A LATTICE BOLTZMANN METHOD APPROACH TO THE ADVECTION-DIFFUSION OF A CONTAMINANT IN AN AQUIFER

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Abstract

The Lattice Boltzmann Method (LBM) is a powerful method which has been introduced recently in numerical hydraulics. Since then, many important results have been obtained. The main advantage of the LBM with respect to other numerical methods, based on the classical governing equations (Navier-Stokes or shallow water), is its intrinsic linearity and versatility.
The aim of this work is to present the formulation and the application of the LBM to the advection-diffusion of a contaminant in a porous medium. After having stated the advection diffusion problem in a porous medium and having presented the correspondent LBM formulation, some numerical results are presented.

Introduction

The Lattice Boltzmann Method (hereinafter LBM) is a powerful method which has been introduced in the Computational Fluid Dynamics field a couple of decades ago. The development of the LBM has been tremendous and many interesting and excellent results have been obtained in several fields of the Fluid Dynamics. The review of Aidun and Clausen (2010) gives a perspective of cutting-edge applications of the LBM, while the books of Succi (2001) and Wolf-Gladrow (2005) are good introductions into the method, with particular regard to its historical development. The book of Zhou (2004) presents the extension of the method to the shallow water flows. The reason of this rapid development is the intrinsic simplicity of the LBM with respect to any classical CFD method, based on the mass, momentum and energy balance equations. This simplicity comes from the fact that the LBM is based on a mesoscopic representation of the fluid, instead of a macroscopic representation, from which the well known mass, momentum and energy balance equations are obtained. In other words, the fluid is seen as a set of particles, which can travel undisturbed for a while and then collide with each other. The distance covered by a fluid particle between two subsequent collisions has a meaning analogous to the mean free path of a perfect gas molecule and has an order of magnitude much smaller than that of the characteristic length-scale of the fluid domain. The description of the state of the fluid is made by means of probability distribution functions (hereinafter PDF), which give the probability, at a given instant of time, of finding a particle in a given position and with a given velocity. The evolution of these PDF is governed by a number of linear kinetic equations equal to the number of PDF. The linearity of the evolution equations is the main advantage of the LBM with respect to methods based on the macroscopic balance equations (Navier-Stokes or shallow water equations).
The aim of this work is to present a LBM being able to simulate the advection-diffusion of a contaminant in a porous medium. The starting point is the mathematical model developed by Nithiarasu et al. (1997) and adopted by Guo and Zhao (2002). This mathematical model is obtained by averaging the continuity and Navier-Stokes equations over a small volume partially occupied by the liquid and partially by the solid. The presence of the porous medium is accounted for by means of additional forces at right hand side (hereinafter RHS) of the momentum equation. This approach has been given recently a solid formal framework by Lasseux et al. (2008).
The structure of this paper is as follows: firstly, the mathematical model is presented; secondly, the LBM equivalent to the mathematical model is formulated; thirdly some numerical results are presented.

The mathematical model

In the following we will consider a 2D, homogeneous and isotropic aquifer, inside of which the flow of a contaminated fluid occurs. The flow is represented by equations obtained (Nithiarasu et al., 1997) by averaging the mass and momentum equations over a small volume containing both the liquid and the solid phase. The presence of the contaminant affects the fluid density ρ and is accounted for by the concentration C. The local fluid density ρ is given by:

$$\rho = \rho_0 + (\rho_s - \rho_0)C \tag{1}$$

ρ_s is the density of the contaminant, ρ_0 the density of the ambient fluid (freshwater). If the condition:

$$\frac{\rho - \rho_0}{\rho_0} = \frac{\rho_s - \rho_0}{\rho_0} C << 1 \tag{2}$$

is fulfilled, the effect of the varying density is felt only in the gravity force term of the momentum equation. Following Nithiarasu et al. (1997), the latter assume the form:

$$\begin{aligned} &\nabla \cdot \mathbf{u} = 0 \\ &\rho_0 \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \frac{\mathbf{u}}{\varepsilon} \right) + \nabla(\varepsilon p) - \mu \nabla^2 \mathbf{u} = \\ &-\varepsilon \left(\rho g \mathbf{k} + \frac{\mu}{k} \mathbf{u} - \frac{\rho_0 c_d}{\sqrt{k}} \mathbf{u}|\mathbf{u}| \right) \end{aligned} \tag{3}$$

ε is the porosity, k is the permeability of the porous medium, μ is the dynamic viscosity, c_d is the dimensionless drag coefficient and $\mathbf{u}$ is the filter velocity. c_d and k can be expressed in terms of the porosity and of the sediment's diameter, as in Guo and Zhao (2002).

