Development of an in-House Lattice-Boltzmann Simulator Towards Bioreactors for Wastewater Treatment: Underlying Concepts

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Abstract. Lattice Boltzmann method (LBM) has become a powerful technique to simulate bioprocesses in porous media. Based on a relatively simple dynamic 1-D model, the present work is a first step towards a comprehensive LBM simulator of bioreactor for vinasse treatment, taken as case study. Species concentrations were LBM-simulated at appropriate order of magnitude.

Keywords: Mathematical modelling · Numerical simulation · Lattice boltzmann method

1 Introduction

Comprehensive knowledge of bioprocesses is prone to rely on equations whose complexity invokes numerical methods. This is the case of bioreactors for wastewater treatment where bioprocesses are combined with transport phenomena (Głuszcz et al. 2011). Besides the variability in terms of chemical kinetics and composition, mathematical hurdles arise due to the mutual interference between fluid flow velocity and species concentrations (Parco et al. 2007). Computational fluid dynamics (CFD) arises as helpful tool (Brannock et al. 2010) and the importance of computational modelling towards bioprocesses has been recognized while innovative methods have been developed and applied (Datta and Sablani 2007).

Envisaged in (McNamara and Zanetti 1988), lattice Boltzmann method (LBM) has become a powerful technique to numerically simulate bioprocesses (van der Sman 2007). As it does not directly solve Navier-Stokes equations (Succi 2001), LBM renders relatively simpler computer codes (Mohamad 2011). LBM can quite straightforwardly deal with single-phase or multiphase flow, whether or not coupled to transport phenomena and/or chemical reactions (Sukop and Thorne Jr. 2006). Bearing in mind the computational modelling of continuous-flow bioreactors via LBM, one may numerically simulate biofilm formation and detachment (Picioreanu et al. 2001) as well as biogas bubbles generation and transport (Chen 2010).

This work is part of ongoing research whose goal is to develop in-house LBM simulators of food and bioprocesses (Durán et al. 2015; Okiyama et al. 2015; Rabi and Kamimura 2016; Rosa et al. 2016). While there is no doubt about the efficiency of

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classic numerical methods (and off-the-shelf software) to perform analogous simulations, LBM is herein pointed as an alternative route to computationally model bioreactors for wastewater treatment.

2 Material and Methos

2.1 Theory: Bioreactor Modelling and Lattice-Boltzmann Simulation

This work is a preliminary step towards the development of an in-house LBM simulator of continuous-flow bioreactors for wastewater treatment. In view of that, an existing cylindrical laboratory-scale APBR (anaerobic packed bed reactor) for sugarcane vinasse treatment is taken as case study (Ferraz Jr. 2013). Resulting from sugarcane juice distillation, vinasse is an effluent from sugar-ethanol industries, whose large-scale use has pointed to fertirrigation in sugarcane crops after it undergoes anaerobic treatment (Vlissidis and Zouboulis 1993).

Figure 1(a) depicts the aforementioned experimental APBR. As sketched in Fig. 1 (b), it comprises feeding module (FM), bed section (BS), effluent collection area (EC) and biogas collection area (BC). Low-density polyethylene cylinders randomly fill up BS module (as the supporting medium), thus yielding porosity ε. Let $\dot{V}$ be the volumetric flow rate of vinasse so that interstitial fluid velocity in BS becomes $v = 4\dot{V}/(\varepsilon\pi d^2)$, where d is bed diameter.

