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LATTICE-BOLTZMANN ASSESSMENT OF THE TORTUOSITY OF A 2D SIERPINSKI CARPET TYPE OF POROUS MEDIUM

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Abstract. *This study presents a numerical investigation of the porous medium tortuosity as a function of its porosity, assuming a two-dimensional, Sierpinski carpet type of geometry using the lattice-Boltzmann method. It has been shown that naturally occuring porous media have properties that allow for a fractal-like characterization. The Sierpinski carpet is a self-similar geometry that leads to a fractal shape upon infinite iterations; the carpet is widely used in the morphological representation of heterogeneous porous media upon a finite number of iterations. The lattice-Boltzmann method is an innovative method that has its origins in the Kinetic theory—a non-equilibrium thermodynamical description of systems at mesoscopic scales, in which the governed quantity is the probability distribution function of molecule momenta; thus sitting in a level that is intermediate between the discrete microscopic and the continuous macroscopic modeling levels—that is nowadays under intense development. The method presents itself as an alternative for solving macroscopic hydrodynamic problems and presents ease of implementation of its dynamics and of the no-slip boundary condition type, making it a suitable method for simulating engineering scale fluid flow in complex geometries, such as those of geometrically resolved, pore-level, porous media. The correlation between tortuosity and porosity for two-dimensional Sierpinski carpet fractal-like porous media is presented and compared with other correlations available for porous media in the literature and the present correlation adequately linearizes the relationship between tortuosity and fractal order, demonstrating a good fit for high porosity values.*

Keywords: *Sierpinski carpet, fractal, porous media, tortuosity, lattice-Boltzmann method*

1. INTRODUCTION

Transport phenomena in porous media are present both in nature as in technological processes, as for example, rainwater percolation through geological systems, fluid filtering by natural rocks, oil recovery in reservoirs, and fluid retention in beds (Sahimi, 1995; Dietrich *et al.*, 2005). Nield and Bejan (2006) described the porous media as a solid with interconnected voids inside through which fluid flow can occur.

The determination of properties related to the structure of a given porous medium, such as porosity, surface area, tortuosity and effective length are essential for characterization of properties of the transport process, such as fluid flux and permeability of the medium. Real porous media geometry is at the same time complex as to make it difficult to determine the performance parameters analytically, and also sufficiently irregular as to render empirical measurements less representative (Dullien, 1992; Faruk, 2011).

One of the earliest and well-known correlations between permeability, porosity, and tortuosity is the Kozeny-Carman correlation (Kozeny, 1927; Carman, 1937), given by

$$k = \frac{\phi^3}{\beta\tau^2 S^2}, \tag{1}$$

where k represents the permeability, ϕ the porosity, β the shape factor, τ the tortuosity, and S the specific surface area.

The Kozeny-Carman correlation was the first to introduce the tortuosity term defined by

$$\tau = \frac{L_{\text{eff}}}{L} \tag{2}$$

where L_{eff} is the effective length, which represents the total length traveled by the fluid and L is the porous medium length, which represents the smallest possible crossing path.

In the course of time some correlations have been developed in order to determine the tortuosity for a generalized porous medium from its porosity $\phi = V_p/V$, where V_p is the volume of the pore and V represents the total volume.

Comiti and Renaud (1989) obtained a correlation experimentally in the form

$$\tau = 1 + P \ln(1/\phi), \tag{3}$$

where P is an empirical constant that for a porous medium of solid cubes is $P = 0.63$ and for a medium of solid spheres is $P = 0.41$.

Koponen *et al.* (1996) using the numerical method of automated cellular lattice-gas obtained empirically the correlation

$$\tau = 0.8(1 - \phi) + 1, \tag{4}$$

solving the flow of a two-dimensional incompressible newtonian fluid in a porous medium of rectangles of equal size, randomly distributed and allowed overlap. Later Koponen *et al.* (1997) observed that their previous correlation given by the Equation (4) presented good results only for a range of $\phi = [0.5, 1]$ and therefore they proposed a new correlation with good results for a range $\phi = [0.4, 1]$, given by

$$\tau = 1 + a\frac{(1 - \phi)}{(\phi - \phi_c)^m} \tag{5}$$

where a and m are some empirical parameters e ϕ_c represents system percolation threshold.

