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Lattice Boltzmann Modeling From the Macro- to the Microscale

- An Approximation to the Porous Media in Fuel Cells -

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Abstract:
Fuel cell (FC) is a device that gives us electrical and thermal energy from the chemical energy present in the fuels involved during the conversion process. The chemical conversion process occurs thanks to the different constitutive layers in the FC, i.e., active layer, anode/cathode support layer, catalyst layer, gas diffusion later and electrolyte. Most of them have the characteristic to allow the flow of the reactants. Understanding the behavior of the fluids in porous media help to improve the efficiency of fuel cells.
Modeling different transport phenomena that occur inside fuel cells during the energy conversion process are important at microscale. Lattice Boltzmann method appears as a powerful tool for solving problems in complex geometries. In the first part of this work the solution of some physical problems at macroscale are presented. Finally, the solution of the momentum equation and the calculation of porosity and tortuosity in a simple and artificially generated porous domain are presented.

Keywords: FC, macroscale, microscale, modeling, LBM, porous media

1. Introduction

Modeling different transport phenomena that occur inside fuel cells have been gaining interest during the last years. The most realistic FC model has to be a 3-Dimensional, non-steady state and with the coupling of the different transport phenomena over all the range of scales from the micro- to the macroscale.

When modeling FC at microscale is important to in deeply understand the behavior of the fluids throughout the porous media presents in the different layers of the FC. That is because the porous media helps the reactants getting in contact with the electrolyte to produce the energy conversion. Then solving transport phenomena in complex geometries, such as porous media, is considered one of the problems to deal with. Lattice Boltzmann method (LBM) can handle with problems at different scales, and has proven to be suitable for solving problems in porous media, and modeling different transport phenomena in fuel cells [1-2].

The aim of this work is to show the solution of physical problems using the LBM at macroscale as a bridge with the physical problems at microscale. The first part of the paper is a briefly description about LBM. Second, the results and discussions of different physical problems are shown. Finally, the porosity and tortuosity values for a simple and artificially generated porous domain are presented.

2. Lattice Boltzmann Method

LBM consider a group of particles and their connections with their neighbors. LBM can solve different problems related to momentum, diffusion, advection, and energy equations [3]. There are different schemes for solving the different transport equations. Normally, the schemes are represented as follows:

$$DnQm \tag{1}$$

where n refer to the dimension (2 dimensional or 3 dimensional) and m the number of connections with the vicinity.

The basic equation for applying LBM is the Boltzmann equation, which be expressed as [3]:

$$\frac{\partial f(r,t)}{\partial t} + c.\nabla f(r,t) = \Omega \tag{2}$$

where f is the particle distribution function that depends on position (r), velocity (c) and time (t). Ω is the collision operator which is a function of f. There are different ways for approximating the collision operator; the most common is the Bhatnagar, Gross and Krook (BGK) approximation.

In this work, using LBM, the momentum equation is solved. The models are developed in D2Q9 schemes, i.e., two dimensional problems and each group of particles has nine interconnections with its neighbors.

3. Results and Discussions

The solution of the momentum equation for two macroscale models are obtained. The velocity field is calculated for each of them. The physical characteristics are given according to the problem to solve, and subsequently the validation of the models is presented. In the artificially generated porous domain, the momentum equation is solved and parameters such as porosity and tortuosity are calculated.

3.1 Macroscale models

3.1.1 Channel flow

The velocity field for a fluid (Re=1000) in a channel is solved. In order to get the solution, the bottom and up boundaries were established as non-slip boundaries. Figure 1 shows the solution of the velocity field.

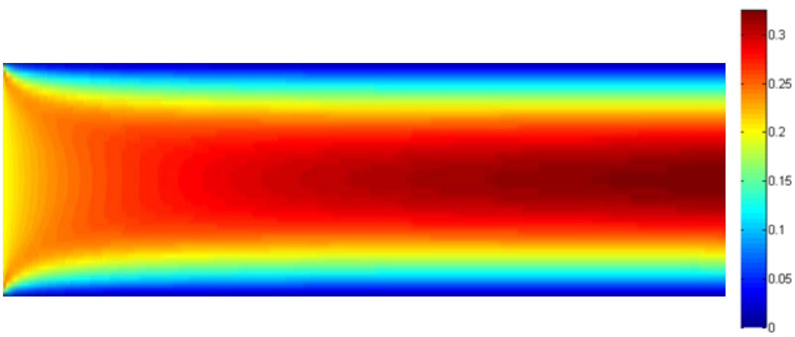


Fig. 1 Velocity field in a Channel flow (Re = 1000).

