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Potential of Lattice Boltzmann Method to Determine the Ohmic Resistance in Porous Materials

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Abstract. The lattice Boltzmann method (LBM) is a suitable tool for solving transport phenomena that occur in gas- and liquid phases at different length scales, especially when complex geometries such as porous media are involved. However, investigations about applications of LBM in the solid electrical conducting material have not been carried out yet. Since in fuel cells (FCs) the multifunctional layers play an important role during the energy conversion process, and such layers consist of porous material, the ohmic resistance of porous materials represents a crucial characteristic to be studied to predict the internal ohmic losses. The purpose of this paper is to show the feasibility of LBM to determine the ohmic resistance of electrical conducting materials whose dimensions are modified considering the cross-sectional area and length. Characteristics, limitations and recommendations of LBM applied to solid electrical conducting materials calculating the ohmic resistance are presented considering the coupling of the methodology with the Ohm's Law. Additionally, the behavior of the ohmic resistance for a given porous material is presented.

1. Introduction

Predicting the internal ohmic losses involved in the energy conversion process is crucial in order to improve the microstructural architecture of the different multifunctional layers inside fuel cells (FCs). Most of these multifunctional layers are porous materials which represent a complex study of fluid and solid interactions.

Given the mentioned characteristics, several studies of the fluid behavior through porous media have been carried out, by the authors, using the lattice Boltzmann method (LBM) [1 – 2]. However, LBM has not been applied to analyze the similarities between the hydraulic and electrical behavior. Considering the mentioned analogy, LBM can result in a powerful tool to analyze certain electrical variables in solid conducting materials such as current density (flow of electrons) and ohmic resistance.

The purpose of this work is to prove the feasibility of applying the LBM in the solid conducting material instead of the fluid phase. The use of LBM in the solid conducting material gives us the opportunity to calculate the ohmic resistance in conductive materials and the possibility to predict the ohmic resistance for porous materials. Since LBM was originally a methodology for recovering hydraulic behavior from the Navier-Stoke equations, some considerations should be taken into account when it is applied to the flow of electrons. For this study the momentum and continuity equations are solved using LBM, which allow to determine the equivalent variables in the electrical system. The corresponding analogies are given in Table 1.

Table 1. Equivalences between hydraulic and electric variables with corresponding units.

	Hydraulic			Electric		
Type	**Variable**	**Symbol**	**Units**	**Variable**	**Symbol**	**Units**
Quantity	Volume	V	m^3	Charge	q	C
Potential	Pressure	p	N/m^2	Potential	φ	$N\,m/C$
Flux	Volumetric flow rate	ϕ_V	m^3/s	Current	I	C/s
Flux density	Velocity	v	m/s	Current density	j	$C/m^2\,s$

2. Methodology

The models are developed using the D3Q19 scheme, and the studied domains are shaped as 3D volumes with uniform cross-sectional areas along the length. The first stage of the investigation is to find the range of values of the equivalent current density, i.e., can be related with the velocity in hydraulic studies, in which LBM can present an equivalent ohmic behavior. The ohmic behavior implies: if the potential difference increases, also the current density increases. Additionally, the relationship between these two variables must be direct and linear. This measure is required since LBM has some limitations and would not give accurate results in higher velocities [3]. For this part, the domain is constructed as 5 lu side of the cross-sectional area and 15 lu length to assure excellent agreement of description in hydraulics [4]. The same domain is modified with the inclusion of non-conducting solid particles in the last part of this study.

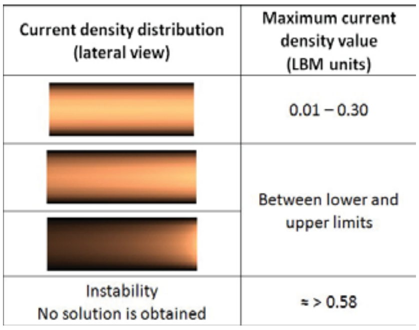

Figure 1. Lateral view of the current density distribution when potential difference is increasing. Higher current density values lead to instability.

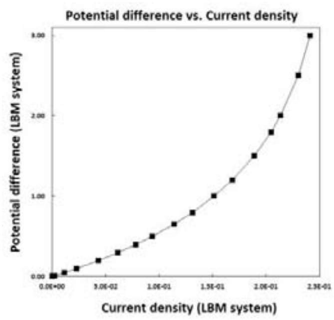

Figure 2. Potential difference vs. current density for the first domain analyzed. The ohmic behavior is obtained at lower current density values.

The first results show that there is a limitation on the maximum current density value obtained within the LBM implementation. Considering the material resistivity as a constant and that the flow of electrons is uniformly distributed, the current density values are not allowed to reach certain values to avoid instabilities.

Ohm's law establishes a relationship between the gradient of the applied potential and the current density:

$$j = -\sigma\, \nabla\varphi \tag{1}$$

where j is the current density (in A/m^2), φ is the potential function (in V), and σ the conductivity of the material (in $\Omega^{-1}m^{-1}$). Several values of potential differences are applied to domains with different sizes in order to demonstrate the validity of the equivalent Ohm's law. The results are presented in the next section.

