

# LATTICE-BOLTZMANN AND FINITE-DIFFERENCES SIMULATIONS OF 1-D TIME-DEPENDENT PROCESSES IN FIXED-BED EQUIPMENT OF FOOD INDUSTRIAL INTEREST

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**Abstract.** *Lattice-Boltzmann Method (LBM) has become a powerful numerical tool to simulate macroscopic transport phenomena in porous media, which is the case of several processes involving foodstuff or biotechnological products of industrial interest such as biospecific affinity chromatography (BAC) and supercritical fluid extraction (SFE) in fixed-bed equipment. Time-dependent one-dimensional model frameworks for such processes occurring in porous media are quite (and appealingly) similar and they have basically evoked phase-equilibrium (sorption-desorption) kinetics, plug-flow, and species (mass) transport by either convection or dispersion (diffusion). By supposing that fluid-phase species concentration may vary in time as well along the bed axial coordinate, the present work considered a simplified and dimensionless form of the corresponding governing partial differential equation. Such equation assumes exactly the same form for either BAC or SFE and it was numerically solved employing both LBM and finite-difference-method (FDM). As the main purpose of this work was to check proper implementation of both computational codes, numerical results from LBM and FDM simulations are compared and discussed accordingly.*

**Keywords:** *numerical simulation, lattice-Boltzmann method, finite-difference method, porous media, mass transfer*

## 1. INTRODUCTION

One may adopt distinct methods in order to simulate transport phenomena in porous media (Mohamad, 2007). The macroscopic approach leads to differential equations so that properties are interpreted as average values referring to a particle ensemble. On the opposite end, the microscopic approach pays attention to each constituent particle and the idea is to simulate overall medium behavior from each possible particle interactions. Last but not least, the mesoscopic approach deals with global effects of all particles through the so-called distribution function and based on such function (and concept) lattice-Boltzmann method (LBM) is implemented.

In LBM simulation, macroscale medium is thought as a collection of particles occupying a discrete space (i.e., sites of a lattice). Based on an equally discrete set of lattice speeds, constituent particles “travel” from one site to another along pre-defined directions (i.e., lattice links) during discrete time intervals and they mutually collide at those sites (Santos, 2000; Succi, 2001; Mohamad, 2007). Such particles dynamics is depicted by two processes respectively referred to as streaming and collision. During the later particles are rearranged at lattice sites preserving their quantity as well as their momentum whereas in the former particles move between neighboring sites according to their speeds. By assuming that such dynamics obeys conservation principles (besides being isotropic), macroscopic medium behavior can be properly described and numerically simulated (Santos, 2000).

LBM has already been applied to processes involving foodstuff or biotechnological products, which is the case of emulsions, suspensions, polymer solutions and flows inside porous media (van der Sman, 2007). In particular, the present work aims at applying LBM to biospecific affinity chromatography (BAC) and to supercritical fluid extraction (SFE). These two processes are of food industry interest and they usually take place inside fixed-bed equipment.

## 2. THEORY

### 2.1. Model framework for biospecific affinity chromatography (BAC) and for supercritical fluid extraction (SFE)

BAC models have basically evoked phase-equilibrium (sorption-desorption) kinetics, plug-flow, and species (mass) transport by both convection and dispersion (diffusion). In accordance to many approaches (Chase, 1984; Cowan *et al.*, 1986; Sridhar *et al.*, 1994; Kempe *et al.*, 1999; Leickt *et al.*, 2001; Özdural *et al.*, 2004; Yun *et al.*, 2005), species concentration in either fluid or solid phase has been assumed to vary in time  $t$  as well along the fixed-bed (equipment) axial coordinate  $x$ . As a result, the aforementioned species concentrations have been respectively modeled as  $\phi = \phi(x,t)$  and  $\theta = \theta(x,t)$  and governing partial differential equations (PDEs) for such concentrations have been expressed as:

$$\text{In fluid phase: } \frac{\partial \phi}{\partial t} + v_x \frac{\partial \phi}{\partial x} = E \frac{\partial^2 \phi}{\partial x^2} - \frac{1-\epsilon}{\epsilon} \dot{r} \quad , \quad \text{in solid phase: } \frac{\partial \theta}{\partial t} = \dot{r} = k_1 \phi (\theta_{\max} - \theta) - k_2 \theta \quad (1)$$

where  $v_x$  is interstitial flow velocity,  $E$  is (porosity-corrected) mass diffusivity,  $\varepsilon$  is bed porosity,  $k_1$  and  $k_2$  are sorption and desorption kinetics coefficients and  $\theta_{\max}$  is the maximum adsorption capacity of the chromatographic column. As far as necessary conditions are concerned, the following have been prescribed:

$$\text{Initial condition: } \phi = 0 \text{ (for fluid-phase concentration)} \quad \text{and} \quad \theta = 0 \text{ (for solid-phase concentration)} \quad (2)$$

$$\text{Boundary conditions for fluid-phase concentration: } \phi = \phi_{\text{in}} \text{ at } x = 0 \text{ (inlet)} \quad , \quad \partial\phi/\partial x = 0 \text{ at } x = L \text{ (outlet)} \quad (3)$$

SFE models have equally evoked phase-equilibrium kinetics, plug-flow and species transfer by both convection and dispersion. Though the later mass transport mechanism has been sometimes neglected (Sovová, 1994; Reverchon, 1996; França and Meireles, 2000; Wu and Hou, 2001; Lucas *et al.*, 2007), diffusive mass transport can be influential in fairly large equipment, therefore justifying its inclusion in the model framework (Gaspar *et al.*, 2003). Relying on a first-order kinetics approach, species concentrations have been modeled as  $\phi = \phi(x,t)$  and  $\theta = \theta(x,t)$  respectively in fluid and solid phases, while related governing PDEs have been expressed as:

$$\text{In fluid phase: } \frac{\partial\phi}{\partial t} + v_x \frac{\partial\phi}{\partial x} = E \frac{\partial^2\phi}{\partial x^2} - \frac{1-\varepsilon}{\varepsilon} \dot{r} \quad , \quad \text{in solid phase: } \dot{r} = \frac{\partial\theta}{\partial t} = \frac{1}{t_i} \left( \frac{\phi}{k_p} - \theta \right) \quad , \quad t_i = \mu \frac{l_p^2}{D_i} \quad (4)$$

where again  $v_x$  is interstitial flow velocity,  $E$  is (porosity-corrected) mass diffusivity and  $\varepsilon$  is bed porosity, whereas  $k_p$  is partition coefficient and  $t_i$  is intra-particle diffusion time. The later has been assessed based on particle characteristics as given by a (dimensionless) shape coefficient  $\mu$ , a typical length  $l_p$ , and an internal mass diffusivity  $D_i$ . If  $\theta_{\max}$  is the maximum extraction capacity of the bed, the following conditions have been prescribed:

$$\text{Initial condition: } \phi = 0 \text{ (for fluid-phase concentration)} \quad \text{and} \quad \theta = \theta_{\max} \text{ (for solid-phase concentration)} \quad (5)$$

$$\text{Boundary conditions for fluid-phase concentration: } \phi = 0 \text{ at } x = 0 \text{ (inlet)} \quad , \quad \partial\phi/\partial x = 0 \text{ at } x = L \text{ (outlet)} \quad (6)$$

It is worth noting that the previous model frameworks for BAC and SFE are considerably and attractively similar to each other, despite these two processes are quite distinct. As a matter of fact, recalling Eqs. (1) and (4), corresponding governing PDEs for fluid-phase species concentration  $\phi$  are basically the same except for the source (or sink) term  $\dot{r}$  concerning sorption-desorption kinetics, which depends on the governing PDE for solid-phase species concentration  $\theta$ . Bearing in mind preliminary implementation of lattice-Boltzmann method computational codes, this work attempts to take advantage of such similarity between those model frameworks.