To validate the velocity field in the channel, the velocity profile for different cross sections were calculated and represented in the Figure 2. The fully developed region is reached when the velocity profile is 1.5 times the inlet velocity [4]. It is important to notice that in LBM the length unit is called lattice unit (lu) and the velocity unit is lattice unit per time step (lu/ts).

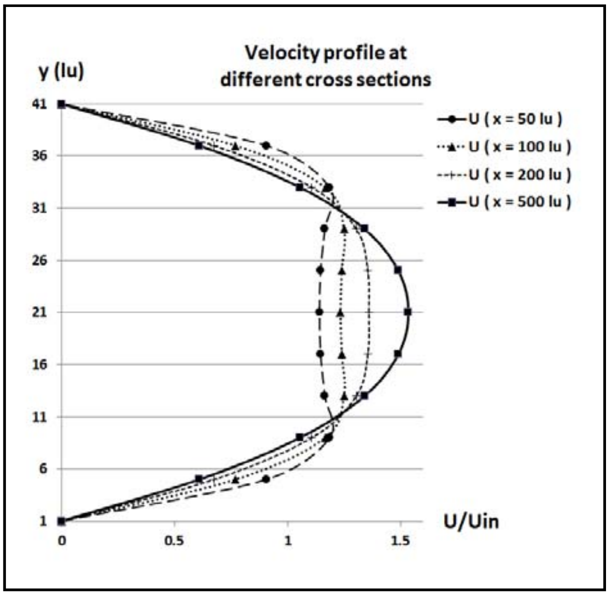


Fig. 2 Velocity profiles at different cross sections in a Channel flow (Re = 1000).

3.1.2 Lid-Driven cavity

The momentum equation for a fluid (Re = 1000) in a square cavity is solved. Initially the velocity is only acting in the top (lid). Figure 3 shows the velocity field at steady state with the maximum velocity at the top and zero velocities at the bottom corners.

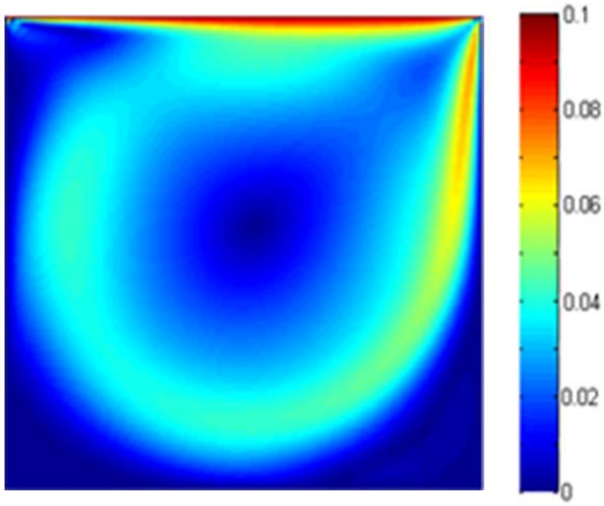
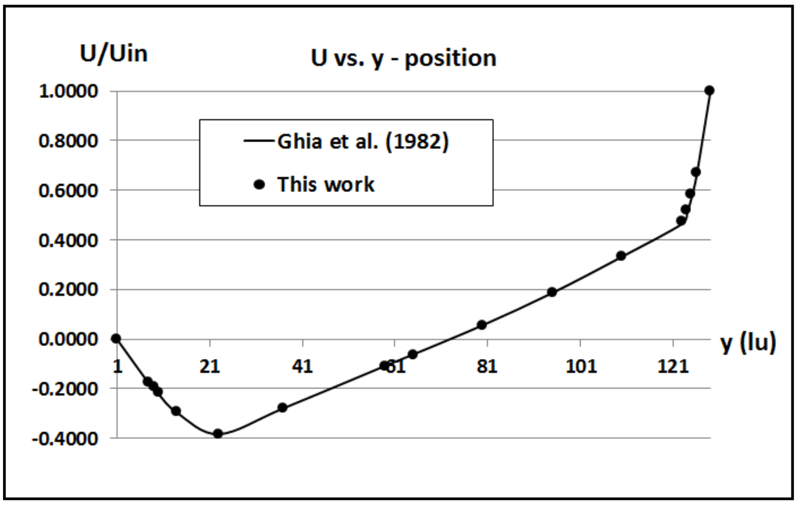
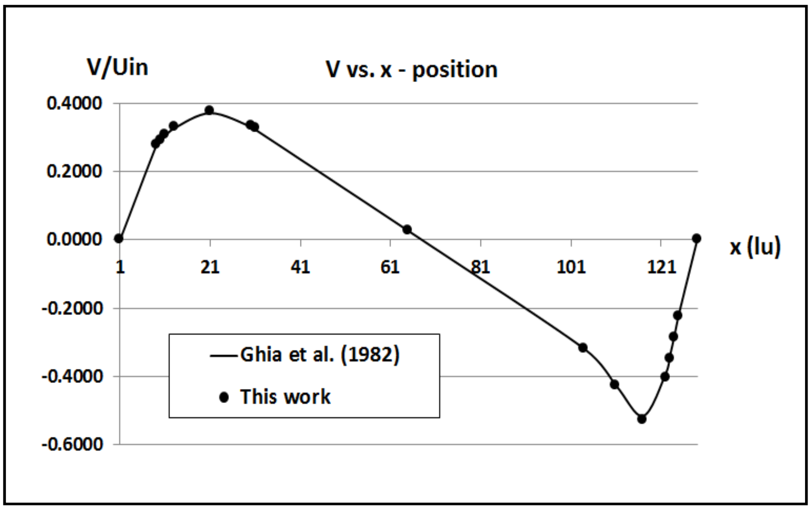