Yu and Li (2004) obtained the analytical correlation for tortuosity

$$\tau = \frac{1}{2}\left[1 + \frac{1}{2}\sqrt{1-\phi} + \frac{\sqrt{(\sqrt{1-\phi}-1)^2 + (1-\phi)/4}}{1-\sqrt{1-\phi}}\right], \tag{6}$$

for a simple two-dimensional porous geometry, considering that some particles that constitute the porous medium overlap and others do not.

Matyka *et al.* (2008), like Koponen *et al.* (1996), obtained a numerical correlation for a porous medium of randomly distributed and allowed overlapping squares. The correlation obtained by Matyka *et al.* (2008) using the lattice-Boltzmann method is given by

$$\tau \propto R\frac{S}{\phi} + 1 \tag{7}$$

where R is the hydraulic ratio of obstacles. This correlation is proportional to Equation (3) obtained by Comiti and Renaud (1989).

The mathematical concept of fractal geometry, introduced by Mandelbrot (1982), has been applied throughout the decades in different branches of science and technology. In the area of porous media research, many have used the fractal concept; although with finite iterations, in the morphological representation of real porous media, as by Li and Yu (2011), Luo *et al.* (2014) and Khabbazi *et al.* (2015).

Real, rocky porous media have formations that exhibit properties that allow for its characterization as a self-similar, fractal-like medium (Sahimi, 1995). The Sierpinski carpet is a self-similar geometry that leads to a fractal shape upon infinite iterations; the carpet is widely used in the morphological representation of heterogeneous porous media-such as aquifers and oil reservoirs-upon a finite number of iterations (Dullien, 1992). Figure 1 shows the first 4 iterations towards the Sierpinski carpet, for details of geometry representation see Mandelbrot (1982).

Li and Yu (2011) obtained a analytical correlation for tortuosity based on a creeping flow of a Newtonian fluid on orders of Sierpinski carpet iteration. The correlation can be given in terms of the order of fractal iteration

$$\tau = \left(\frac{19}{18}\right)^n, \tag{8}$$

where n is the order, or by the respective porosity of each order

$$\tau = \left(\frac{19}{18}\right)^{-8,49\ln(\phi)}, \tag{9}$$

where $\phi = (8/9)^n$.

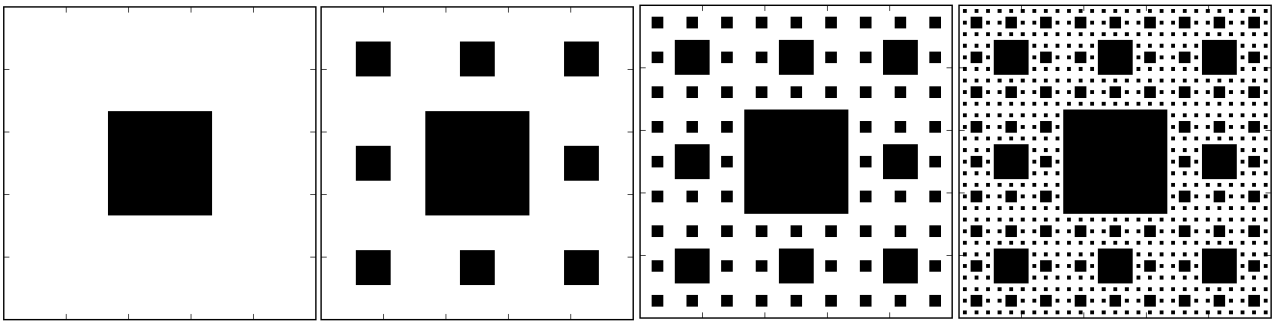


Figure 1. The first 4 iterations towards the Sierpinski carpet fractal.

