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Lattice-Boltzmann code for a multiphase fluid flow through reconstructed porous media

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Abstract: In this paper, we present a Lattice Boltzmann simulation of multiphase flow in a homogeneous two-dimensional porous media. For this study, we develop a program based on lattice Boltzmann equation. The underlying theoretical model makes it possible to couple the state equation of a non-ideal fluid with the pressure tensor at the interface and uses the excess free-energy density formalism. The fluid properties can be prescribed in a thermodynamically consistent manner, which remains accurate at states close to the critical point. We have simulated some known two-phase flow configurations, like displacement of vapor by its liquid in homogeneous two-dimensional porous media reconstructed by image treatment under the action of an external flow field. We present also results for the averaged velocity as a function of time iteration and the permeability of two dimensional porous media as a function of kinematic viscosity and mesh resolution. Our results confirm that the LBM scheme reproduces Darcy's law through the analysis of the dependency of the permeability on the kinematic viscosity.

Keywords: Lattice Boltzmann method, multiphase flow simulation, Darcy law, porous media, kinematic viscosity.

1. Introduction

In recent years, there has been significant progress in the development of the lattice Boltzmann equation (LBE) method [1], a novel technique developed for modeling complex systems. One particular application of the lattice Boltzmann method which has attracted considerable attention is the modeling of heterogeneous fluids, such as multi-phase or multi-component fluids [2, 3]. These flows are important, but are difficult to simulate by conventional techniques of solving the Navier-Stokes equations. The main difficulty conventional techniques face is the existence of interfaces in inhomogeneous flow. There is ample evidence that the lattice Boltzmann models based on mesoscopic theory are particularly suitable for these systems [3].

Historically, the lattice Boltzmann equation was first developed empirically [1] from its predecessor the lattice-gas automata [4]. This empiricism influences even the most recent lattice Boltzmann models [2]. Empirical lattice Boltzmann models usually have someinherent artifacts which are not yet fully understood. One particular problem with multi-phase or multi-component lattice Boltzmann models is the thermodynamic inconsistency: the equilibrium state in these models cannot be described by thermodynamics [5]. Although this issue has been raised previously [5], no progress has been made in solving this problem, despite its paramount importance. It has been recently demonstrated [6] that the lattice Boltzmann equation can be directly derived the continuous Boltzmann equation.

Flow through porous media has been a topic of longstanding interests in many areas of science and engineering [7]. The lattice Boltzmann discrete numerical schemes were found to be easily applied to fluid flows in different porous structures immediately after their elaboration, while recent applications are dealing with packed beds of fibers [8]. Previous numerical simulations, including finite difference schemes [9] and networking models [10],

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were either limited to simple physics, small geometry size, or both. Lattice gas automata (LGA) were also used to simulate porous flows and check Darcy's law in simple and complicated geometries [11]**.**Succi& al. [12] used the LBM to measure the permeability in 3-D random media Darcy's law was confirmed. Flows through sandstones measured using X-ray micro tomography were simulated by Buckles & al. [13]**,**Soll& al. [14], and Ferréol& Rothman [15]**.** They found that the permeability for these sandstones, although showing large variation in space and flow directions, in general agreed well with experimental measurements within experimental uncertainty. H. Hidemitsu [16] also studied the effect of grid resolution on permeability. He found that the viscosity dependence decreases with the increase the grid resolution and the dependence of permeability on the grid resolution decreases as the viscosity decreases.

This paper main objective is the simulation of a low Reynolds number two-phase flow in porous media, using a discrete numerical scheme. The method is based on the lattice Boltzmann approach with an external force. In the first section, we outline the essential back-ground of the LBM method with external force. Application to two dimensional porous media flow is detailed.