In the considered case, the pressure p can be expressed as the sum of the hydrostatic pressure distribution and of the dynamic pressure distribution:

$$p = p_d + \rho g (H - z) \tag{4}$$

H is the constant reference hydrostatic head. Substituting the expression (4) for p in (3) and accounting for the expression of the density (1), the following equation is obtained:

$$\begin{aligned} &\rho_0 \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \frac{\mathbf{u}}{\varepsilon} \right) + \nabla(\varepsilon p) - \mu \nabla^2 \mathbf{u} = \\ &-\varepsilon \left((H - z)(\rho_s - \rho_0) g \nabla C + \frac{\mu}{k} \mathbf{u} + \frac{\rho_0 c_d}{\sqrt{k}} \mathbf{u}|\mathbf{u}| \right) \end{aligned} \tag{5}$$

According to Nithiarasu et al. (1997), the time evolution of the concentration C is governed by the following convection-diffusion equation:

$$\frac{\partial C}{\partial t} + \frac{\mathbf{u}}{\varepsilon} \cdot \nabla C - (\nabla \cdot D \nabla C) = 0 \tag{6}$$

D is the molecular diffusivity of the contaminant. The mathematical model of the flow, consists then of the continuity equation (3), the modified Navier-Stokes (5) and advection-diffusion (6) equations.

The LBM formulation of the problem

An alternative formulation of the mathematical model is given by the Lattice Boltzmann Method (LBM). The main idea of the LBM is to represent the flow as a set of particles which, in analogy to a perfect gas, travel undisturbed for a while and then interact with each other by means of collisions.

The duration Δt and the distance Δx of the fluid particle's undisturbed travelling are small with respect to macroscopic time- and length-scales, i.e. the scales of the fluid domain as a whole. Moreover, define the ratio e as:

$$e = \frac{\Delta x}{\Delta t} \tag{7}$$

The latter is the velocity with which the fluid particle travels. Consider, at a given spatial position x, a finite number N of velocities, each with a different direction. Each velocity is directed toward another spatial point, with a distance Δx from the previous point. The set of spatial points endowed with the set of velocities is the lattice. In two spatial dimensions it is usual to assume the so-called 2DQ9 lattice reproduced in Fig. 1.

The nine velocities (represented as vectors numbered from 0 to 8 in Fig. 1) have different directions but the same intensity e, except for the vector numbered with 0, which represents the zero velocity.

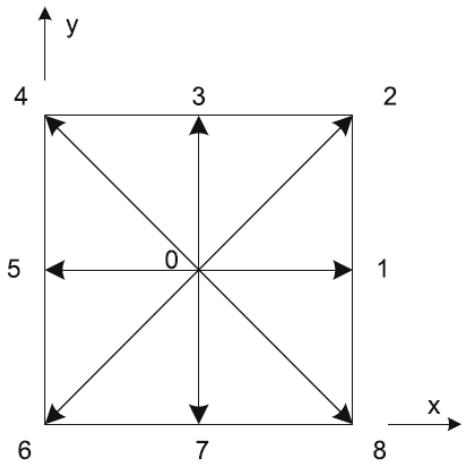

Figure 1: The 2DQ9 lattice.

For the 2DQ9 lattice, these vectors can be defined as:

$$\begin{aligned} &\mathbf{e}_0 = \{0,0\}, \mathbf{e}_i = \left\{ e\cos\left((i-1)\frac{\pi}{4} \right), e\sin\left((i-1)\frac{\pi}{4} \right) \right\}, \quad i = 1,3,5,7 \\ &\mathbf{e}_i = \left\{ \sqrt{2}e\cos\left((i-1)\frac{\pi}{4} \right), \sqrt{2}e\sin\left((i-1)\frac{\pi}{4} \right) \right\}, \quad i = 2,4,6,8 \end{aligned} \tag{8}$$