Luo *et al.* (2014) proposed a solution for the flow around of orders of Sierpinski carpet iteration to an incompressible Newtonian fluid, obtained a correlation approaching the results of the tortuosity by a line with respect to the order of the fractal iteration, which written in term of the porosity is given by

$$\tau = 0,946 - 0,408\ln(\phi). \tag{10}$$

Khabbazi *et al.* (2015) obtained an analytical correlation for tortuosity using a methodology close to that used by Li and Yu (2011), also considering a two-dimensional creeping flow for orders of Sierpinski carpet iteration, the correlation is given by

$$\tau = \frac{3}{2} - \frac{\phi}{2}, \tag{11}$$

also obtained a correlation for a variation of the Sierpinski carpet using circles instead of squares in their respective orders, which is given by

$$\tau = (1 - \frac{4}{\pi})\phi + \frac{4}{\pi}. \tag{12}$$

2. PROBLEM FORMULATION

In this work the numerical study for the flow around a porous medium determined by the Sierpinski carpet iteration is proposed, seeking a correlation for the results of tortuosity obtained for each order of the fractal geometry. The numerical study is based on the lattice-Boltzmann method, as a method that presents some advantages over conventional numerical methods such as the easy implementation of its bounce-back boundary condition, which makes it the ideal method for simulating complex flow geometries such as the case of porous media (Chen and Doolen, 1998).

The Figure 2 shows schematically the representation of a porous media using the geometry of the Sierpinski carpet in a channel. The channel has an aspect ratio of $A = H/L = 1$, where L and H are the length and the height of the channel, respectively. Being the velocity components u and v for the x and y directions, respectively, as $\mathbf{u} = \sqrt{u^2 + v^2}$ and $\mathbf{x} = \sqrt{x^2 + y^2}$. The boundary conditions are the non-slip on the surface of each block and the on channel walls, and the flow is given by the pressure difference between the inlet and outlet of the channel, the channel is considered as periodic.

The conservation equations of mass and momentum, respectively, that were solved numerically for the specified problem are expressed in dimensional form by

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}}(\rho \mathbf{u}) = 0, \tag{13}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla_{\mathbf{x}}(\rho \mathbf{u}\mathbf{u}) = -\nabla_{\mathbf{x}}(p) + \nabla_{\mathbf{x}}\left[\rho\nu(\nabla_{\mathbf{x}}\mathbf{u} + \nabla_{\mathbf{x}}\mathbf{u}^T\right], \tag{14}$$

where ρ , p and ν are the density, pressure and kinematic viscosity, respectively, and t the time.

The tortuosity is evaluated in accordance with the method proposed by Matyka and Koza (2012), given by

$$\tau = \frac{\sum |\mathbf{u}(x,y)|}{\sum |u(x,y)|}. \tag{15}$$

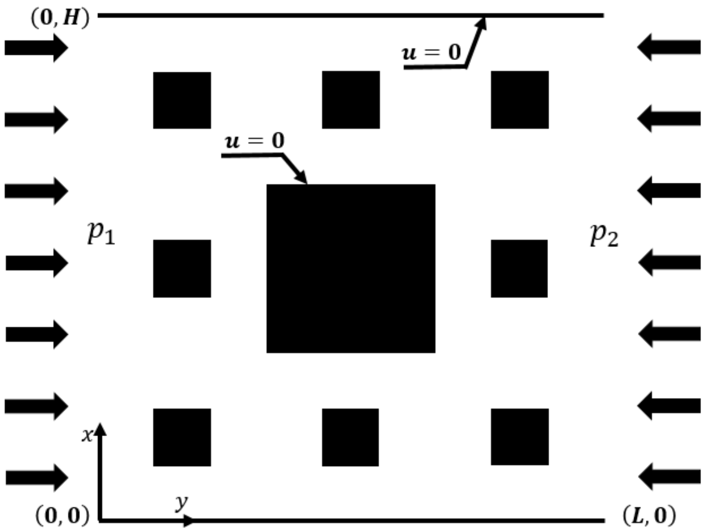


Figure 2. Representation of the fractal porous media in channel and its boundary conditions.