## 2.2. Lattice-Boltzmann method (LBM) for transport phenomena

LBM replaces the knowledge about each particle position and velocity by the description of global effects by means of a distribution function  $f(\vec{r}, \vec{c}, t)$  giving the probability of finding particles at time  $t$  and about position  $\vec{r}$  with speeds between  $\vec{c}$  and  $\vec{c} + d\vec{c}$ . Provided that function  $f$  is known, macroscopic properties like density  $\rho$ , bulk flow velocity  $\vec{v}$  or pressure  $p$  can be obtained (van der Sman, 2007). The governing equation for  $f$  is the so-called Boltzmann equation, which in the absence of external forces results in the following advection equation with a source (or sink) term:

$$\frac{\partial f}{\partial t} + \vec{c} \cdot \vec{\nabla} f = \Omega(f) \quad \Rightarrow \quad \frac{\partial f}{\partial t} + \vec{c} \cdot \vec{\nabla} f = \frac{1}{\tau} (f^{\text{eq}} - f) \quad (7)$$

where the collision operator  $\Omega = \Omega(f)$  measures the variation rate of function  $f$  due to collisions between particles. The above final form of Eq. (7) evoked a linear approximation for  $\Omega$ , namely  $\Omega(f) = (f^{\text{eq}} - f)/\tau$ , which is referred to as BGK approximation (after Bhatnagar, Gross and Krook), where  $\tau$  is the relaxation time whereas  $f^{\text{eq}}$  is the local equilibrium distribution function (Qian *et al.*, 1992).

In LBM, Eq. (7) is discretized along pre-defined directions (lattice links) so that distances between sites are given in lattice units. Time is also a discrete variable in LBM. Distinct lattice arrangements are indicated as  $DnQm$ , where  $n$  is problem dimension (e.g.,  $n = 1 = 1\text{-D} = \text{one dimension}$ ) and  $m$  is the number of lattice velocities (distribution functions). Comprising a central site and two linked neighboring sites, Fig. 1 sketches a 1-D structure known as D1Q3, which is similar to another 1-D structure referred to as D1Q2. Along such two links, particles may “stream” with lattice velocity  $\vec{c}_k$  (subscript  $k$  refers to a given lattice link) so that  $\vec{c}_1 = +c \hat{i}$  (to the right) and  $\vec{c}_2 = -c \hat{i}$  (to the left), where  $c = \Delta x/\Delta t$  is the lattice speed and  $\hat{i}$  is a unit vector. Central velocity is null, i.e.,  $c_0 = 0$ .



Figure 1. Either D1Q3 or D1Q2 lattice arrangement for 1-D LBM.

By writing Eq. (7) for a given direction  $k$  at any position  $x$  and time  $t$ , one obtains 1-D lattice-Boltzmann equation (LBE) under BGK approximation, namely:

$$\frac{\partial f_k}{\partial t} + \bar{c}_k \cdot \bar{\nabla} f_k = \Omega_k \Rightarrow \frac{\partial f_k(x,t)}{\partial t} + c_k \frac{\partial f_k(x,t)}{\partial x} = \frac{1}{\tau} [f_k^{\text{eq}}(x,t) - f_k(x,t)] \quad (8)$$

Space-time discretization of Eq. (8) results in the following algebraic equation (Mohamad, 2007):

$$f_k(x + \Delta x_k, t + \Delta t) = [1 - \omega] f_k(x, t) + \omega f_k^{\text{eq}}(x, t) \quad (9)$$

where  $\omega = \Delta t/\tau$  is the relaxation parameter and  $c_k = \Delta x_k/\Delta t$ . For D1Q3 Eq. (9) is written for  $k = 0, 1$  and  $2$  (i.e., for  $f_0, f_1$  and  $f_2$ ) while for D1Q2 Eq. (9) is written only for  $k = 1$  and  $2$  because  $f_0$  ( $k = 0$ ) is disregarded. Evolution of Eq. (9) is numerically accomplished in two steps. During the so-called collision step, distribution functions  $f_k$  for each direction  $k$  are updated (i.e., from  $t$  to  $t + \Delta t$ ) at each lattice site as:

$$f_k(x, t + \Delta t) = [1 - \omega] f_k(x, t) + \omega f_k^{\text{eq}}(x, t) \quad (10)$$

whereas during the streaming step collision results are then transported to neighboring sites according to:

$$f_k(x + \Delta x_k, t + \Delta t) = f_k(x, t + \Delta t) \quad (11)$$

LBM physics is governed by the equilibrium distribution function  $f_k^{\text{eq}}$  concerning the transport nature together with the relaxation parameter  $\omega$  regarding the related transport coefficient. For species (mass) transport, the later refers to the mass diffusivity  $D$  as (Mohamad, 2007; van der Sman, 2007):

$$D = c_s^2 \left( \frac{1}{\omega} - \frac{1}{2} \right) \Delta t \Leftrightarrow \omega = \left( \frac{D}{c_s^2 \Delta t} + \frac{1}{2} \right)^{-1} \quad (12)$$

The so-called lattice sound speed results as  $c_s = c$  for both D1Q2 and D1Q3, where  $\Delta t$  is a discrete advancing time step (Mohamad, 2007). As far as the equilibrium distribution function  $f_k^{\text{eq}}$  is concerned, for low velocities  $\bar{v}$  the following expression applies (Mohamad, 2007; van der Sman, 2007):

$$f_k^{\text{eq}} = w_k \rho(\bar{r}, t) \left[ 1 + \frac{(\bar{c}_k \cdot \bar{v})}{c_s^2} + \frac{(\bar{c}_k \cdot \bar{v})^2}{2c_s^4} - \frac{(\bar{v} \cdot \bar{v})}{2c_s^2} \right] \quad (13)$$

For D1Q2, weighting factors are  $w_0 = 0$  (because  $f_0$  is disregarded, as already cited) and  $w_1 = w_2 = 1/2$ .

### 3. APPLICATION OF LBM TO NUMERICALLY SIMULATE BAC / SFE PROCESSES

#### 3.1. Preliminary approach: dimensionless simulation of species concentration in the fluid phase alone

As far as the previously described model frameworks for both BAC and SFE are concerned, it is worth noting that there is no explicit dependence on the bed axis (spatial) coordinate  $x$  in governing differential equations for the species concentration in the solid phase. Because the porous matrix is stationary ( $v_x = 0$ ), LBM evolution in such phase can be implemented by suppressing the corresponding streaming step while another possibility is to impose periodic boundary conditions (Rabi and Mohamad, 2008).

Nevertheless, as a first step towards LBM simulation of BAC and SFE processes and in order to take advantage of the resemblance between their model frameworks, the present work was particularly concerned with applying LBM to the fluid-phase concentration alone. With the help of such preliminary approach, a simplified form for the first of Eqs. (1) and (4) was considered by simply disregarding the source (or sink) term  $\dot{r}$ , which is influenced by and dependent on

the solid-phase kinetics. As a result, fluid-phase species concentration  $\phi$  in either BAC or SFE becomes governed by exactly the same PDE, namely:

$$\dot{r} = \frac{\partial \theta}{\partial t} = 0 \Rightarrow \frac{\partial \phi}{\partial t} + v_x \frac{\partial \phi}{\partial x} = E \frac{\partial^2 \phi}{\partial x^2} \quad (14)$$

One may obtain a dimensionless form of the previous PDE by introducing the following dimensionless variables for fluid-phase species concentration, axial coordinate and time, respectively:

$$\Phi = \frac{\phi}{\phi_{\text{ref}}} \quad , \quad X = \frac{x}{\Delta x} \quad , \quad \tau = \frac{t}{\Delta t} \quad (15)$$

where the reference concentration can be identified to a non-null inlet concentration,  $\phi_{\text{ref}} = \phi_{\text{in}} \neq 0$ , while  $\Delta x$  and  $\Delta t$  are lattice parameters. Recalling that  $c_s = c = \Delta x / \Delta t$  and  $\|\bar{v}\| = v = v_x$  for 1-D problems, Eq. (14) can be rewritten into the following dimensionless form:

$$\frac{\partial \Phi}{\partial \tau} + \text{Ma} \frac{\partial \Phi}{\partial X} = \frac{1}{\text{Pe}_m} \frac{\partial^2 \Phi}{\partial X^2} \quad , \quad \text{Ma} = \frac{v}{c_s} \quad \text{and} \quad \text{Pe}_m = \frac{c \Delta x}{E} = \frac{c^2 \Delta t}{E} = \frac{(\Delta x)^2}{\Delta t E} \quad (16)$$

where Ma and  $\text{Pe}_m$  are lattice-based Mach number and mass-transfer Peclet number, respectively. Bearing in mind Eqs. (2) and (3), one may impose the following conditions for the dimensionless fluid-phase concentration:

$$\text{Initial condition: } \Phi = 0 \quad (17)$$

$$\text{Boundary conditions: } \Phi = 1 \text{ at } X = 0 \text{ (inlet)} \quad , \quad \partial \Phi / \partial X = 0 \text{ at } X = N_x = L / \Delta x \text{ (outlet)} \quad (18)$$

where  $N_x + 1$  is the number of lattice sites along the axial direction (including both end points).

### 3.2. LBM implementation aiming at both BAC and SFE

In order to apply LBM to numerically simulate BAC or SFE processes, one needs in fact two distinct distribution functions  $f_k(x,t)$  and  $s_k(x,t)$  “sharing” the same lattice. Each distribution function refers to the species concentration in each phase,  $\phi(x,t)$  and  $\theta(x,t)$ , respectively in the fluid and solid phases. Bearing in mind the underlying physics in each corresponding governing PDE, Eqs. (1) and (4), the following simplified equilibrium distribution functions might be adopted (Mohamad, 2007):

$$\text{Fluid (diffusion-convection): } f_k^{\text{eq}}(x,t) = w_k \phi(x,t) \left[ 1 \pm \frac{v_x}{c} \right] \quad , \quad \text{solid (stationary): } s_k^{\text{eq}}(x,t) = w_k \theta(x,t) \quad (19)$$

where the sign of  $v_x/c$  depends on the streaming direction. Despite weighting factors  $w_k$  are the same for  $f_k^{\text{eq}}$  and  $s_k^{\text{eq}}$ , relaxation factors are different for each phase in line with corresponding governing PDEs, Eqs. (1) and (4), namely:

$$\text{Fluid phase } (E \neq 0): \quad \omega_f = \left[ \frac{E}{c \Delta x} + \frac{1}{2} \right]^{-1} \quad , \quad \text{solid phase } (E = 0): \quad \omega_s = 2 \quad (20)$$

Considering the dimensionless formulation, LBM was applied for a D1Q2 arrangement. Bearing in mind Eqs. (16), the following expressions hold for the fluid-phase concentration alone:

$$f_1^{\text{eq}}(X, \tau) = w_1 \Phi(X, \tau) [1 + \text{Ma}] \quad \text{and} \quad f_2^{\text{eq}}(X, \tau) = w_2 \Phi(X, \tau) [1 - \text{Ma}] \quad (21)$$

$$\omega_f = \left[ \frac{1}{\text{Pe}_m} + \frac{1}{2} \right]^{-1} \quad \text{and} \quad \Phi(X, \tau) = \sum_k f_k(X, \tau) = f_1(X, \tau) + f_2(X, \tau) \quad (22)$$

where the weighting factors are  $w_1 = w_2 = 1/2$ , this way satisfying the condition  $\sum w_k = 1$  (Mohamad, 2007). In line with Eq. (17), initial condition is imposed as:

$$f_1(X,0) = w_1 \Phi(X,0) \quad \text{and} \quad f_2(X,0) = w_2 \Phi(X,0) \quad (23)$$

At the inlet ( $X = 0$ ), boundary condition for  $f_2(0,\tau)$  was obtained through streaming from the neighboring site  $f_2(1,\tau)$  so that  $f_1(0,\tau)$  is the only unknown. By imposing  $\Phi(0,\tau) = 1$  as given by the first of Eqs. (18), then the second of Eqs. (22) provides the following expression:

$$\Phi(0,\tau) = f_1(0,\tau) + f_2(0,\tau) \Rightarrow f_1(0,\tau) = 1 - f_2(0,\tau) \quad (24)$$