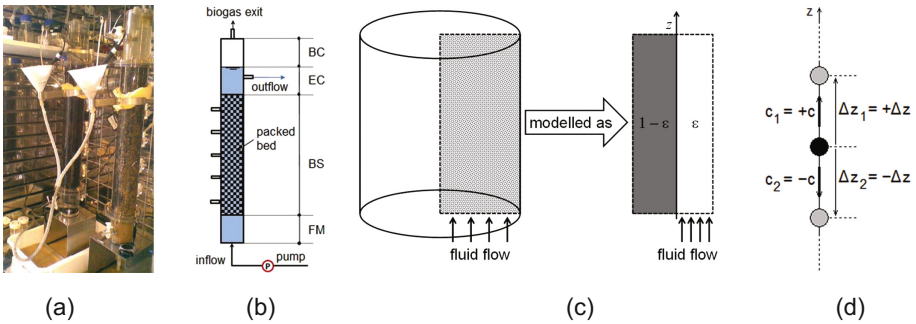

Fig. 1. LBM simulation of APBR for vinasse treatment: (a) picture of experimental bioreactors; (b) APBR sketch comprising feeding module (FM), bed section (BS), effluent collection area (EC) and biogas collection area (BC); (c) dynamic 1-D approach for BS with porosity ε; (d) basic and repetitive linear structure of D1Q2 LBM lattice

In line with LBM simulators implemented in our research (Durán et al. 2015; Okiyama et al. 2015; Rabi and Kamimura 2016; Rosa et al. 2016), a dynamic 1-D model is herein put forward. Coordinate axis z is oriented along with vinasse up-flow so that inlet is at $z = 0$ while exit is at $z = L$, where L is the total length. After considering an axisymmetric plane as shown in Fig. 1(d), stratification is assumed so that chemical species concentrations (or any other quantity) become functions of time t and coordinate z., i.e. $y_i = y_i(z, t)$.

In view of comprehensiveness and scale-up towards large equipment, convective-diffusive transport in the fluid phase has been considered since early versions of our LBM simulators, which can cope with concentrations y_i modelled by partial differential equations of the form:

$$\frac{\partial y_i}{\partial t} + v\frac{\partial y_i}{\partial z} = D_i\frac{\partial^2 y_i}{\partial z^2} + \dot{r}_i \tag{1}$$

where v is interstitial flow velocity (which is the same for all species), D_i is species diffusivity in the fluid phase, and rate $\dot{r}_i$ includes source and/or sink terms related to species generation and/or consumption via chemical reactions. Inspired by ADM1 - IWA Anaerobic Digestion Model No 1 (Batstone et al. 2002), Table 1 lists chemical species concentrations intended to be accounted for in the LBM simulator of continuous-flow APBR for vinasse treatment.

Table 1. Species to be accounted for in the LBM simulator of continuous-flow APBR for vinasse treatment.

y_i	Concentration of	Units	ρ_n	Concentration of	Units
y_1	chemical oxygen demand (COD)	kg-COD/m^3	y_8	acetate (ethanoate) ion	M = kmol/m^3
y_2	acetic (ethanoic) acid	kg-COD/m^3	y_9	propionate (propanoate) ion	M = kmol/m^3
y_3	propionic (propanoic) acid	kg-COD/m^3	y_{10}	butyrate (butanoate) ion	M = kmol/m^3
y_4	butyric (butanoic) acid	kg-COD/m^3	y_{11}	hydrogen ion (H^+)	M = kmol/m^3
y_5	dissolved hydrogen gas (H_2)	kg-COD/m^3	y_{12}	inorganic carbon	kmol-C/m^3
y_6	ethanol (ethyl alcohol)	kg-COD/m^3	y_{13}	dissolved carbon dioxide	kmol-C/m^3
y_{71}	biomass for sugar degradation	kg-COD/m^3	y_{14}	bicarbonate ion	kmol-C/m^3
y_{72}	biomass for H_2 degradation	kg-COD/m^3	y_{15}	carbon dioxide in the biogas	kmol-C/m^3
y_{73}	biomass for propionic acid degradation	kg-COD/m^3	y_{16}	hydrogen gas (H_2) in the biogas	M = kmol/m^3
y_{74}	biomass for butyric acid degradation	kg-COD/m^3			

LBM considers any medium (whether solid or fluid) as comprised by fictitious constituent particles following a sequence of synchronised streaming and collision steps in a discrete space, namely a fictitious lattice. During streaming, particles travel from one site to another through links defined by the fictitious lattice. As particles simultaneously arrive at sites, they mutually collide so that their velocities become rearranged for subsequent streaming-collision steps. By imposing conservation

principles (e.g. mass and momentum) to such repetitive particle dynamics, macroscopic medium can be numerically simulated (Succi 2001).

