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FLUID FLOW SIMULATION IN RANDOM POROUS MEDIA AT PORE LEVEL USING THE LATTICE BOLTZMANN METHOD

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Abstract

Fluid flow in two dimensional random porous media is simulated at pore level using the Lattice Boltzmann Method. Random media are constructed by placing identical rectangles with a random distribution and free overlapping. Different domain resolutions are examined and it is shown that the effect of the domain resolution is negligible in the range examined. Simulations clearly indicate, for the same porosity, the permeability of the random porous media is lower than the permeability of the regularly ordered medium; the permeability, independently of the porous media organization, varies exponentially with the porosity. Average tortuosity of the flow is calculated and it is proposed its correlation with the porosity. The effect of the aspect ratio of the randomly placed obstacles on the predicted tortuosity and permeability is studied, and it is found that an increase of the obstacles' aspect ratio (height to width ratio) yields an increase of the tortuosity and consequent decrease of the permeability. The predicted values of the permeability and tortuosity are in close agreement with the data available in the literature.

Keywords: lattice Boltzmann Method, Permeability Prediction, Random Porous Media, Pore Level Analysis

1. Introduction

The prediction of the permeability of porous media has been a challenge for engineers and scientists. Literature dealing with permeability prediction is vast, but most methodologies, and in particular those based on experimentally-based correlations, suffer from lack of generality primarily due to the assumptions that they embody.

Nomenclature

A_0	obstacle area
C	Kozeny constant
c_i	lattice discrete velocity set
c_s	lattice sound speed
D	space dimension (2)
Dx	obstacles' width (in x direction)
Dy	obstacles' height (in y direction)
f	particle distribution function
K	perrmeability
Kn	Knudsen Number
P	pressure
P_0	obstacle perimeter
R_0	hydraulic radius of an obstacle
S	specific surface area
t	time
u	fluid velocity
x	spatial position
Greek letters	
φ	porosity
δt	lattice time step
τ	tortuosity
T	transformed tortuosity
ω	inverse of the lattice relaxation time
β_i	weighting factor for the lattice directions
λ	constant parameter in Box-Cox transformation
μ	fluid viscosity
Superscripts	
eq	equilibrium

In recent years, fluid flow simulation at pore level has received considerable attention as a powerful tool for the permeability prediction. In this approach, fluid flow is simulated in the inter-grain regions and inside the pores of the porous medium. The permeability of the medium can be calculated using the Darcy law [1] by averaging the local velocities over the flow domain and by using the pressure gradient, namely:

$$\langle u \rangle = \frac{K}{\mu}\left(-\frac{\partial P}{\partial x}\right) \tag{1}$$

The very first challenge in these analyses is to determine the structure of the medium at pore level. Applied experimental and imaging techniques have had some success in the determination of these structures [2]; even so, experimental methods have their own limitations and, in general, are costly. An alternative approach, which has been popular with many researchers in this field, is to simulate the fluid flow in a reconstructed virtual medium capable of reproducing the real medium behavior. The medium can be formulated, as a first approximation, by considering ordered or random packing of spheres, cylinders or rectangular parallelepipeds. It should be noted that for pore level analyses, the length scale is usually taken as the average size of the pores; therefore, the Knudsen number (Kn) can be locally high ($0.01 < Kn < 0.1$) and the flow may fall into the slip flow regime, for which the Navier Stokes equation is still applicable, but some velocity slip should be allowed.

The Lattice Boltzmann Method (LBM) [3, 4] is an alternative methodology to the Navier Stokes equations for the fluid flow simulation at the pore level. The LBM is capable of dealing with the complex geometries of the porous media at pore level, and can handle both the continuum or slip flow regimes with no need for further modifications.

