). Distinct species diffusivities were successfully examined in LBM simulations. Yet, a thorough study on the sensitivity as well as fine-tuning of process parameters (e.g. bed porosity, kinetic coefficients, volumetric flow rate, and maximum adsorption or extraction capacity) falls beyond the scope and purpose of the present work.

At their current development stage, LBM simulators can deal with dynamic one-dimensional models, involving as many chemical species as necessary. Moreover, LBM simulators based on dimensionless (i.e. non-dimensional) form of the governing differential equations have already been implemented and tested. The coupling of best-fitting routines (i.e. parameter fine-tuning against real-operation and/or experimental data) to the LBM simulation code is currently under way.

As far as future developments are concerned, LBM simulators will be extended to two (and eventually three) dimensional solution domains, therefore allowing for the simulation of bed hydrodynamics, i.e. the simulation of the interstitial fluid flow. Future extensions will equally comprise additional physical-chemical phenomena such as degradation, pH-related, and thermal effects.

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References


