JITH 2017
18èmes Journées Internationales de Thermique (JITH 2017)
Monastir (Tunisie), 25 - 27 Octobre 2017

Lattice Boltzmann simulation of liquid transport through gas diffusion layer of PEMFC

Mohamed El Amine Ben Amara
Sassi Ben Nasrallah
Adresse des auteurs Laboratoire d'Études des Systèmes Thermiques et Énergétiques, École Nationale d'Ingénieurs de Monastir, Monastir 5019 Tunisie
ben.amara.amin@gmail.com
Sassi.bennasrallah@enim.rnu.tn

Résumé: This work is about two phase flow in a gas diffusion layer of a polymer electrolyte membrane fuel cell using a lattice Boltzmann Shan-Chen algorithm which is an efficient numerical scheme for the time dependent simulation of multiphase fluid flow problems. This method is especially useful for modelling complicated boundary conditions and multiphase interfaces and it is based on microscopic models and macroscopic kinetic equation. A numerical code is used to simulate two-dimensional flow through an idealized and a real GDL to characterize density distributions in the layer. The porous medium is firstly constructed by random discs of different diameters, next a real GDL will be used in the simulation after being binarized.

Key words: GDL, lattice Boltzmann, Fuel Cell, Shan-Chen.

1. Introduction

A fuel cell is a device that generates electricity by a chemical reaction. There are different types of fuel cells. A fuel cell proton exchange membrane (PEM) is composed of an anode, a cathode, two bipolar plates, two catalysts and a membrane. The hydrogen and oxygen are fed to the anode and cathode by the flow channels and the gas-diffusion-layers (GDL), while the water produced in the porous membrane is then shunted out to the exterior of the fuel cell. The polymer membrane must be hydrated to ensure high conductivity of protons. Diffusion layers must have sufficient pores to provide reactant gas access from flow-field channels to catalyst layers and providing passage for removal of product water from catalyst-layer area to flow-field channels which must have a well-defined shape. The bipolar plate containing the channels must have an adequate geometry for improving the performance of a fuel cell. PEM operating at reduced temperature and pressure levels, which triggers the development of two-phase flows inside the bipolar plates channels and the gas diffusion layer. The gas diffusion layer commonly referred as GDL consists of a porous support, electronic and thermal conductor, which is conventionally composed of a carbon cloth or paper (Figure 1). In a PEMFC fuel cell, the diffusion layers must simultaneously lead the gases of the channels into the active zone and evacuate the products of the reaction. For this the GDL must be permeable to reagents and products in all directions. The best material which respects the constraints imposed by the operation of the fuel cells is a material based on carbon fibers whose diameter is approximately 10 µm. The GDL is in the form of cloth or felt whose thickness is between 200 and 400 µm. The GDLs have a strong anisotropy: the fibers have a privileged orientation. The GDLs have porosities of the order of 80%. Gdls are compressed between the bipolar plates and the membrane / electrode assembly and their effective thickness decreases by 10 to 40%.

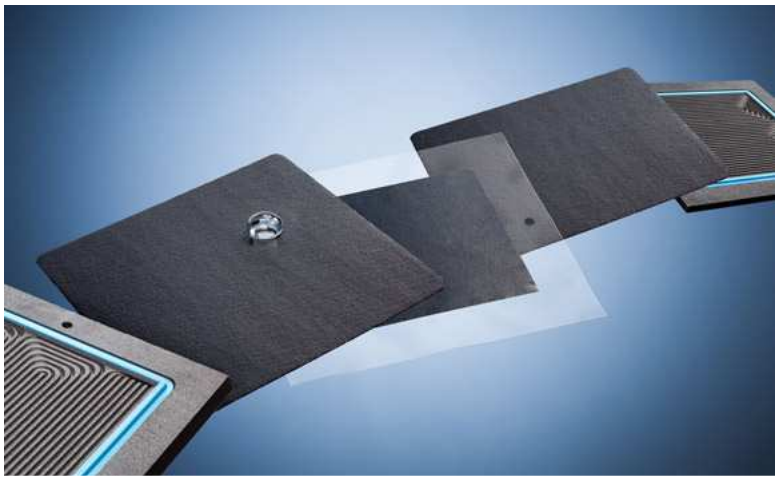

Figure 1: Gas Diffusion Layers in FC Stack (Freudenberg Fuel Cell Products R)