LBM mathematically relies on the so-called particle distribution function $f(\vec{r}, \vec{c}, t)$ giving, at time t and about position $\vec{r}$, the number of particles per unit volume with velocities between $\vec{c}$ and $\vec{c} + \mathrm{d}\vec{c}$. One may then retrieve observable properties (e.g. species concentration) by taking suitable moments of function f, which is governed by Boltzmann's transport equation. In the absence of external forces while invoking BGK approach (after Bhatnagar, Gross and Krook) for the collision operator, Boltzmann's transport equation is written as:

$$\frac{\partial f}{\partial t} + \vec{c} \cdot \vec{\nabla} f = \frac{1}{\Delta t_{\text{relax}}} (f^{\text{eq}} - f) \tag{2}$$

where Δt_{relax} and f^{eq} are relaxation time and equilibrium distribution function respectively.

LBM is implemented to solve Eq. (2) as written in terms of the fictitious lattice assigned to the true medium, when it becomes known as lattice Boltzmann equation (LBE). Functions f_k are allocated to each streaming velocity c_k in the lattice. LBM lattices are identified as *DnQm*, being n the dimension of the problem (e.g. $n = 1$ for 1-D problem) whereas m refers to the number of particle distribution functions f_k to be solved for each observable property.

As this work proposes a dynamic 1-D model, D1Q2 lattice is employed, whose basic and repetitive linear structure comprises a central lattice site linked to two neighbouring sites, one at each side. As shown in Fig. 1(d), let $k = 1$ and $k = 2$ respectively refer to forward (i.e. upward) and backward (i.e. downward) streaming directions. LBE-BGK is written for each particle distribution function f_k (related to each streaming link k) at position z and time t:

$$\frac{\partial f_k(z,t)}{\partial t} + c_k \frac{\partial f_k(z,t)}{\partial z} = \frac{f_k^{\text{eq}}(z,t) - f_k(z,t)}{\Delta t_{\text{relax}}} \tag{3}$$

If Δt is the advancing time step then $c_1 = +\Delta z/\Delta t$ and $c_2 = -\Delta z/\Delta t$ are upward and downward streaming speeds respectively. The numerical solution method of Eq. (3) is addressed next.

2.2 Numerical Solution Method

There are two approaches to simulate species transport in multicomponent systems via LBM. Species can be simulated either as an active component (so that an increase of its local concentration leads to a local decrease in background fluid concentration) or as a passive solute carried by the solvent (Sukop and Thorne Jr. 2006). In this work we follow the latter approach as it has been adopted in LBM simulators previously implemented in our research.

Accordingly, particle distribution functions $f_{i,k}$ are assigned to each concentration y_i invoked in the model. At time t and position z, functions $f_{i,k} = f_{i,k}\ (z, t)$ become known by numerically solving Eq. (3) and the corresponding species concentration can be

retrieved simply as:

$$y_i(z,t) = \sum_k f_{i,k}(z,t) \quad \xrightarrow{\text{D1Q2 lattice}} \quad y_i(z,t) = f_{i,1}(z,t) + f_{i,2}(z,t) \tag{4}$$

Space-time discretisation of Eq. (3) renders an algebraic equation whose computational evolution is implemented in two separate iterative steps. Time evolution is accomplished in the collision step where particle distribution functions $f_{i,k}$ are updated from instant t to $t + \Delta t$ for all lattice links k and lattice sites at positions z in the solution domain. Eventual source or sink terms $\dot{r}_i$ (e.g. species generation or consumption by means of chemical reactions) are included at this LBM step so that the following algebraic expression holds:

$$f_{i,k}(z, t + \Delta t) = (1 - \omega_i) f_{i,k}(z,t) + \omega_i f_{i,k}^{\text{eq}}(z,t) + w_k \, \Delta t \, \dot{r}_i \tag{5}$$