The first LBM simulation of the fluid flow in porous media was performed by Foti and Succi [5] and since then the literature associated with the LBM simulation of fluid flow in porous media has been steadily growing. Cancelliere et al. [6] studied the fluid flow in a three dimensional porous medium constructed by randomly positioning spheres of equal radii. They reported that the predicted permeability at the high solid fractions agreed with the Kozeny-Carman equation, and at low solid fractions it approaches the lower limit of the variational bounds. Heijs & Lowe [2] discussed the flow in a random array of spheres and a clay soil sample using the LBM. They used the bounce back scheme for modeling the solid wall boundary condition, and they found the LBM yields acceptable results even with very coarse lattice. In their study, it was assumed the flow only occurs in the connected pores identified experimentally by computed tomography (CT) imaging in the sample under study. This means that the flow in the small pores, which may have not been detected by the CT imaging, was neglected, so the results may have underestimated the permeability. Koponen et al. [7] studied the creeping flow through large three dimensional random fibers web using the LBM with the D3Q19 lattice. For the faces of the flow domain, the periodic boundary condition was implemented. The solid walls were treated by employing the bounce back scheme, which, as it was found, led to results that were sensitive to the lattice resolution. It was also noted the Knudsen effect may occur in the small pores. The Darcy law was used to calculate the permeability, and they reported that it was exponentially dependent on the porosity and independent of whether the fibrous porous medium was random or not. No theoretical explanation was given for this observation. They compared with good agreement their results against experimental data. Clague et al. [8] studied the permeability of three dimensional ordered and disordered fibrous media. They analyzed wall bounded and unbounded media cases and the effect of the wall on the overall permeability of the fibrous media; for the wall boundary treatment, the bounce back method was used. Three dimensional lattices with 15 velocities and 19 velocities were employed, and for the low Reynolds number flows, both models yielded nearly identical results. Their predictions were in very good agreement with the available data. A phenomenological relation was developed by curve fitting the calculated values for the permeability of both the bounded and unbounded three dimensional fibrous media. Pan et al. [9] studied the flow through random packing of spherical particles with random diameter using the LBM along with the pore network modeling approaches for the low Reynolds number flow. A log-normal sphere size distribution, as proposed by Yang et al. [10] was used, along with a D3Q15 lattice.

In the present study, fluid flow in two dimensional random porous media was simulated at pore level using the LBM; rectangle obstacles were placed randomly in the flow domain with a uniform distribution. Domain resolution and particles geometry were studied for their effect upon the predicted permeability and tortuosity. The simulation results, as it will be shown, are in very good agreement with the previously published correlations.

2. Methodology

In the present study, fluid flow in two dimensional random porous media was simulated at pore level using the single relaxation time Lattice Boltzmann Equation (LBE) [3]; the evolution equation of the particles, which governs the fluid dynamics, is written in the following form:

$$f_i(\vec{x} + c_i\delta t, t + \delta t) - f_i(\vec{x}, t) = -\omega\left[f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)\right] \tag{2}$$

where δt, ω and c_i are the lattice time step, inverse of the lattice relaxation time and the lattice discrete velocity set, respectively, and f is the particle distribution function.

The discrete velocity set of the particles for a D2Q9 lattice, which is used in the present study, is defined as

$$\begin{aligned} &c_0 = 0 \\ &c_i = c\left(\cos(i-1)\pi/4), \sin(i-1)\pi/4)\right) \qquad i = 1,3,5,7 \\ &c_i = \sqrt{2}c\left(\cos(i-1)\pi/4), \sin(i-1)\pi/4)\right) \quad i = 2,4,6,8 \end{aligned} \tag{3}$$

The equilibrium distribution function, which is the second order truncated expansion of the Maxwell-Boltzmann equilibrium function, is written as

$$f_i^{eq} = \rho\beta_i\left[1 + \frac{3}{c^2}c_i.u + \frac{9}{2c^4}(c_i.u)^2 - \frac{3}{2c^2}u.u\right] \tag{4}$$

where β_i is the weighting factor and is equal to

$$\beta_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1,3,5,7 \\ 1/36 & i = 2,4,6,8 \end{cases} \tag{5}$$