It's very important to study the flow behavior in gas diffusion layer of PEFC in order to test the fuel cell performance. In this work, two phase flow distribution in GDL is modeled using the lattice Boltzmann method in two dimensions. Simulations are carried out by the incompressible LBGK 2D 9-velocity (D2Q9) model. Firstly the GDL is considered as a porous media constructed by fixed disks after that a two-dimensional slice of a real GDL will be studied.

2. Lattice Boltzmann method

Over the last decade the lattice-Boltzmann (LB) methods (Qian et al (1992), Chen et al (1998), Succi et al (1991)) have achieved great success as alternative and efficient numerical schemes in the simulation of a variety of transport phenomena in porous media, modeling fluid flow in fuel cells, and microfluidics.
Due to its simple calculation procedure, efficient implementation, simplicity of boundary condition's implementation, easy and robust handling of complex geometries, LBM is considered as the best alternative to traditional conventional computational fluid dynamics solvers which basically solve the macroscopic transport equations.
This method is a mesoscopic approach inheriting many of the advantages of molecular dynamics and kinetic theories without using complicated kinetic equations.
The starting point of the lattice Boltzmann method is to solve, on a discrete lattice, the following Boltzmann equation for the discrete velocity distribution:

$$\frac{\partial f_i}{\partial t} + e_i \bullet \vec{\nabla} f_i = \Omega(f_i) \qquad (1)$$

Where e_i is the speed of a particle at a position x_i and time *t* and $\Omega(f_i)$ is the collision operator controlling the rate of change in the distribution function *f* during the collision, the term $\vec{e}_i.\vec{\nabla} f_i$ models the change in the distribution function due to the spread of the particles during their movement.
The collision function represents the collision of fluid molecules at each node and has the following form (Bhatnagar et al. (1954)):

$$\Omega_i = -\frac{f_i(x,t) - f_i^{eq}(x,t)}{\tau} \qquad (2)$$

Where $f_i^{eq}(x,t)$ is the equilibrium distribution function and τ is the relaxation time which is related to the viscosity of the fluid ($\nu = (2\tau - 1)/6$, where ν is the kinematic viscosity)
The equilibrium distribution functions for different models were derived by He and Luo (1997). The function is given in the following form for the two-dimensional LB model with nine microscopic velocity vectors (D2Q9) (Figure 2):

$$f_i^{eq}(\vec{\mathbf{x}},t) = w_i\,\rho(\mathbf{x},t)\times\left[1+\frac{\vec{\mathbf{e}}_i\cdot\vec{\mathbf{u}}(\mathbf{x},t)}{c_s^{\,2}}+\frac{(\vec{\mathbf{e}}_i\cdot\vec{\mathbf{u}}(\mathbf{x},t))^2}{2c_s^{\,4}}-\frac{\vec{\mathbf{u}}(\mathbf{x},t)\cdot\vec{\mathbf{u}}(\mathbf{x},t)}{2c_s^{\,2}}\right] \qquad (3)$$

Where ρ and $\vec{\mathbf{u}}$ are the density and the macroscopic velocity of the node.

w_i is the weight factor for i^{th} direction; we also assume that these factors are the same for directions having the same velocity , these variables satisfy the following relationship: $\sum_i W_i = 1$. For D_2Q_9 model the weighting factors are defined by:

$$w_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1,3,5,7 \\ 1/36 & i = 2,4,6,8 \end{cases} \qquad (4)$$

c_s is the isothermal speed of sound, it is obtained by the Chapman-Enskog expansion.

$c_s = 1/\sqrt{3}$ for D2Q9 lattice (Chen et al, (1992) ; Frisch et al, (1987) ; He and Luo, (1997))

The D_2Q_9 model is the most popular scheme in two-dimensional problems:

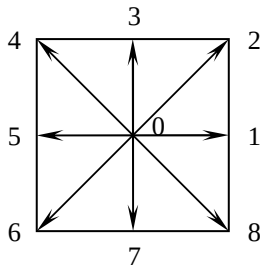

Figure 2: D_2Q_9 model.