where $\omega_i = \Delta t_{\text{relax},i}/\Delta t$ is known as relaxation parameter and w_k are weighting factors, namely $w_1 = w_2 = 1/2$ for D1Q2 lattice. Space evolution is achieved in streaming step as collision outcomes are transmitted to adjacent lattice sites in all streaming directions simply as:

$$f_{i,k}(z + \Delta z_k, t + \Delta t) = f_{i,k}(z, t + \Delta t) \tag{6}$$

Collision and streaming steps, Eqs. (5) and (6), are repeated until final simulation instant is reached. Besides Eq. (4), LBM simulation becomes connected to macroscopic medium via relaxation parameters and equilibrium distribution functions. In a dynamic 1-D model (which is the present case), the latter refer to the bulk fluid (i.e. effluent) velocity v as:

$$f_{i,k}^{\text{eq}}(z,t) = w_k \, y_i(z,t) \, (1 \pm \text{Ma}) \tag{7}$$

while the former are related to individual species diffusivities D_n according to:

$$\frac{1}{\omega_i} = \frac{D_i \, \Delta t}{(\Delta z)^2} + \frac{1}{2} \quad \Rightarrow \quad \frac{1}{\omega_i} = \frac{\text{Ma}}{\text{Pe}_i} + \frac{1}{2}, \quad \text{Ma} = \frac{v \, \Delta t}{\Delta z} \quad \text{and} \quad \text{Pe}_i = \frac{v \, \Delta t}{D_i} \tag{8}$$

where Ma and Pe_i are lattice-based Mach number and lattice-based mass-transfer Péclet number, respectively. In Eq. (7), the sign before Ma is positive for forward (i.e. upward, $k = 1$) streaming and negative for backward (i.e. downward, $k = 2$) streaming.

With regard to inlet boundary conditions, one obtains $f_{i,2}(0,t) = f_{i,2}(0 + \Delta z, t)$ via backward streaming from adjacent lattice site while $f_{i,1}(0,t)$ is the unknown. One may impose Dirichlet condition by combining first-order finite-differences estimate of $\partial \rho_i / \partial z$ with Eq. (4) to obtain:

$$\text{At } z = 0: \quad f_{i,1}(0,t) = y_{i,\text{in}} - f_{i,2}(0,t) \tag{9}$$

where $y_{i,\text{in}}$ is the species concentration in the feeding effluent. Danckwerts inlet condition is addressed in (Rabi and Kamimura 2016). At exit, $f_{i,1}(L,t) = f_{i,1}(L - \Delta z, t)$ is obtained from forward streaming while $f_{i,2}(L, t)$ is the unknown. Null Neumann condition is imposed by again combining first-order finite-differences estimate of $\partial y_i/\partial z$ with Eq. (4) and the final result is:

$$\text{At } z = L: \quad f_{i,2}(L,t) = f_{i,2}(L - \Delta z, t) \tag{10}$$

Last but not least, if $y_i(z,0)$ is the initial condition imposed to species concentration, initial conditions for corresponding particle distribution functions are implemented as:

$$\text{At } t = 0: \quad f_{i,k}(z,0) = w_k\, y_i(z,0) \tag{11}$$

3 Results and Discussions

A first-round LBM simulator was implemented to numerically solve Eq. (1) for species $i = 1$ to 5 in Table 1, together with single (i.e. "unified") biomass species y_7 (instead of using species y_{71} to y_{74}). For such rather simplified scenario, Table 2 shows generation and consumption rates $\dot{r}_i$, which are expressed in terms of the common auxiliary parameter A defined as:

$$A = k_{\text{m,su}} \frac{y_1(z,t)}{K_{\text{S,su}} + y_1(z,t)} y_7(z,t), \quad \text{with} \quad k_{\text{m,su}} = 30\ \text{day}^{-1} \quad \text{and} \quad K_{\text{S,su}} = 0.5\ \frac{\text{kg - COD}}{\text{m}^3} \tag{12}$$