Fig. 3 Velocity field for a Lid-Driven cavity (Re=1000).

The results of the velocity field in this model were compared with previous studies and figure 4 shows the velocities in the *x*- and *y* directions for some selected positions and the solution obtained by Ghia *et al.* [5].



(a) *x*- velocities at the mid-section.



(b) *y*- velocities at the mid-height.

Fig. 4 Velocity profiles at the mid-section and at the mid-height of the cavity. (Re=1000).

3.2 Microscale model

As mentioned, one of the advantages of LBM is to solve problems in complex geometries. The porous media presented in this section is artificially generated for showing the feasibility for applying the LBM.

The momentum equation is solved and the porosity and tortuosity are calculated. The up and bottom boundaries are established as periodic boundaries and the fluid direction is from left to the right.

The size of the porous domain is 300 lu and 150 lu at the *x*- and *y* directions respectively. The LBM solution is an equivalent to the real problem that is solved. For example, the aspect ratio in LBM is 300lu/150lu, i.e., 2:1. It can be considered that the real problem solved has the size of 10 µm x 5 µm for giving an example. Figure 5 shows the velocity field for the porous domain.

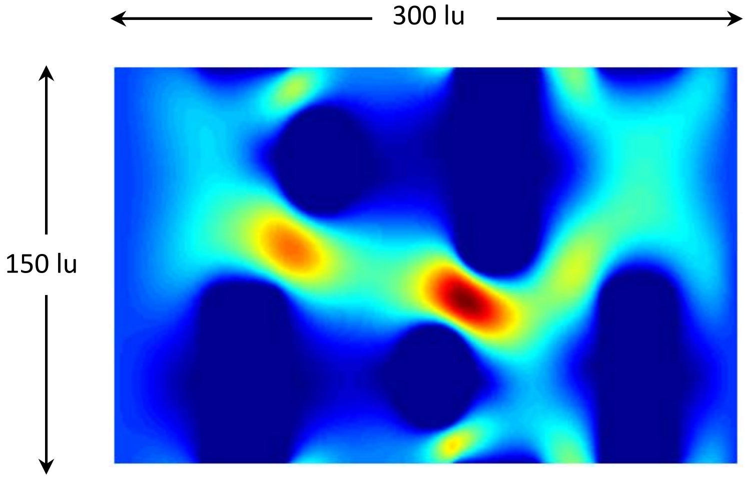


Fig. 5 Velocity field representation in an artificially generated porous domain. (High velocities in red color, the obstacles are represented in blue color).

Two variables were calculated in the porous domain, i.e., the porosity, the ratio between the void surface and the total surface, was established in 0.76; and the tortuosity, defined as the ratio between the actual length path and the shortest length path, was calculated in 1.17. Those values agreed with the values shown by Nabovati and Sousa [6].

4. Conclusions

A 2D LBM was developed to model the velocity field for two physical problems at the macroscale. Based on previous studies results were validated. In both, channel flow and lid-driven cavity the results obtained were as expected. An artificially generated porous domain was presented to show the feasibility to model transport equations in the porous media. The porosity and tortuosity obtained using LBM agreed well with previous studies.

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