The discretized Lattice Boltzmann equation is as follow:

$$f_i(\vec{x}+\vec{e}_i.\Delta t, t+\Delta t) - f_i(\vec{x},t) = \frac{1}{\tau}(f_i^{eq}(\vec{x},t) - f_i(\vec{x},t)) \qquad (5)$$

There are two basic recurrent steps during simulation of viscous flow in a typical LB algorithm:
-Collision step: the arriving particles at the points interact with another and change their velocity directions, thus, at time t the particles at node x come into collision with each other which changes the distribution function from $f_i(\vec{x},t)$ to $f_i^*(\vec{x},t) = f_i(\vec{x},t)+\frac{1}{\tau}(f_i^{eq}(\vec{x},t) - f_i(\vec{x},t))$

-Streaming step: particles move during the time step Δt , along lattice bonds to the neighbouring lattice nodes and the distribution function $f_i^*(\vec{x},t)$ spreads along the vector $\vec{e}_i$, more formally: $f_i(\vec{x}+\vec{e}_i.\Delta t, t+\Delta t) = f_i^*(\vec{x},t).$

The two macroscopic properties, density (ρ) and velocity (**u**) of the nodes, are calculated using the following relations:

$$\rho(\mathbf{x},t) = \sum_{i=1}^{9} f_i(\mathbf{x},t) \qquad (6)$$

$$\mathbf{u}(\mathbf{x},t) = \frac{\sum_{i=1}^{9} f_i(\mathbf{x},t)\,\vec{\mathbf{e}}_i}{\rho(\mathbf{x},t)} \qquad (7)$$

2. Lattice Boltzmann boundary conditions

One of the main advantages of the lattice Boltzmann method is the easy introduction of boundary conditions; the

most popular boundary condition for (LBE) method is the bounce back scheme, in this rule, particles which are incident upon a solid boundary are reversed and leave in the direction from which they came.(D'Humières et al (1987)). This method makes the resolution of complex solid boundaries straightforward. (Figure 3)

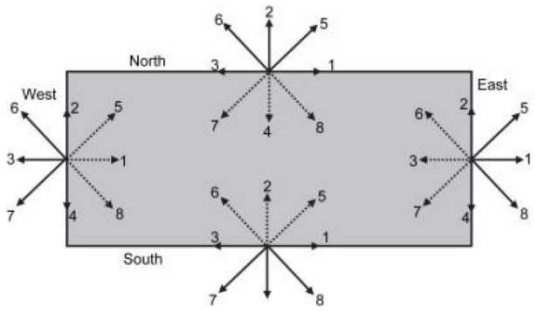

Figure 3: Rebound conditions at a wall

As the lattice Boltzmann method is a kinetic method, macroscopic boundary conditions do not have direct equivalents. They have to be replaced by appropriate microscopic rules which induce the desired macroscopic behavior. For the bounce back rule on wall nodes:

$$f_i(\vec{x},t) = f_{\bar{i}}(\vec{x},t) \quad / x \in wall \qquad (8)$$

With $\vec{\mathbf{e}}_{\bar{i}} = -\vec{\mathbf{e}}_i$.

3. Shan and Chen-type lattice Boltzmann

Shan and Chen proposed a multiple phases LBM model by introducing an interparticle potential between fluid components and based on the BGK collision model. In this model, one distribution function is introduced for each of the fluid components.

In the Shan-Chen model, a force, between the two fluids is introduced that effectively perturbs the equilibrium velocity for each fluid.

In D2Q9 model, this force is given by:

$$F(x,t) = -G\psi(x,t)\sum_i w_i \psi(x + e_i \Delta t, t) e_i \quad (9)$$

Where G is the interaction strength, w_i is weight coefficient, and ψ is the interaction potential:

$$\psi(\rho) = \psi_0 (1 - e^{(-\rho_0/\rho)}) \quad (10)$$

ψ_0 and ρ_0 are arbitrary constants.