Null Neumann boundary condition ($\partial y_i/\partial z = 0$) was imposed to all species at the exit while the feeding values $y_{i,\text{in}}$ for Dirichlet inlet condition are shown in Table 2. Initial conditions $y_i(z,0) = 0$ were set to species $i = 1$ to 5 while $y_7(z,0) = 0.1$ kg-COD/m^3 was set to species $i = 7$. Further APBR and LBM parameters used in simulations comprise: $L = 1$ m, $v = 2$ m/s, $k_{\text{d1}} = 0.02\ \text{day}^{-1}$, $Y_{\text{su}} = 0.1$, $f_{\text{C2,su}} = 0.41$, $f_{\text{C3,su}} = 0.27$, $f_{\text{C4,su}} = 0.13$, $f_{\text{H2,su}} = 0.19$, $D_i = 0.02\ \text{m}^2/\text{day}^{-1}$ (small diffusivity arbitrarily set for all species), $\Delta z = 0.01$ m, and $\Delta t = 0.0005$ day.

Table 2. Reaction rates and inlet concentrations for species considered in the preliminary LBM simulator

Chemical species	$i = 1$	$i = 2$	$i = 3$	$i = 4$	$i = 5$	$i = 7$
Reaction rate $\dot{r}_i$	A	$(1 - Y_{\text{su}})\cdot f_{\text{C2,su}}\cdot A$	$(1 - Y_{\text{su}})\cdot f_{\text{C3,su}}\cdot A$	$(1 - Y_{\text{su}})\cdot f_{\text{C4,su}}\cdot A$	$(1 - Y_{\text{su}})\cdot f_{\text{H2,su}}\cdot A$	$Y_{\text{su}}\cdot A - k_{\text{d1}}\cdot y_7$
Inlet $y_{i,\text{in}}$ (kg-COD/m^3)	24.7	0.5013	0.0801	0.5266	0.0001	0.1

While the LBM simulator can provide concentrations $y_i(z, t)$ at any position z and time t, for brevity and grouping results with similar order of magnitude, Fig. 2 shows time-dependent concentrations at the exit $y_i(L, t)$ for (a) $i = 1$ (COD) and (b) $i = 2$ to 5 and 7 (further species). As far as the experimental APBR is concerned, COD was measured as 26.1 kg-COD/m^3 at $t = 1$ day, which is consistent with simulations shown in Fig. 2(a). Figure 2(b) suggests that acidogenesis, H_2 and biomass generation were successfully simulated via as well.

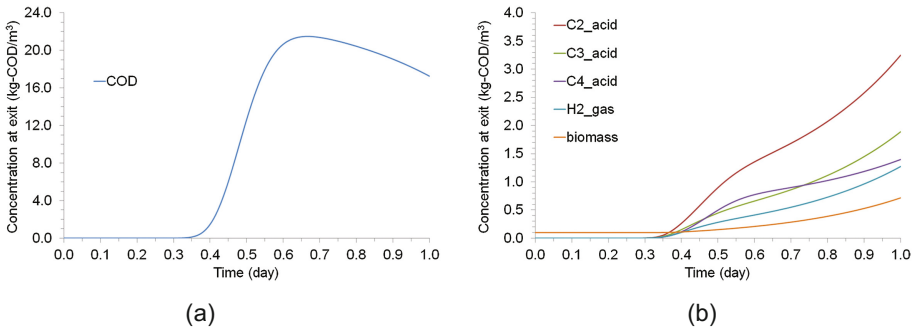

Fig. 2. LBM-simulated time-dependent species concentrations at the exit $y_i(L, t)$: (a) $i = 1$, (b) $i = 2$ to 5 and 7

4 Conclusions

Although relatively simple at its current development, the dynamic 1-D model for continuous-flow APBR was successfully implemented via LBM. Species concentrations were numerically simulated at suitable order of magnitude. Future developments of the LBM simulator point to the inclusion of further chemical species as well as fine-tuning model parameters.

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