2. Lattice Boltzmann Method

In the LB method, a typical volume element of fluid is described as a collection of particles that are represented in terms of a particle velocity distribution function at each point of space. The single particle distribution function, $f_i(x) = f_i(x, e_i)$ defined for each lattice vector $\vec{e}_i$ at each site x. Taking for simplicity a single-time relaxation approximation (BGK), the evolution of equation for a given f_i takes the form [5]**:**

$$f_\alpha(x + \vec{e}_i\Delta\mathrm{t}, t + \Delta\mathrm{t}) = f_i(\vec{x}, t) - \frac{1}{\tau}\left[f_i(x, t) - f_i^{(eq)}(x, t)\right] \quad (1)$$

Where $\Delta\mathrm{t}$ is the time step and τ is the relaxation parameter. $f_i^{(eq)}$ is an equilibrium distribution function. For a one component non-ideal fluid. The density ρ and the fluid momentum ρu are related to the distribution functions by:

$$\rho = \sum_i f_i = \sum_i f_i^{eq} \quad (2)$$

$$\rho u_\alpha = \sum_i \mathrm{e}_{\mathrm{i}\alpha} f_i = \sum_i \mathrm{e}_{\mathrm{i}\alpha} f_i^{eq} \quad (3)$$

3. Lattice Boltzmann for Multiphase Flow

There have been a number of LB multiphase flow models presented in the literature. The first immiscible multiphase LB model proposed by Gunstensen*et al.* uses red and blue colored particles to represent two kinds of fluids [17]. The phase separation is then produced by the repulsive interaction based on the color gradient and color momentum. The model proposed by Shan and Chen (SC) imposes a non-local interaction between fluid particles at neighboring lattice sites [18]. The interaction potentials control the form of the equation of state (EOS) of the fluid. Phase separation occurs automatically when the interaction potentials are properly chosen. There is also the so-called free-energy-based approach proposed by Swift et al. [5]. In this model, the description of non-equilibrium dynamics, such as Cahn-Hilliard's approach, is incorporated into the LB model by using the concepts of the free energy function. The free energy model has a sound physical basis, and, unlike the SC model, the local momentum conservation is satisfied. However, this model does not satisfy Galilean invariance and some unphysical effects will be produced [19] in the simulation.

4. Free Energy Approach

The higher moments of $f_i^{(eq)}$ must be chosen such that the resulting continuum equations correctly describe the hydrodynamics of nonideal, one-component fluid [5]. Defining the second moment as:

$$\sum_i f_i^0 e_{i\alpha} e_{i\beta} = P_{\alpha\beta} + \rho u_\alpha u_\beta , \qquad (4)$$

Where α and β represent a Cartesian coordinates and, as usual, a summation over repeated indices is assumed.

The van der Walls fluid for nonideal system at a fixed temperature has the following free-energy functional within a gradient-squared approximation:

$$\Psi = \int d\vec{r} \left(\psi(T, \rho) + \frac{k}{2} (\nabla \rho)^2 \right) \qquad (5)$$

The first term in the integral is the bulk free-energy density at a temperature T, which is given by:

$$\psi(T, \rho) = \rho T \ln \left(\frac{\rho}{1 - \rho b} \right) - a\rho^2 \qquad (6)$$

And the second term gives the free-energy contribution from density gradients in an inhomogeneous system and is related to the surface tension through the coefficient k . To produce two-phase behavior, the pressu

re tensor must be generalized beyond the usual diagonal hydrostatic pressure tensor to include off-diagonal terms. The form used in these calculations is the Cahn-Hilliard pressure tensor which is related to the free energy in the usual way:

$$P_{\alpha\beta}(\vec{r}) = P(\vec{r}) \delta_{\alpha\beta} + k \frac{\partial \rho}{\partial x_\alpha} \frac{\partial \rho}{\partial x_\beta} \qquad (7)$$

With

$$P(\vec{r}) = p_0 - k\rho \nabla^2 \rho - \frac{k}{2} \left| \vec{\nabla} \rho \right|^2 \qquad (8)$$

Where $p_0 = \rho \psi'(\rho) - \psi(\rho)$ is the equation of state of the fluid.