Adhesive forces between the fluid and solid phases are introduced into the model by Martys and Chen, (1996) :

$$F_{ads}(x,t) = -G_{ads}\psi(x,t)\sum_i w_i s(x + e_i \Delta t, t) e_i \quad (11)$$

Here s=0, 1 for nodes in the liquid and on solid walls, respectively.

G_{ads} represents the particle interaction strength between fluid and solid walls, and varying the parameter allows simulation of the complete range of contact angles.

With these definitions, in simulation, the cohesive force and the attractive force are added to the velocities that compute the equilibrium distribution function with the following formula:

$$u^{eq} = u + \frac{\tau}{\rho}(F + F_{ads}) \quad (12)$$

4. Results

We consider a simple network as illustrated in Figure 4 in which the GDL are made of randomly packed disks with porosity p = 0.5023. This can be considered as a layer of unit thickness of a three-dimensional porous media. The centers and radii of the disks are generated according to a normal law with a non-intersection condition between the circles.

We implemented the lattice Boltzmann model for non-ideal fluids to simulate the external force driven two phase flow through the simplified GDL. The two steps “stream and collide” algorithm for a (D2Q9) lattice is

used to simulate lattice Boltzmann equation on 400 x 400 site lattices. Bounce back boundary conditions are imposed on the solid walls.

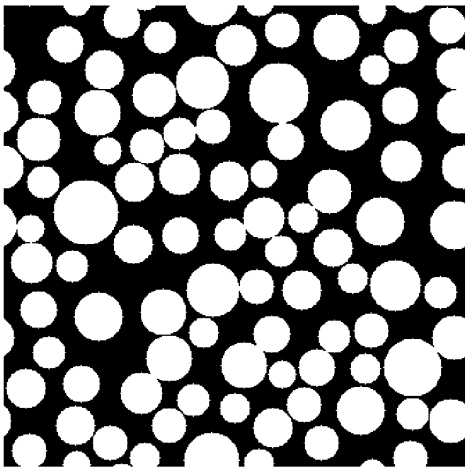

Figure 4: GDL as a porous medium with circular solids

Generally, diphasic flow in a porous medium involves low infiltration rates and capillary forces due to fluid / fluid and fluid / solid interactions, which is reflected by low Reynolds and capillary numbers. In this part of simulation, the dimensionless numbers are set as following: *Ca*= 0.091 *Re*=0.45 and *Bo*= 0.087. Normalized density plots at various time steps were generated. Figure 5 show the evolution of the phase distribution patterns.
According to the phase diagram presented by Lenormand et al the values of these non-dimensional numbers indicate that the diphasic flow in the porous model falls in the so called capillary fingering, which consists of a liquid front characterized by the development of one or more fingers.
The next step is the two dimensional simulation of flow into a real GDL, the idea is to binarize a real image of gas diffusion layer to output the first binary slice of this porous media.(Figure 5).
Figure 7 show the density distribution of the flow through the gas diffusion layer we can confirm that the flow is also in the so called capillary fingering regime.
It is also observed that flow blockages can occur which caused by the constrictions formed by the fibers in certain zones, we then speak of trapped vapor regions. Figure 8 show the saturation versus time in the GDL.
After a time greater than $6x10^4$ ts, the fluid distribution in the fibrous media varies very slowly and the penetration is extremely slow, the calculation has been stopped because the saturation has converged substantially to a constant value.