At the opposite boundary (outlet,  $X = N_x$ ), null Neumann condition can be approximated by finite differences as:

$$\frac{\Phi(N_x,\tau) - \Phi(N_x - 1,\tau)}{\Delta X} = \frac{[f_1(N_x,\tau) + f_2(N_x,\tau)] - [f_1(N_x - 1,\tau) + f_2(N_x - 1,\tau)]}{\Delta x} = 0 \quad (25)$$

so that at  $X = N_x$  one may impose:

$$f_1(N_x,\tau) = f_1(N_x - 1,\tau) \quad \text{and} \quad f_2(N_x,\tau) = f_2(N_x - 1,\tau) \quad (26)$$

#### 4. RESULTS AND DISCUSSION

The resulting LBM-BGK computational code was implemented in FORTRAN language (standard 90/95). DIQ2 arrangement was adopted with  $N_x = 150$  (i.e., 151 lattice sites including sites at  $X = 0$  and  $X = N_x$ ). Lattice-based Mach number and mass-transfer Peclet number were respectively and arbitrarily set as  $Ma = 0.1$  and  $Pe_m = 4/5$ . From the later, the first of Eqs. (22) provided  $\omega_f = (1/Pe_m + 1/2)^{-1} = 4/7$  as relaxation factor. Besides such LBM code, a finite-difference-method (FDM) simulator was additionally implemented in order to compare numerical results from both simulators. Aiming at relatively more complex LBM simulation of either BAC and SFE processes, the main purpose of this work was to check proper implementation of such preliminary LBM code with respect to the fluid-phase concentration.

At  $\tau = 600$ , Fig. 2 compares dimensionless fluid-phase concentration distribution as simulated by LBM and FDM, where differences are observed between profiles. As far as the governing PDE is concerned, the first of Eqs. (16), in the FDM simulator it is worth mentioning that (i) time derivative was discretized utilizing first-order accurate forward-differences and (ii) convective term was discretized according to an upwind scheme. While the later might cause false (i.e., numerical) diffusion, the former can be replaced by a fully or partially implicit (e.g., Crank-Nicholson) scheme (Patankar, 1980; Ferziger and Peric, 2002).

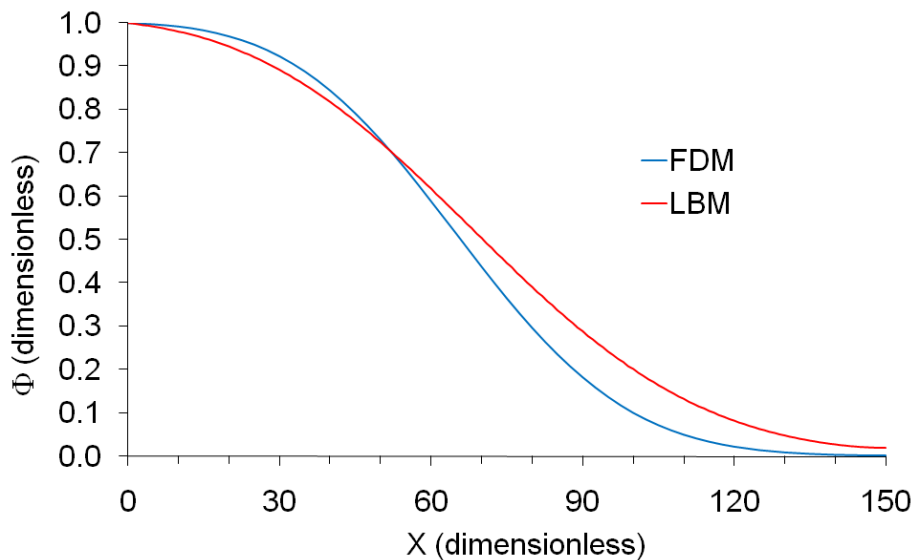


Figure 2. Comparing LBM and FDM results for 1-D time-dependent convective-diffusive mass transfer.