The shear viscosity ν is given by:

$$\nu = \frac{1}{8} (\tau - 1/2) \Delta t \, c^2 \qquad (9)$$

Where c is the sound velocity.

The Van Der Waals theory gives the following expression for the interfacial tension at a flat interface [20]**:**

$$\sigma = k \int_{-\infty}^{+\infty} \left(\frac{\partial \rho}{\partial z} \right)^2 (z) dz \qquad (10)$$

where z is the coordinate perpendicular to the interface.

Applying the approximation done for the density near the critical temperature this expression becomes [19]**:**

$$\sigma = 2k \frac{(\rho_2 - \rho_1)^2}{3D} \qquad (11)$$

where D is a measure of the interface thickness.

And the capillary number is given by [21]**:**

$$C_a = \frac{\mu_d u}{\sigma} \qquad (12)$$

In Eqn. (13), $\mu$is viscosity, subscript d represents the displacing fluid, u is the velocity of the displacing fluid, and σ is the interfacial tension between fluids.

5. Application of two Dimensional Flows in Porous Media

The LBM method presented in the previous section takes the density and the velocity as independent variables. To simulate fluid flow in porous media, we use an LBM scheme for incompressible fluid, in which pressure and velocity are independent variables. This LBM is convenient for confirming the conservation of flow, which, for an incompressible fluid, must be constant over a porous media [16]. One fundamental information necessary for the understanding of such a flow is the relation between applied pressure gradient and the resulting fluid flux. In the limit of zero Reynolds number, the pressure-flux relation becomes linear, commonly known as Darcy's law. This empirical based relation is shown to be valid by rigorous methods of homogenization and volume averaging **[7]**. Permeability, as a fundamental physical quantity of a porous media, is defined using Darcy's law [16], which takes the average values over this area:

$$\langle u\rangle = -\frac{K}{\mu}(\nabla p - \rho_0 f) and f = -\frac{1}{\rho_0}\nabla p \qquad (13)$$

Where u is the fluid velocity, $\langle ... \rangle$ is the average over the porous media, K represent the intrinsic permeability, ∇p is the pressure gradient, $\rho_0 f$ is the external force operating on the unit volume of the fluid and μ the viscosity related to the kinematic viscosity through $\mu = \rho_0 . v$.

For the purpose of numerical calculations, it is convenient to introduce the dimensionless permeability, which is related to the permeability of a square with side length L_c[16]**:**

$$K_{tpl} = (1/L_c^2) \times K \qquad (14)$$

S.D.C. Walsh et al derive an analytical expression that relates the intrinsic permeability to the solid fraction [22]**:**

$$K = \frac{(1-n_s)v}{2n_s} = \frac{\varepsilon . v}{2(1-\varepsilon)} \qquad (15)$$

Where n_s present solid fraction and ε represent the porosity of porous media.

6. Results and discussion

We implemented the lattice Boltzmann model for non-ideal fluids to simulate two-phase flow in homogeneous two-dimensional porous media reconstructed by image treatment. The two steps “stream and collide” algorithm [23] for a hexagonal lattice (D2Q7) is used to simulate lattice Boltzmann equation on 100×100 and 170×170 site lattices. The domain can be decomposed into unit cells of length L and only the content of such unit cell is displayed. The fluid chosen by Swift et al. [20] was selected for our study, which has as coefficients $a = 9/49$ $and b = 2/21$, corresponding to a critical density $\rho_c = 7/2$, and a critical temperature $T_c = 4/7$, throughout this work $k = 0.01$. No slip boundary conditions are imposed on the walls and periodic boundary conditions are imposed on the two domain ends, the parameter values are:

$\rho_1 = 2\,\text{kg/m}^3$, $\rho_2 = 6\,\text{kg/m}^3$, D = 1 and σ = 0.107

Fig.1 shows the variation of the average velocity over the porous media as a function of time iteration in the section of the media located at the position (x=Lx/2), the stationary regime was reached only after 500 simulation iterations. After this time the mode of flow is permanent what results in a constant average velocity at moment (t+1), this curve is a good indicator for the convergence of the results obtained.