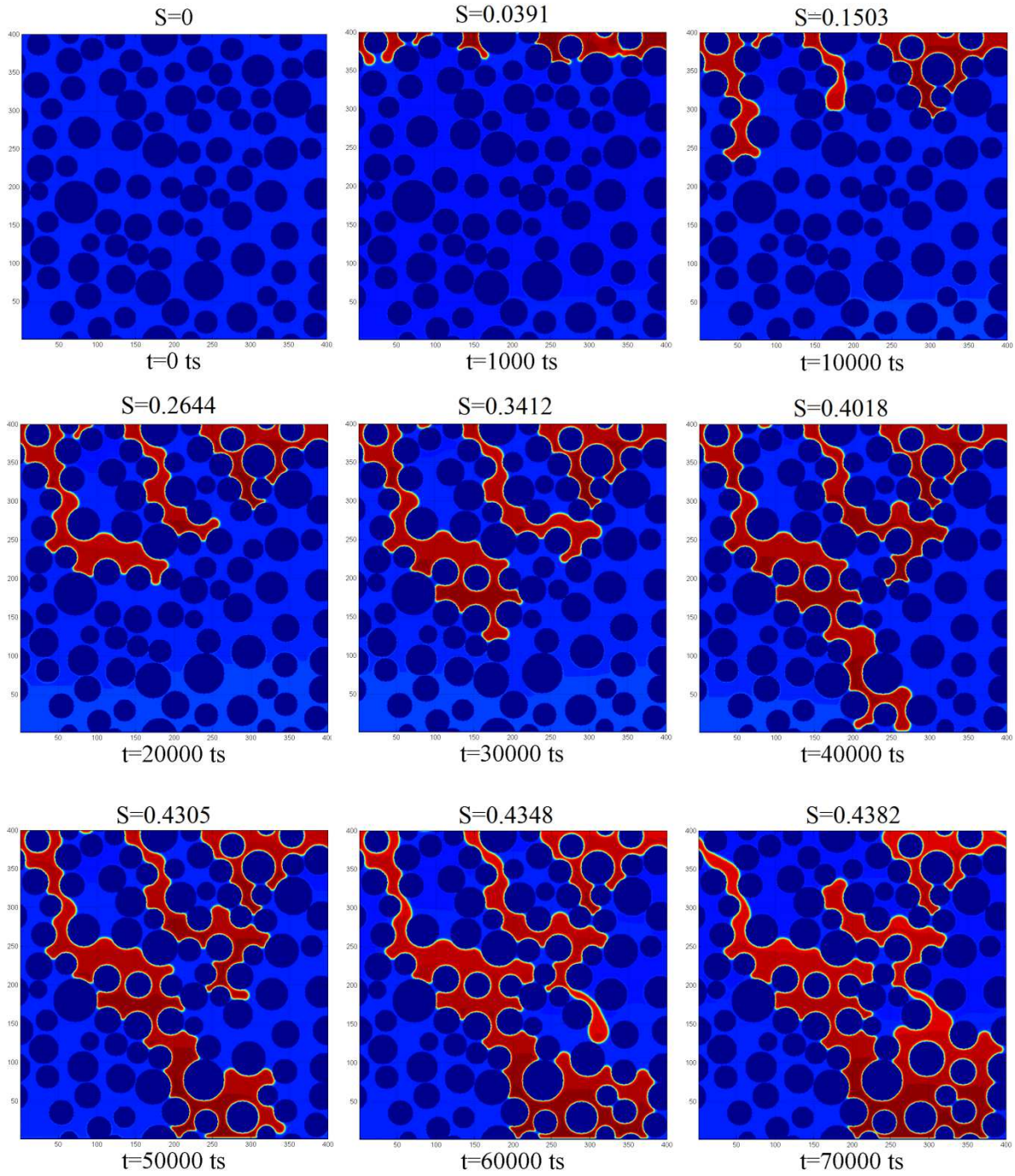

Figure 5: Partial invasion of the GDL. The liquid phase is red.

Figure.6 Original image and image after being binarized.