As an attempt to additionally investigate the comparison between LBM and FDM numerical results, the first of Eqs. (16) was simplified by neglecting the convective term (i.e., by imposing  $v_x = 0 \Leftrightarrow \text{Ma} = 0$ ). Accordingly, the following diffusive-dominant governing PDE resulted:

$$\frac{\partial \phi}{\partial t} = E \frac{\partial^2 \phi}{\partial x^2} \xrightarrow{\text{dimensionless}} \frac{\partial \Phi}{\partial \tau} = \frac{1}{\text{Pe}_m} \frac{\partial^2 \Phi}{\partial X^2} \quad (27)$$

while equilibrium distribution functions resulted as:

$$f_1^{\text{eq}}(X, \tau) = w_1 \Phi(X, \tau) \quad \text{and} \quad f_2^{\text{eq}}(X, \tau) = w_2 \Phi(X, \tau) \quad (28)$$

Imposing the same initial and boundary conditions as given by Eqs. (23), (24) and (26), Fig. 3 compares dimensionless fluid-phase concentration distribution as simulated by LBM and FDM at  $\tau = 1200$ . It is interesting to notice that both simulated profiles are now practically coincident (so that FDM results are plotted as a few dots instead of a solid line in order to avoid superimposition). In the vicinity of  $X = 150$  it is also worth noting that simulated  $\Phi$  values by both LBM and FDM are slightly above zero and not practically zero as simulated by FDM in Fig. 2.

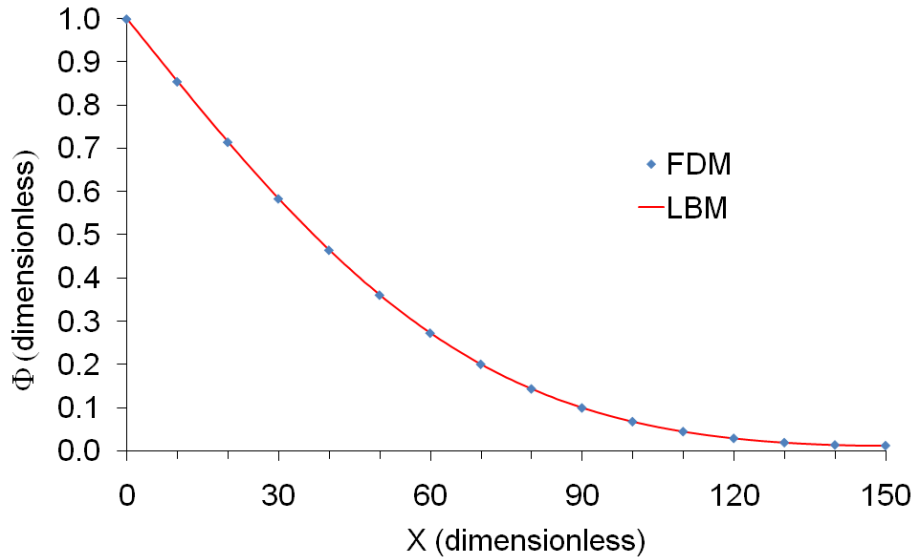


Figure 3. Comparing LBM and FDM results for 1-D time-dependent diffusive mass transfer.

A further comparison was accomplished by introducing a constant source term  $\dot{r} > 0$  into the previous governing PDE for the fluid-phase species concentration so that Eq. (27) became:

$$\frac{\partial \phi}{\partial t} = E \frac{\partial^2 \phi}{\partial x^2} + \dot{r} \xrightarrow{\text{dimensionless}} \frac{\partial \Phi}{\partial \tau} = \frac{1}{\text{Pe}_m} \frac{\partial^2 \Phi}{\partial X^2} + \dot{R} \quad , \quad \dot{R} = \frac{\dot{r} \Delta t}{\phi_{\text{ref}}} \quad (29)$$

In LBM, source (or sink) terms are directly introduced into the right-hand side of Eq. (7) (Mohamad, 2007) so that the corresponding BGK discrete approximation, Eq. (9), was extended to:

$$f_k(X + \Delta X_k, \tau + \Delta \tau) = [1 - \omega] f_k(X, \tau) + \omega f_k^{\text{eq}}(X, \tau) + w_k \dot{R} \Delta \tau \quad (30)$$

where weighting factors were again  $w_1 = w_2 = 1/2$  whereas initial and boundary conditions, Eqs. (23), (24) and (26), were kept the same as well. For the sake of demonstration, further LBM and FDM simulations were carried out utilizing  $\dot{R} = 0.01$  and  $\Delta \tau = 1.0$  and Fig. 4 shows the dimensionless concentration profiles obtained at  $\tau = 1200$ . Once again, it is worth observing the coincidence between the numerical solutions (so that FDM results are again plotted as a few dots in order to avoid superimposition).