The macroscopic density and velocity on each lattice site are calculated using the distribution function on that site and the neighboring sites, namely:

$$\rho = \sum_{i=0}^{8} f_i = \sum_{i=0}^{8} f_i^{eq} \tag{6}$$

$$\rho u = \sum_{i=0}^{8} c_i f_i = \sum_{i=0}^{8} c_i f_i^{eq} \tag{7}$$

Fluid viscosity is calculated using the relaxation frequency and the lattice sound speed as follows:

$$\upsilon = \left(\frac{1}{\omega} - \frac{1}{2}\right) c_s^2 \tag{8}$$

Two dimensional rectangle obstacles were placed in the flow domain with a random distribution and free overlapping. Periodic boundary conditions were implemented in the flow direction; solid wall boundary conditions are set in the transverse direction and they are modeled using the bounce back method [4, 12]. Along the flow direction, a gravitational body force was applied by adding a specified portion of the momentum at each time scale to all the particles within the pore space. To generate the random porous medium, three different sizes of the domain and obstacles were used, namely: 10×10 obstacles in a 100×100 domain, 8×8 obstacles in an 80×80 domain and 5×5 obstacles in a 50×50 domain. The actual porosity of the medium was calculated as the ratio of the number of the lattice sites in the fluid area to the total number of the lattice sites. For each domain resolution, several runs were conducted with porosities ranging between 0.5 and 0.97. All the three domain resolutions yield nearly similar average results. The increase of the domain size will reduce the error resulting from the bounce back solid wall treatment [13]; therefore, the remaining part of the study is conducted with the 100×100 domain and the 10×10 obstacles, unless otherwise mentioned.

The relaxation time for all the simulations was set to 1.25, resulting in a lattice viscosity of 0.1 in a D2Q9 lattice; therefore the effect of the viscosity on the predicted permeability was negligible [14]. The predicted permeability using the Darcy law [1] is reported as K / R_0^2 , where R_0 is the hydraulic radius of an obstacle defined as:

$$R_0 = \frac{DA_0}{P_0} \tag{9}$$

where A_0, P_0 and D are the obstacle area, obstacle perimeter and the number of space dimensions considered, respectively. In the present case, D is equal to 2, because the study was conducted for a two-dimensional space.

3. Results

Figure 1 shows the comparison between the predicted permeability for a random medium and for a regularly ordered medium, and the value determined from the modified Kozeny relation; to take into account the effect of the dead-end and non-connecting pores in a random medium, the effective porosity was introduced into the Kozeny equation as proposed by Koponen et al. [15], namely:

$$K = \frac{\varphi_{eff}^{3}}{C\tau^{2}S^{2}} \tag{10}$$

where φ_{eff}, τ and S are the effective porosity, tortuosity and specific surface area, respectively; the Kozeny coefficient, C, takes the values of 5.8, as given by Koponen et al. [15]. Effective porosity was defined as the ratio of the volume of conducting pores to the total volume and can be mathematically described as a function of the porosity [15]. At low porosity, the fraction of the dead end and non-conducting pores is higher, therefore higher is the difference between the actual and effective porosity.

It can be noted that the agreement between the predicted average permeability and the Kozeny equation is very good. For porosities less than 0.9, the permeability of the ordered medium is higher than the random medium permeability and its predicted values are in very good agreement with the results given by the Kozeny equation based on the effective porosity. In this region, the permeability is an exponential function of the porosity whether it is an ordered medium or a random medium. For porosities higher than 0.9, the Kozeny equation tends to overestimate the permeability. In high porosity media, as obstacles are distributed sparsely in the flow domain, the contribution to the permeability of dead end pores and tortuous flow passages tends to be reduced, because they are more likely to occur in lower porosities. Even so, these particular flow obstacles may explain why the average permeability of a random medium is lower than the permeability of a regularly arranged medium with the same porosity.