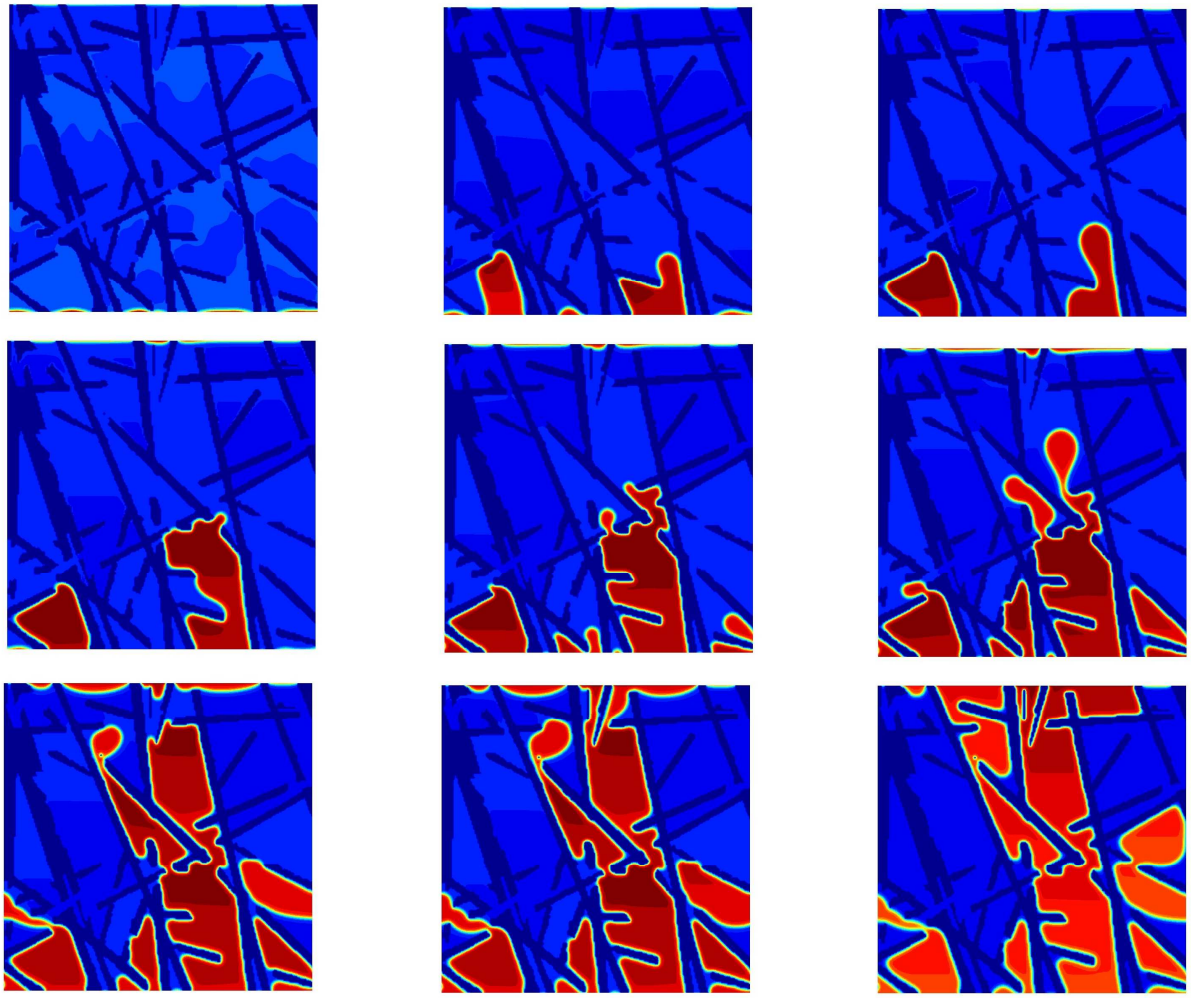

Figure.7 Original image and image after being binarized.