The state of the fluid is described by means of N+1 probability density functions f_i (i=0,…,N) each giving the probability of finding a fluid particle, at a given instant of time, at a given position, travelling with the velocity $\mathbf{e}_i$. The evolution of the probability density functions is governed by the following set of N+1 kinetic equations:

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = \Omega_i + \frac{\mathbf{e}_i \cdot \mathcal{F}}{N_c e^2} \quad (i = 0,\ldots,N) \tag{9}$$

The meaning of the symbols is the following: Ω_i is the collision operator, i.e. the term which describes the interaction between the particles, the vector $\mathcal{F}$ represents the external forces, per unit volume, acting on the flow, N_c a constant integer, defined by (Liu et al., 2010):

$$N_c = \frac{1}{e^2}\sum_{i=0,N} e_{ix}e_{ix} = \frac{1}{e^2}\sum_{i=0,N} e_{iy}e_{iy} \tag{10}$$

The vector of the external forces is defined as:

$$\mathcal{F} = -\varepsilon\left(g(H-z)(\rho_s - \rho_0)\nabla C - \frac{\mu}{k}\mathbf{u} - c\frac{\rho_0}{\sqrt{k}}\mathbf{u}|\mathbf{u}| \right) \tag{11}$$

The macroscopic quantities, which in the considered case are the liquid density and the velocity field, are obtained from the probability density functions by means of the simple operations (Succi, 2001):

$$\rho_0 = \sum_{i=0,N} f_i \,,\; \rho_0 \mathbf{u} = \sum_{i=0,N} \mathbf{e}_i f_i \tag{12}$$

The latter can be seen as the zeroth and first order statistical moments of the probability density functions with respect to the velocity $\mathbf{e}_i$. Once the collision operator is defined, the formulation of the LBM is complete. Although the original structure of this operator, defined by Ludwig Boltzmann to describe the interactions among the molecules of a perfect gas, was very complicated and highly nonlinear, it has been found that a linear approximation (Chen and Doolen, 1998) is good enough to obtain reliable results.

$$\Omega_i = -\sum_{j=1,N} M_{ij}\left(f_j - f_j^{eq}\right) \quad (i = 1,\ldots,N) \tag{13}$$

M_{ij} are the elements of the collision matrix and f_j^{eq} is the equilibrium probability density function, which is assigned. In this work we assume for the collision matrix the simple isotropic form of Bhatnagar, Krook and Gross (Succi, 2001).

$$M_{ij} = \frac{1}{\tau^*}\delta_{ij} \tag{14}$$

δ_{ij} is the Kronecker delta and τ^* the relaxation time. The latter is an indication of the rapidity with which the system goes toward to the instantaneous equilibrium, represented by the equilibrium probability density function f_j^{eq}. The difference $f_j - f_j^{eq}$ is the deviation from the equilibrium. Despite of its simplicity, the Bhatnagar, Krook and Gross form of the collision operator (14) is very often and successfully used also for complex flows (Succi, 2001; Aidun and Clausen, 2010). Finally, adopting the following definition of the equilibrium probability density functions (Guo and Zhao, 2002):

$$\begin{cases} f_i^{eq} = \rho_0 a_i\left[1 + 3\dfrac{\mathbf{e}_i \cdot \mathbf{u}}{e^2} + \dfrac{9}{2}\dfrac{(\mathbf{e}_i \cdot \mathbf{u})^2}{\varepsilon e^4} - \dfrac{3}{2}\dfrac{\mathbf{u}\cdot\mathbf{u}}{\varepsilon e^2}\right], \quad i = 0,\ldots,N \\ a_0 = \dfrac{4}{9}, a_1 = a_3 = a_5 = a_7 = \dfrac{1}{9}, a_2 = a_4 = a_6 = a_8 = \dfrac{1}{36} \end{cases} \tag{15}$$

it is possible to show that, following the Chapman-Enskog procedure (Chen and Doolen, 1998), the LBM consisting of the equations (9), with definitions (10), (11), (12), (13) and (14) is "approximately" equivalent to the Navier-Stokes equation (5) with a kinematic viscosity defined by (Liu et al. 2010):

$$\nu = \frac{e^2 \Delta t}{6}\left(2\frac{\tau^*}{\Delta t} - 1\right) \tag{16}$$

In literature, the dimensionless ratio $\tau^*/\Delta t$ is often defined as the relaxation time τ. The error of approximation of the equivalence between the LBM and the Navier Stokes equation (5) is proportional to a small parameter, which can be identified with the Mach number of the flow (Succi, 2001; Wolf-Gladrow, 2005).