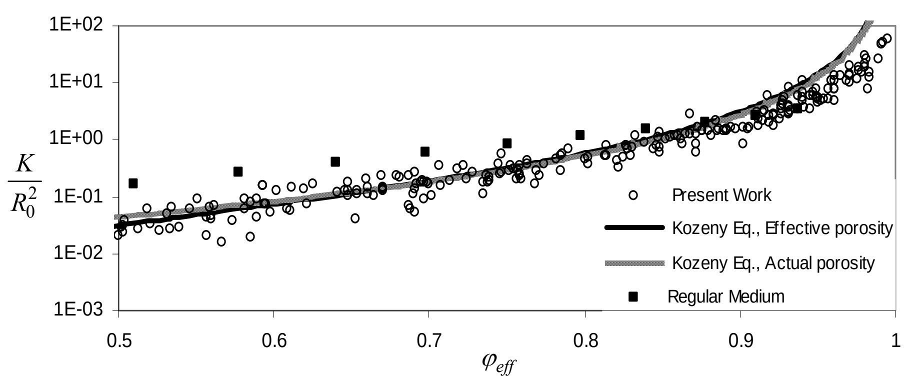


Fig.1. Comparison between the permeability predicted in the present study and the permeability obtained with the Kozeny equation using the actual and effective porosity.

One of the important features of the flow in the random porous medium is the tortuosity of the flow and it can be defined as the ratio of the length of the actual path of the fluid particles to the shortest path length in the direction of the mean flow. In the present study, the volume averaged tortuosity is calculated as follows:

$$\tau = \frac{\sum_{i,j} u_{mag}(i,j)}{\sum_{i,j} \left| u_x(i,j) \right|} \tag{11}$$

where the mean flow is in x direction and u_{mag} is the velocity magnitude, namely:

$$u_{mag}(i,j) = \sqrt{u_x(i,j)^2 + u_y(i,j)^2} \tag{12}$$

Koponen et al. [15] studied the permeability and tortuosity of two dimensional random porous media using the LGA. The tortuosity was correlated as a function of the porosity as follows

$$\tau = 1 + a\frac{(1-\varphi)}{(\varphi-\varphi_c)^m} \tag{13}$$

where a, m and φ_c are equal to 0.19, 0.65 and 0.33, respectively.

Koponen et al. [16] studied the tortuosity of the flow in a random two dimensional porous medium using the LGA with periodic boundary conditions in both directions. Obstacles were defined as randomly placed squares with free overlapping. Different formulations for the tortuosity calculation were discussed and the following correlation for the tortuosity as a function of the porosity was presented:

$$\tau = 0.8(1-\varphi) + 1 \tag{14}$$

Figure 2 presents the predicted tortuosity versus porosity; tortuosity is always greater than one, and as the porosity approaches one, it should tend to one, as expected; the tortuosity increases with decreasing porosity.

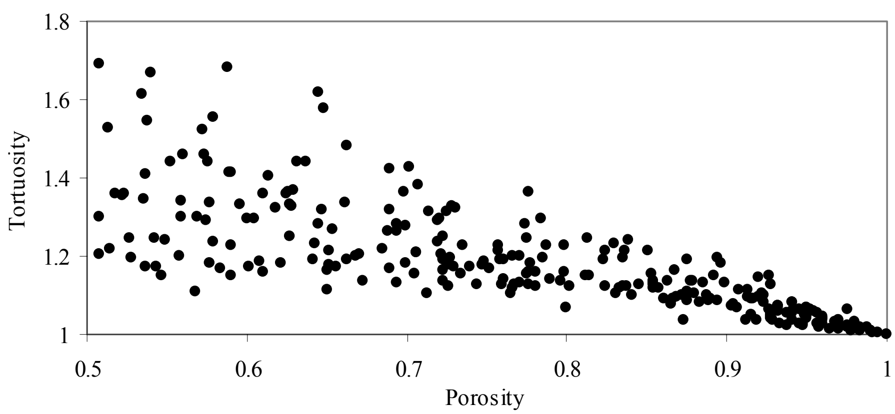


Fig.2. Predicted tortuosity as a function of the porosity

A third order polynomial can be used to fit the simulation results for the averaged tortuosity as a function of the porosity. Its formulation is as follows:

$$\tau = -0.5191\varphi^3 + 0.879\varphi^2 - 1.1657\varphi + 1.8058 \tag{15}$$

The fitted polynomial has the least error in comparison with the straight line correlations [16], and the curve fitting error is nearly the same for both high and low porosity regions. In addition, this polynomial is capable of capturing the nonlinear dependence of the tortuosity on the porosity at high porosities; the condition of τ(1) equal to 1 is satisfied with no need for further tuning up of the fitting parameters. But as it can be clearly seen in Fig. 2, the variance of the data point around the mean value is not constant and the lower the porosity, the higher variance and more scatter data points. To overcome this problem, the data points can be transformed using a power transformation known as Box-Cox transformation [17], namely:

$$\mathrm{T} = \begin{cases} \dfrac{\tau^{\lambda} - 1}{\lambda} & \lambda \neq 0 \\ \ln \tau & \lambda = 0 \end{cases} \tag{16}$$

where λ is an arbitrary real constant number. The optimum value of λ should minimize the Sum of Squared Errors (SSE), which is defined as:

$$SSE = \sum_{i=1}^{n} {e_i}^2 = \sum_{i=1}^{n} \left(\tau_i - \hat{\tau}_i\right)^2 \tag{17}$$

where $\hat{\tau}$ is the value obtained using the fitted polynomial. Testing of the SSE for different values of λ, it yields the optimum value of λ equal to -3.99, when approximately 300 data points are employed. Using this value of λ and transforming the data points, a polynomial of order of 3 can be fitted to the results as follows:

$$\mathrm{T} = -3.7148\varphi^3 + 6.8942\varphi^2 - 4.6039\varphi + 1.4318 \tag{18}$$

Figure 3 shows the plot of $\tau - \varphi$ and $\mathrm{T} - \varphi$ and the fitted polynomials to each set of data. It can be seen that the transformed values of tortuosity are scattered more uniformly around the fitted polynomial for whole range of the porosity. Equations 16 and 18 can be used together to explicitly calculate the tortuosity as a function of the porosity.

Previous work by the authors [18] has demonstrated the obstacles' geometry has major effect on the flow pattern and on the predicted permeability of a regular ordered porous medium; by increasing the height to width ratio of the obstacles, while keeping the porosity constant, the permeability decreases. Figure 4 presents the streamlines and continuous contours of the velocity magnitude for three different obstacle aspect ratios - 0.5, 1 and 2; darker regions indicate higher local velocity magnitudes. The high tortuosity path of the flow in the region bound by the randomly placed obstacles is clearly apparent for the cases presented. Obstacles with larger height to width ratio exert more resistance to the mean flow path and are more likely to obstruct or eliminate the flow passages. The size of the obstacles is chosen with the purpose of keeping the total area of the obstacles nearly constant.

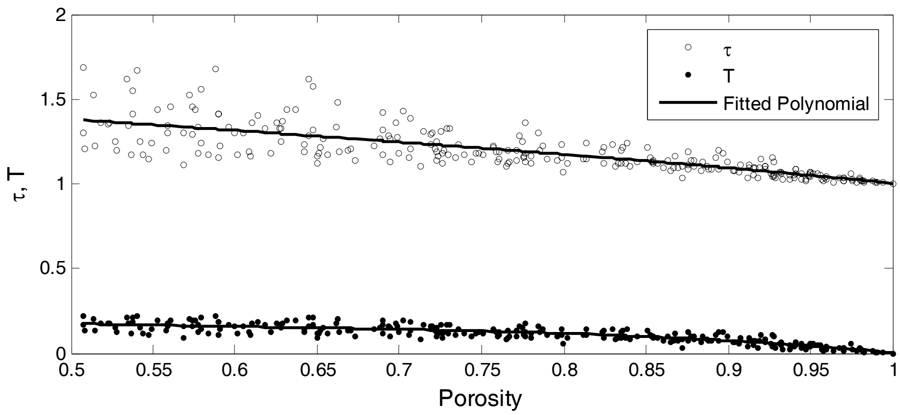
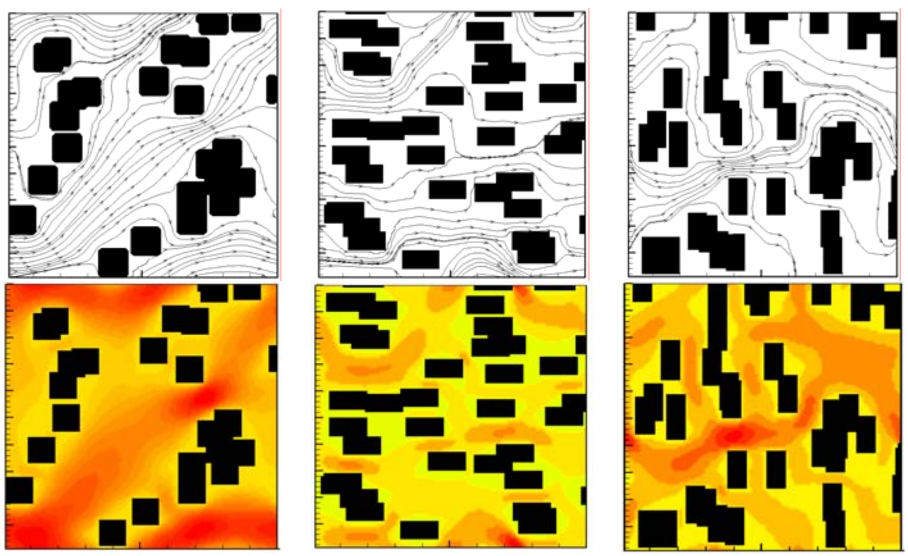