3. Results and discussion

Considering equation (1) and knowing that the conductivity is the reciprocal value of the resistivity (ρ), the simplified version of the Ohm's law is expressed as I = V/R; where I is the electric current, V is the potential difference applied, and R is the ohmic resistance of the studied material. Figure 3 shows the results obtained when the dimensions of the conducting material are varied.

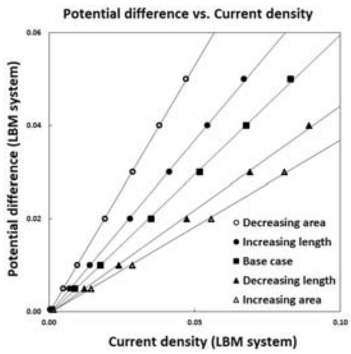

Figure 3. Ohmic region behavior for several domain sizes. Base case corresponds to a 20 *lu* side cube.

Ohm's law tells that the slope of the curves is proportional to the ohmic resistance materials. To corroborate the obtained results and to analyze the behavior of the ohmic resistance as a function of the material length and cross-sectional area, several measurements were effected.

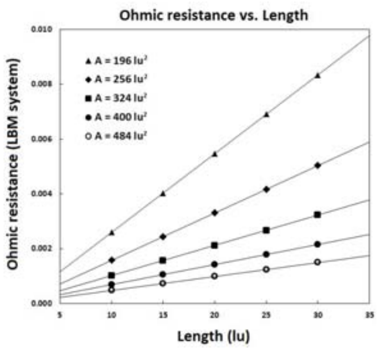

Figure 4. Obtained ohmic resistance values for a certain potential difference when the length varies.

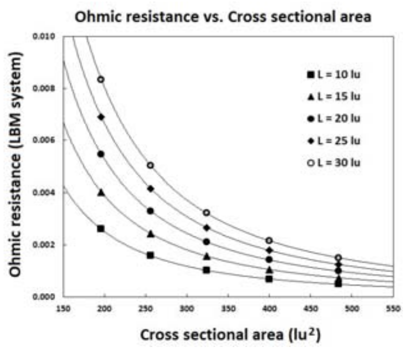

Figure 5. Obtained ohmic resistance values for a given potential difference when the cross-sectional area varies.

In physics, Ohm's law is expressed as E = ρ j; where E is the electric field (in V/m). If the electric field is assumed constant along the length of the conductor (L), the potential difference can be determined as V = E L. Using the mentioned relationships in equation (1) and solving for V/I, the ohmic resistance can be calculated as R = ρ (L/A). Results presented in Fig. 4 and Fig. 5 agree with the latest expression, i.e., the ohmic resistance increases in a linear manner when the length increases and decreases as an inverse function when cross-sectional area increases.

Although the behavior of the curves showed in Fig. 4 and Fig. 5 agree with the expected in ohmic materials, it is important to notice that there is an additional issue that should be addressed related to the material resistivity. Independently the size of the material and the potential difference applied, the resistivity is an intrinsic characteristic of the material, i.e., it must be constant. However, the values obtained during our simulations required some adjustments, which can be achieved relating the resistivity and the relaxation parameter in LBM, and also the boundary conditions can be revised.

Finally, some measurements of the incidence over the ohmic resistance when non-conducting particles are included in the material domain, i.e., porous material, are carried out. These non-conducting particles represents the void space volume. Figure 6 shows the variation of the ohmic resistance with a certain percentage of non-conducting particles. As expected, the ohmic resistance increases with the increasing percentage of such particles.

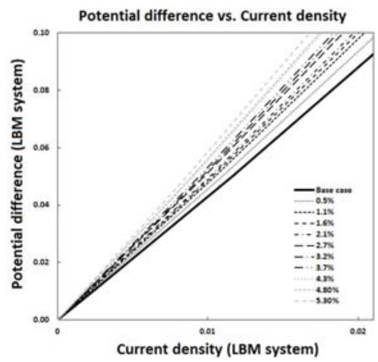

Figure 6. Base case corresponds to a volume domain of 5 *lu* side of cross-sectional and 15 *lu* length.

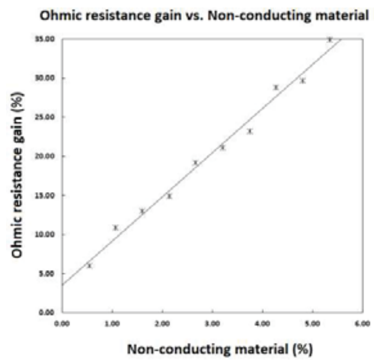

Figure 7. Trend of the ohmic resistance gain relative to the base case.

4. Conclusions and further studies

Although LBM has proven to be suitable to calculate the ohmic resistance for uniform shape conducting materials and porous materials, additional studies with different domain sizes and higher presence of non-conducting materials are required. Another issue to be addressed is related to the material resistivity; which can be associated to the relaxation parameter used in LBM. Additionally, the boundary conditions applied to the electric conductive surfaces can be analyzed.

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