Accordingly to Zhou (2009), the LBM can be extended to the advection-diffusion equation (6). In other words, it can be shown that the kinetic equations:

$$\frac{\partial f_i^c}{\partial t} + \mathbf{e}_i \cdot \nabla f_i^c = -\frac{f_i^c - f_i^{ceq}}{\tau} \quad (i = 0,1,3,5,7) \tag{17}$$

together with the following definition of the equilibrium distribution functions for the concentration f_i^{ceq}:

$$\begin{cases} (1-2\lambda)C, & i = 0 \\ \dfrac{1}{2}\left(\lambda + \dfrac{\mathbf{e}_i \cdot \mathbf{u}}{\varepsilon e^2}\right)C, & i = 1,3,5,7 \end{cases} \tag{18}$$

are equivalent to the advection-diffusion equation (6) with a diffusivity D defined by (Zhou, 2009):

$$D = \lambda e \Delta x\left(\tau - \frac{1}{2}\right) \tag{19}$$

The concentration C is obtained by means of the simple operation:

$$C = \sum_{i=0,1,3,5,7} f_i^c \tag{20}$$

The coefficient λ is a dimensionless dispersion coefficient, while the vector $\mathbf{u}$ in (18) is the velocity field. It is important to observe that the kinetic equations (17) are relative only to five velocities out of the nine defined by the 2DQ9 lattice. In other words the lattice of the concentration

C has a structure simpler than that of the velocity lattice. This fact is due to the intrinsic scalar nature of the concentration *C* (Zhou, 2009).

Results and discussion

Description of the considered flow

The two dimensional fluid domain under consideration is a rectangle, basis *L*, height *H*. At the left vertical boundary (x=0) the concentration of a contaminant is imposed:

$$\begin{cases} C(0,y,t) = c_0, & y_1 \le y \le y_2, \quad t \ge 0 \\ C(0,y,t) = 0, & y < y_1, y > y_2, \quad t \ge 0 \end{cases} \tag{21}$$

At the horizontal boundaries and at the right vertical boundary, the directional derivative of the concentration along the normal to the boundary vanishes.

$$\left.\frac{\partial C}{\partial x}\right|_{x=L} = \left.\frac{\partial C}{\partial y}\right|_{x=0,H} = 0, \quad t \ge 0 \tag{22}$$

The velocity field **u** is imposed at the left vertical boundary. The horizontal boundaries are assumed as impermeable, i.e. the scalar product **u**·**n** (being **n** the unit vector normal to the boundary) vanishes there and a free-slip condition is adopted, while at the right vertical boundary, supposed far enough from the left vertical boundary, the velocity field is imposed, in order to conserve mass.

Validation of the model

The correctness of the model has been verified by comparing the numerical results with analytical results. The validation has been made separately with respect to the LBM formulation of the molecular diffusion process, represented by equation (6) with imposed and constant flow velocity, and to the LBM formulation of the Navier-Stokes equation (5).

The analytical solution of the advection-diffusion equation (6) correspondent to the boundary condition (21) in presence of a constant velocity field directed along the *x* axis has been compared to the numerical solution of the kinetic equations (17). If y_1=0 and y_2=*H*, the analytical solution is given by:

$$c(x,t) = c_0\left(1 + \frac{1}{2}\left(e^{\frac{Ux}{D}}\left(1 - Erf\left(\frac{x+ut}{2\sqrt{Dt}}\right)\right) - \left(1 + Erf\left(\frac{x-ut}{2\sqrt{Dt}}\right)\right)\right)\right) \tag{23}$$