3. NUMERICAL PROCEDURE

The numerical formulation of the problem is made through the lattice-Boltzmann method, which consists of lattice discretization of the continuous Boltzmann equation, expressed by

$$\frac{\partial f}{\partial t} + \mathbf{e} \cdot \nabla_{\mathbf{x}} f + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{e}} f = \Omega, \tag{16}$$

where Ω represents the collision operator, $\mathbf{e}$ the microscopic particle velocity, f the distribution function of molecular momenta, $\mathbf{F}$ an external body force and m the molecular mass. The space is a $2N$-dimensional remnant of the phase-space of the thermodynamic system, where N is the Euclidean spacial dimensionality, since both $\mathbf{x}$ and $\mathbf{e}$ are abscissas.

Using the BGK model of the collision operator and writing the Equation (16) in a discrete lattice form for a system without external forces yields the so-called lattice-Boltzmann equation (Bhatnagar *et al.*, 1954):

$$f_i(\mathbf{x} + \mathbf{e}_i\delta_t, t + \delta_t) - f_i(\mathbf{x}, t) = -\frac{1}{\lambda}\Big[f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)\Big], \tag{17}$$

where f^{eq} is the equilibrium distribution function of molecular momenta and i represents the discrete lattice velocity index, δ_t is the discrete time increment and λ represents the non-dimensional relaxation time given by

$$\lambda = \frac{\nu}{c_s^2} + \frac{1}{2}, \tag{18}$$

where ν and c_s are the kinematic viscosity and speed of sound, respectively.

The equilibrium distribution function of molecular momenta is given by the Maxwell-Boltzmann distribution function, which, written in its discretized form truncated up to second-order terms becomes

$$f_i^{eq} = \rho w_i\Big(1 + \frac{\mathbf{e}_i\mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i\mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2}\Big), \tag{19}$$

where ρ is the density, $\mathbf{u}$ is the macroscopic (flow) velocity vector, and w_i are the weight factors for the corresponding discrete lattice velocity index.

The macroscopic properties of the problem are recovered from the momentum of the probability distribution functions for the molecular moments, i.e.,

$$\rho = \sum_i f_i, \qquad \rho\mathbf{u}^* = \sum_i \mathbf{e}_i f_i, \tag{20}$$

where $\mathbf{u}^*$ is the predicted macroscopic (flow) velocity.

In this work, the above discretized equations are applied to a two-dimensional, nine-velocity lattice, popularly known as the D2Q9 lattice, where

$$\mathbf{e}_0 = (0,0),$$
$$\mathbf{e}_i = \left(\cos\frac{i-1}{2}\pi, \sin\frac{i-1}{2}\pi\right), \qquad i = 1,2,3,4 \tag{21}$$
$$\mathbf{e}_i = \sqrt{2}\left(\cos\frac{i-5}{2}\pi + \frac{\pi}{4}, \sin\frac{i-5}{2}\pi + \frac{\pi}{4}\right), \qquad i = 5,6,7,8.$$

The D2Q9 lattice weight factors are given by $\omega_0 = 4/9$, $\omega_i = 1/9$ for $i = 1,2,3,4$; and $\omega_i = 1/36$ for $i = 5,6,7,8$; and the sound speed by $c_s = 1/\sqrt{3}$.

3.1 Boundary Conditions

The boundary conditions illustrated in Figure 2, are implemented in accordance with the non-equilibrium bounce-back model for non-slip conditions

$$f_i^{neq} = f_i - f_i^{eq} = f_{i'} - f_{i'}^{eq} = f_{i'}^{neq} \tag{22}$$

where f^{neq} is the non-equilibrium distribution function and i' is the opposite direction to i (Zou and He, 1997). For the channel inlet and outlet is used the periodic boundary condition.