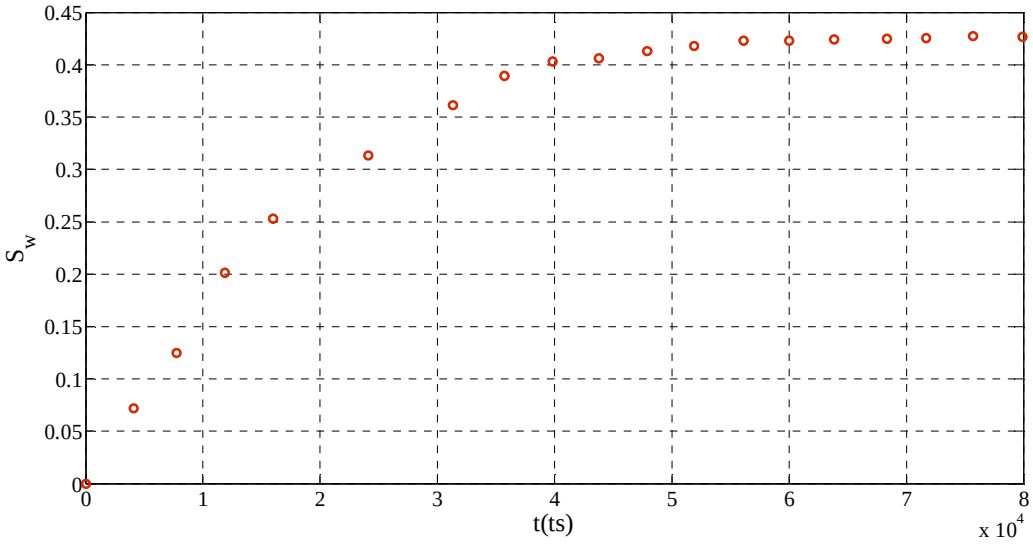

Figure 8: Saturation versus time

Conclusion

We have developed an LB code with an external force for two-phase flow in two-dimensional GDL, in this code the two phase fluid is modeled by Shan-Chen scheme. The present scheme has all the advantages, including good numerical stability and the ability to handle multiphase flow in complex geometry problems.
The density distribution of the flow through a GDL model constructed by random disks packing and a two dimensional slice of a real GDL was simulated.
The results have shown that the flow is in the so called capillary fingering regime according to Lenormand diagram.
Finally, the capability of the lattice Boltzmann method to analyse multiphase problem in fibrous material was shown. The effect of the porosity of the medium on the flow must be included in future work.
Also other geometries must be tested. However, migration to three-dimensional simulation seems inevitable because of its advantages.

Nomenclature

Symbols

$\vec{u}$: Macroscopic velocity

f_i : Distribution function

f_i^{eq} : Equilibrium distribution function

c : Lattice velocity

c_s : Speed of sound

p : Pressure

Ca: Capillary number

Ma : Mach number

R_e : Reynolds number

Δt : Time step

T : Temperature

R : Specific gas constant

u_0 : Top lid velocity

lu : Lattice unit

Δx : Lattice spacing

W : Weighting factor

Greek symbols

ρ : Density

τ : Relaxation time

Ω : Collision operator

ν : Kinematic viscosity

$\vec{\xi}$: Molecular velocity

Indices

i : Lattice streaming vector direction

Références

[1] Bhatnagar P.L., Gross E.P. and Krook M. (1954) 'A model for collision processes in gases, I.small amplitude processes in charged and neutral one-component system', Phys. Rev., Vol. 94, pp.511–525

[2] Chen, H., Chen, S. and Matthaeus, W., H., (1992) Recovery of the Navier-Stokes equations using a lattice-gas Boltzmann method, Phys. Rev. A, 45, pp. 5339-5342

[3] Chen S., Doolen GD., Lattice Boltzmann method for fluid flows. Annual Review of Fluid Mechanics, 30,329 –364, (1998).

[4] D'Humieres, D. and Lallemand, P. Numerical simulations of hydrodynamics with lattice gas automata in two dimensions, Complex Systems, 1 (1987)598.

[5] Frisch, U., Hasslacher, B. and Pomeau, Y., (1986) Lattice-gas automata for Navier-Stokes equations, Phys. Rev. Lett., 56, pp. 1505–1508.

[6] He, X. and Luo, L.-S., (1997) Theory of the lattice Boltzmann method: From the Boltzmann equation to the lattice Boltzmann equation, Phys. Rev. E., 56, pp. 6811-6818.

[7] Martys, N. S., and H. Chen (1996), Simulation of multicomponent fluids in complex three-dimensional geometries by the lattice Boltzmann method, Phys. Rev. E., 53, 743 – 750.

[8] Qian YH., d'Humieres D., Lallemand P., Lattice BGK models for the Navier–Stokes equation. Europhysics Letters, 17,479– 484, (1992).

[9] Succi S., Benzi R., Higuera F., The lattice-Boltzmann equation—a new tool for computational fluid dynamics. Physica D 47, 219 –230, (1991).