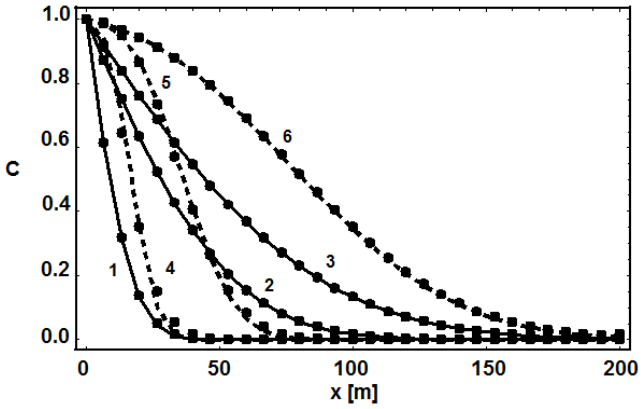

Figure 2. Concentration profiles.1) D=2×10^{-3} m^{2}s^{-1}, u=0. ms^{-1}, t=44000s; 2) D=2×10^{-2} m^{2}s^{-1}, u=0. ms^{-1}, t=44000s; 3) D=2×10^{-1} m^{2}s^{-1}, u=0. ms^{-1}, t=11000s; 4) D=2×10^{-3} m^{2}s^{-1}, u=0.001 ms^{-1}, t=15400s; 5) D=2×10^{-2} m^{2}s^{-1}, u=0.005 ms^{-1}, t=6600s; 6) D=2×10^{-1} m^{2}s^{-1}, u=0.01 ms^{-1}, t=6600s;

In (23) the symbol *Erf* stands for error function. In this case the analytical solution (23) depends only on *x* and *t* and the behavior of the concentration is 1D. *u* is the constant *x* velocity component. In Fig. 2 analytical (solid and dashed curves) and numerical concentration curves (dots) are plotted. They have been obtained assuming different values for the diffusivity and the *x* velocity component (see the figure caption for the details). The agreement between numerical and analytical results is very good, even if the number of computational points was relatively low. Indeed only 30 points have been defined along *L* and *H* which were assumed equal to 200m, with a resulting Δx equal to 6.67m. Moreover, the effect of the advection is clearly shown in Fig. 2, mostly by the curves 5 and 6, relative to a diffusivity of 0.2m^{2}s^{-1} and a velocity of 0.0 and 0.01 ms^{-1} respectively.

If the length of the segment through which the concentration c_0 is imposed at x=0 is less than *H*, the distribution of the concentration becomes fully 2D and the analytical solution is given by the series (Wexler, 1992):

$$c(x,y,t) = c_0 \sum_{i=0}^{\infty} L_i Cos\left(i\frac{\pi}{H}y\right) \times \left[e^{\frac{x(u-\beta_i)}{2D}} Erfc\left(\frac{x-\beta_i t}{2\sqrt{Dt}}\right) + e^{\frac{x(u+\beta_i)}{2D}} Erfc\left(\frac{x+\beta_i t}{2\sqrt{Dt}}\right)\right]$$

$$\begin{cases} L_i = \dfrac{y_2 - y_1}{2H}; \quad i = 0 \\ L_i = \dfrac{1}{i\pi}\left(sin\left(i\dfrac{\pi}{H}y_2\right) - sin\left(i\dfrac{\pi}{H}y_1\right)\right); \quad i = 1,2,3\ldots \end{cases} \tag{24}$$

$$\beta_i = \sqrt{u^2 + \left(i\frac{2\pi}{H}D\right)^2}$$

In (24) the symbol *Erfc* stands for the complementary error function. As highlighted in Wexler (1992), the terms in the

infinite series (24) oscillate, and the series converges slowly for small values of x. A suitable number of terms may be necessary to ensure convergence.