Fig.3. Tortuosity and transformed tortuosity data versus porosity and fitted polynomials.



i) Porosity=0.80, Dx=10, Dy=10 **ii) Porosity= 0.72, Dx=14, Dy=7** **iii) Porosity =0.68, Dx=7, Dy=14**

Fig.4. Streamlines and velocity magnitude contour for three different obstacle aspect ratios (0.5, 1, 2) in a 100×100 domain with randomly placed obstacles

Figure 5 reports on the effect of the obstacles' aspect ratio on the predicted tortuosity. As observed in Fig. 4, the flow tortuosity increases with increasing aspect ratio; the effect of the obstacles' aspect ratio is more pronounced at lower porosities, and at the high porosities, it is practically negligible.

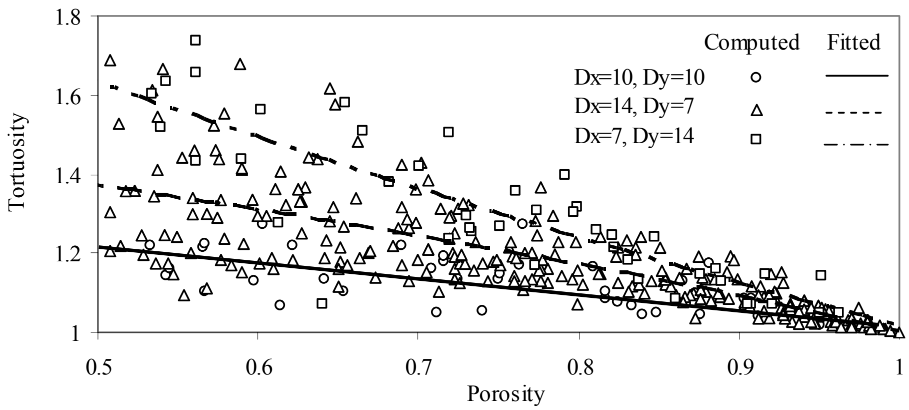


Fig.5. Effect of the aspect ratio of the obstacles on the predicted tortuosity.

5. Conclusion

In conclusion, the effect of the domain resolution on the results for permeability and tortuosity was investigated, and it was concluded the relaxation time and the lattice density used led to lattice independent results. It was found the permeability of a random medium is lower than the permeability of a regularly ordered medium with the same porosity. The permeability, independently of the porous medium structure, varies exponentially with the porosity. Average tortuosity of the flow was also calculated for an extensive set of conditions; the numerical data generated were correlated using a third order polynomial. The proposed correlation for the average tortuosity is in very good agreement with previously published correlations and describes well the asymptotic value of the tortuosity for high and low porosity. It was also found the increase of the obstacles' aspect ratio (height to width ratio) yields an increase of the tortuosity and, consequently, a decrease of the permeability. Like in regularly ordered media, the effect of the obstacles' aspect ratio is augmented at low porosities and it is practically negligible at high porosities.

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