Fig. 2 shows treated image of a porous media. The dark is solid and the white is the pores [24] .The immiscible displacement of the vapor by liquid in reconstructed porous media is analyzed. This network consists of capillaries containing segments of variable cross sections with no preferential wetting as shown in Figure (3). A high capillary number $C_a = 1.6 \times 10^{-2}$ is reached during the flow which leads to a very efficient sweep. After 70000 time steps, the liquid traversed the totality of pores leaving some trapped vapor. For a complete sweep we need to run our program more than 200000 time steps. This type of simulation is useful to predict the flooding process in actual hydrocarbon fields with nonuniforme wettability.

The variation of the dimensionless permeability values, K_{tpl} with the kinematic viscosity is obtained from Equations (13), (14) and (15). Changing the magnitude of the kinematic viscosity, we have calculated the dimensionless permeability K_{tpl}, and the results are given in Fig. 4. The problem wherein the permeability varies with the fluid viscosity has been investigated by H. Hidemitsu **[16]** and has been interpreted to originate from insufficient resolution of the underlying lattice of the LBM. In order to confirm this interpretation, we increased the resolution by preparing a fine grid, in which we have two grids resolutions (100×100) and (170×170) voxel lattice, and calculated the permeability using the fine grid. The results are shown in figure 4. We understand from this figure that the viscosity dependence decreases with the increase in the grid resolution, and the interpretation mentioned above is confirmed. In addition Fig. 4 indicates that the dependence of the permeability on the grid resolution decreases as the viscosity decreases, our results confirmed by an analytical solution [22] (Equations 15). As shown in Fig. 4, LBM method produces the correct result for this requirement for the calculated permeability.

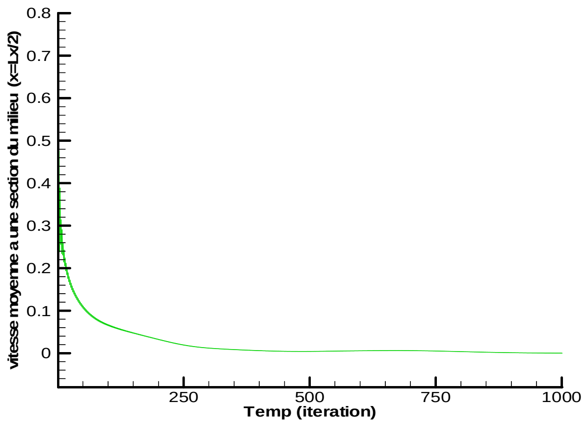

Fig.1. Average axial velocity vs. time iteration

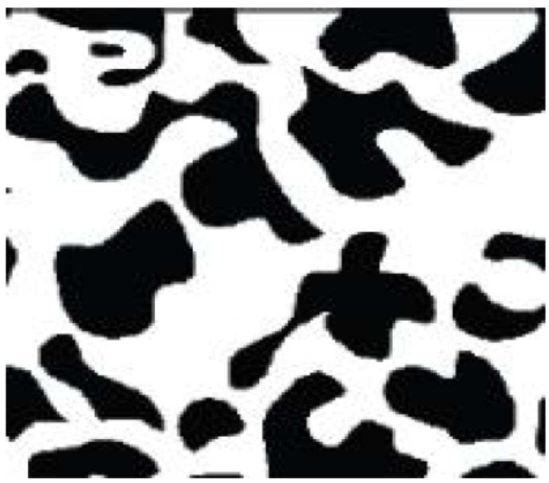

Fig.2. treated image of a porous media. The dark is solid and the white present the pores [24]