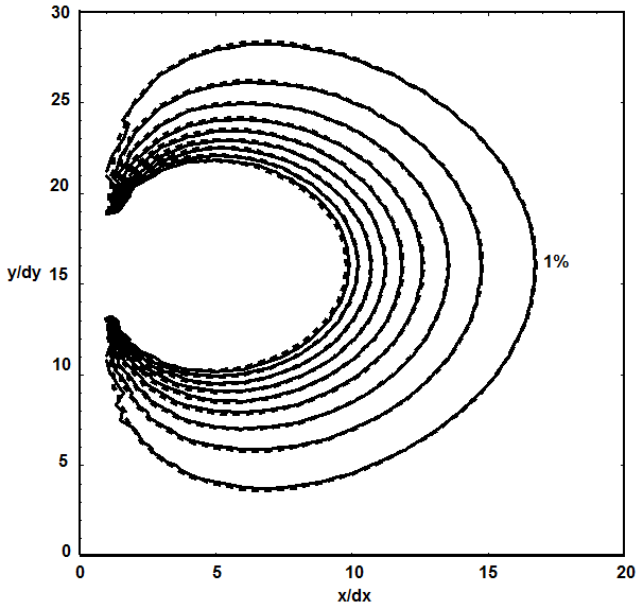

Figure 3. Iso-lines of the concentration. Starting from the external 1% curve, the internal curves increase the concentration regularly of 1%. D=2×10^{-3} m^{2}s^{-1}, u=10^{-5} ms^{-1}, t=528000s; y_1=86.7m ($y/\Delta y$=13) and y_2=113.3m ($y/\Delta y$=17).

Figure 3 shows the fully 2D distribution of the iso-concentration curves at t=528000 s. Analytical (solid lines) and numerical (dashed lines) results plotted in Fig. 4 have been obtained assuming D=2×10^{-3} m^{2}s^{-1}, u=10^{-5} ms^{-1}, y_1=86.7m ($y/\Delta y$=13) m and y_2=113.3m ($y/\Delta y$=17). The agreement is quite good. Small differences appear in the neighborhood of the zone where the contaminant is entered. This is probably due to the fact that in this region the gradients of the concentration are much larger than elsewhere.

Being concerned with the LBM formulation of the Navier-Stokes equation (5), the 1D Poiseuille flow has been considered for the validation. In this case the analytical solution is given by:

$$u = \frac{gJH}{2\nu} y\left(1 - \frac{y}{H}\right) \tag{26}$$

J is the pressure gradient in x direction and ν the kinematic viscosity, determined by means of definition (16). The numerical Poiseuille flow has been obtained in the rectangular domain (H=50m, L=10m) imposing the analytical velocity profile (26) as initial condition and letting the computation run.

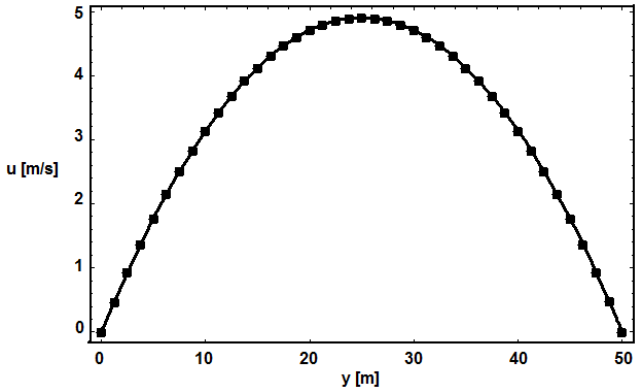

Figure 4. The Poiseuille velocity profile. J=0.01, ν=6.25 m^{2}s^{-1}, t=25000 s.

In Fig. 4 the numerical and analytical Poiseuille velocity profiles are shown. Also in this case the agreement is very good, despite of the low number (n_y=40) of computational points adopted in y direction. Moreover, the numerical solution remains stable for the whole duration of the simulation (25000s).

Advection-diffusion of a contaminant in a porous medium

The contaminant affects the velocity fields, due to the presence of the gravity term at the RHS of equation (5). This term forces the motion in the opposite direction of the concentration gradients. In other words, the forcing is directed towards the direction of diminishing concentration. The other forcing terms at RHS of equation (5) are respectively a viscous and a drag term. Their relative importance is given by the product of the dimensionless numbers of Darcy and Reynolds:

$$\sqrt{Da}\, Re \tag{27}$$

being the Darcy number and the Reynolds number defined as:

$$Da = \frac{k}{H^2}, Re = \frac{UH}{\nu} \tag{28}$$

H is a characteristic length scale. If the dimensionless product (27) is smaller with respect to the unity, the drag term can be neglected in comparison with the viscous term.