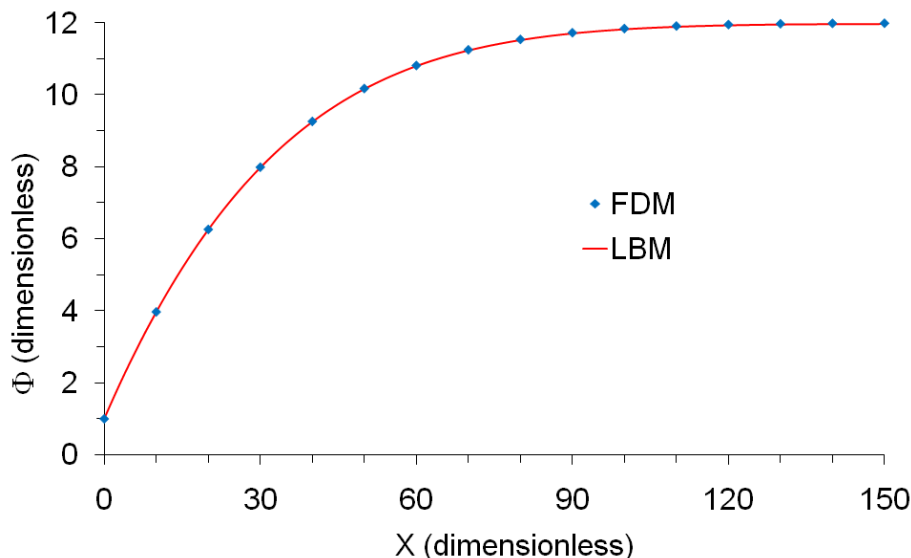


Figure 4. Comparing LBM and FDM results for 1-D time-dependent diffusive mass transfer with source term.

## 5. CONCLUDING REMARKS

Understanding food or biotechnological processes in porous media of industrial interest may claim the solution of differential governing equations of some complexity, which is the case of biospecific affinity chromatography (BAC) and supercritical fluid extraction (SFE). Despite relatively simple models have been assumed, inherent mathematical hurdles justify the use of numerical methods in order to solve corresponding governing differential equations. Lattice-Boltzmann method (LBM) comes forward as an efficient numerical simulation tool as far as process engineering (under distinct operational conditions) is particularly concerned.

As a first step towards LBM simulation of both BAC and SFE, the present work was particularly concerned with applying LBM to species concentration in the fluid phase alone. Evoking sorption-desorption kinetics, plug-flow, and mass transport by either convection or diffusion, model frameworks for BAC and SFE are interestingly similar to each other with respect to the aforesaid concentration and such resemblance helped considerably in implementing related simulators. Along with preliminary LBM simulators, finite-difference-method (FDM) codes were equally implemented based upon a dimensionless time-dependent one-dimensional (1-D) diffusive-convective model, whose fundamental governing partial differential equation (PDE) was exactly the same for either BAC or SFE.

As the main purpose of this work was to check proper implementation and functionality of LBM codes, numerical simulations were carried out to compare LBM results against FDM counterparts. With respect to the common governing PDE, overall behavior of the dimensionless fluid-phase concentration profile was reasonably reproduced whereas LBM and FDM results were practically coincident as far as further variations of such PDE is concerned. It is believed that observed differences are due to the convective term in the governing PDE. Besides considering species concentration in the solid phase, already implemented LBM simulators may become more comprehensive inasmuch as they are extended to comprise additional phenomena such as 3-D domains, thermal effects and bed hydrodynamics.

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