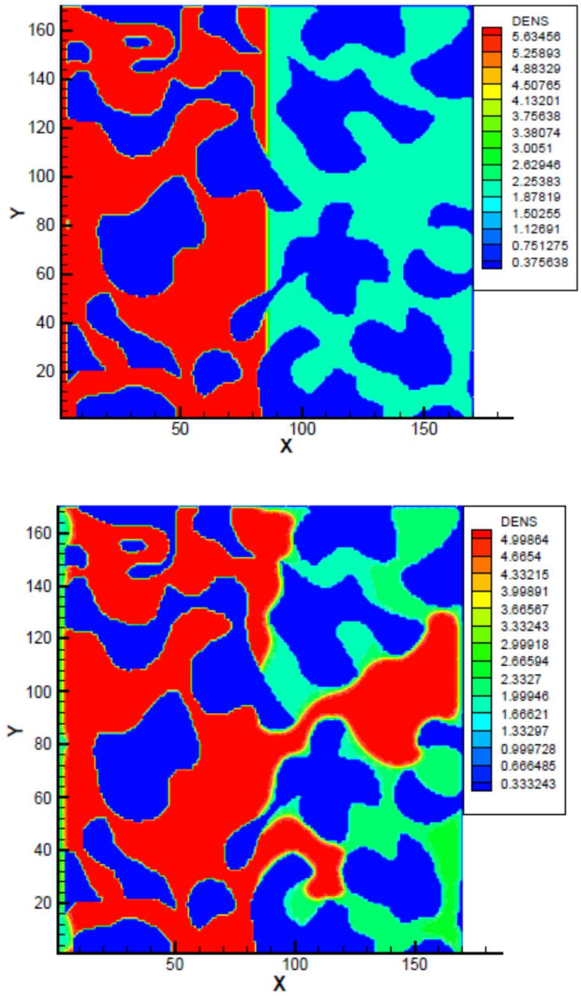

Fig.3. vapor displacement by liquid in reconstructed porous media by image treatment. Blue color presents the solid (the dark color in Fig. 2)

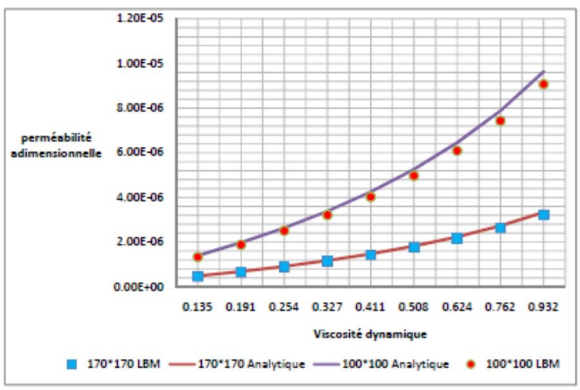

Figure.4. Dimensionless permeability vs. kinematic viscosity for two grid resolutions.(100*100) and (170*170).

Table1. Comparison between Numerical and Analytical of Dimensionless permeability with different values of dynamic

μ	LBM	Analytical	relative error %
0.135	4.63E-07	4.82E-07	3.88E+00
0.191	6.57E-07	6.83E-07	3.75E+00
0.254	8.77E-07	9.10E-07	3.63E+00
0.327	1.13E-06	1.17E-06	3.52E+00
0.411	1.42E-06	1.47E-06	3.44E+00
0.508	1.76E-06	1.82E-06	3.40E+00
0.624	2.16E-06	2.23E-06	3.40E+00
0.762	2.64E-06	2.73E-06	3.45E+00
0.932	3.22E-06	3.34E-06	3.56E+00

6. Conclusions

We have developed an LBM with an external force for two-phase flow in homogeneous two-dimensional porous media reconstructed by image treatment. In which the independence variable are pressure and velocity. Using this LBM, we can impose the periodic boundary condition on the inlet and outlet of the flow driven by external force. This is an advantage of the LBM with an external force, because we can easily code the periodic boundary condition to be applicable to any velocity model, while the fluid mechanic boundary must be prepared for each velocity model. The numerical study is extended to the estimate of the physical parameters characteristic of porous media, our results show the ability of LBM to calculate of the physical parameters correctly like the permeability. We have demonstrated the ability of LBM to predict a complexes phenomenon within a complex geometry.

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