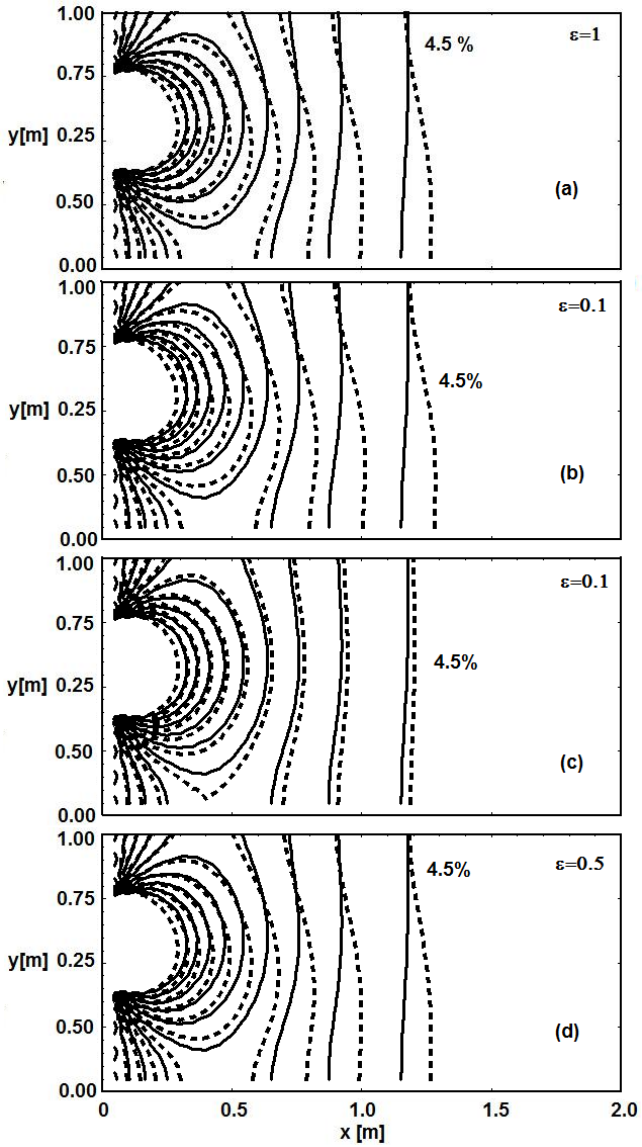

Figure 5. Modification of the concentration field due to the velocity field. a) Absence of viscous and drag forces (ε=1); b) Absence of viscous and drag forces (ε=0.1); c) presence of both viscous and drag forces (ε=0.1); d) presence of both viscous and drag forces (ε=0.5). Analytical results: solid line. Numerical results: dashed line.

In Fig. 5 four different cases are presented. They show the influence of the different forces and the porosity ε in a rectangular fluid domain L=2m, H=1m, with an initial uniform and constant velocity field, directed towards x direction. The x component of the initial velocity field is equal to 0.0001 m/s. The molecular diffusivity is equal to $0.002 m^2 s^{-1}$. The inlet of contaminant occurs through a segment 0.35m long, starting at y=0.35m. The analytical solution (24) is also plotted in figure 5 (the solid line). All of the cases considered in Figure 5 are relative to the instant of time t=123s.

The case with porosity ε=1 and neither viscous nor drag forces is considered in Fig. 5a. The presence of the contaminant, which in this case acts only in the gravity force, modifies sensibly the numerical curves of constant concentration (dashed lines) with respect to the analytical lines (solid lines). A y velocity component is evidently developed, from the initial constant and uniform velocity field. A smaller porosity does not cause evident modification of the concentration field (Fig. 5b), while the presence of the viscous force damps the velocity field and makes the concentration curves of the case shown in Figure 5c more similar to the analytical solution, with respect to the cases shown in the other figures. An increase in porosity (Fig. 5d) affects the gravity force and the result is again similar to those of Figg. 5a, 5b.

In all of the considered cases (except for Fig. 5a where neither viscous nor drag force was considered) the product (27) had an order of magnitude not larger than 10^{-3}, so the influence of the drag force was negligible.

Conclusion

In this paper a Lattice Boltzmann Method approach has been used to model the problem of the advection-diffusion of a contaminant in a porous medium.

The LBM formulation has been validated comparing numerical results with analytical results.

A case of advection-diffusion has been considered in order to show the influence of the several force terms and the porosity. It has been found that for a small porosity (ε=0.1) the influence of the viscous term is such to counterbalance the effect of the gravity force on the concentration field. This influence is vanishing with the increase of porosity.

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