The pressure boundary condition is implemented based on Poisson pressure equation proposed by Inamuro *et al.* (2004),where

$$\mathbf{u} = \mathbf{u}^* - \left[\frac{p_{\mathbf{x}+1} - p_{\mathbf{x}-1}}{2\rho}\right]. \tag{23}$$

3.2 Grid Test Accuracy

The test seeks to minimize the total error related to the method given by the sum of $E_{total} = E_{\mathrm{Ma}} + E_{\delta_x} + E_{\delta_t}$, and E_{total} the total error, E_{Ma} the error associated with compressibility where Ma is the Mach number, E_{δ_t} the temporal error associated with the time step and E_{δ_x} the spatial error associated with mesh, where δ_x is the spacial lattice spacing (Guo and Shu, 2013).

The error related to compressibility to $\mathrm{Ma} < 1$ is order of magnitude Ma^2, calculated by $\mathrm{Ma} = |\mathbf{u}|/c_s$ in the lattice-Boltzmann scale. From the established compressibility error the relationship between the errors is given by

$$E_{\mathrm{Ma}} \propto \frac{E_{\delta_t}}{E_{\delta_x}} \propto \frac{1}{r^2} \tag{24}$$

where E_{δ_x} is of the order δ_x^2, E_{dt} of order δ_t^2 and $r = \delta_x/\delta_t$ is a relationship between the lattice spacing and the time increment (Guo and Shu, 2013).

In the test adopted, an inital mesh with fixed δ_x is considered and δ_t is decreased progressively so as to minimize E_{Ma} and E_{δ_t}, within an acceptable tolerance. This procedure eliminates the temporal errors, leaving the E_{total} dominated by E_{δ_x}, that is $E_{total} \approx E_{\delta_x}$. With the progressive decrease from δ_t to fixed δ_x, the value of r grows progressively.

One factor that impedes the use of relatively low values of δ_t is its influence on the relaxation time λ. Notably, the method stability is hindered when λ close to $1/2$ (Succi, 2001).

Then, refining δ_x by increasing the number of mesh nodes, along with the raise of r in the same proportion, results in a quadratic decrease of δ_t in relation to δ_x, ensuring that $E_{total} \approx E_{\delta_x}$. Therefore, the successive refinement of δ_x ensures that the results converge to a solution independent of δ_x and δ_t, for a given tolerance.

4. RESULTS AND DISCUSSION

The range of investigation of the flow through the Sierpinski carpet parameters are shown in Table 1. The Reynolds number is given by $Re = U_{ref}H/\nu$, where U_{ref} is the mean velocity calculated by

$$U_{ref} = -\frac{1}{12\nu\rho}\frac{\partial p}{\partial x}H^2 \tag{25}$$

where $\frac{\partial p}{\partial x}$ is the difference pressure between inlet and outlet.

The different iterations of the Sierpinski carpet interfere in the amount of obstacles and consequently in the tortuosity and permeability of the channel. In addition, the dimensionless parameter of the Reynolds number is varied from 0.1 to

Table 1. Parameters considered in the simulations of the flow through the Sierpinski carpet

N	1;2;3;4;5
Re	0.1;1;10;100

100 to cover a laminar flow range. The grid test is done for each interaction of the Sierpinski carpet in its critical case, i.e $Re = 100$, considering a tolerance of 0.01% for the variation of the tortuosity in the refinement of δ_t and δ_x. The meshes obtained are presented in the Table 2.

4.1 Reynolds number effect over tortuosity

The results obtained for tortuosity in the numerical simulations can be observed in the Table 2 for different Sierpinski carpet iterations according to the Reynolds number. Remarkably, no value greater 0.5% was observed when calculating the percentage variation between the maximum and minimum values of tortuosity for each iteration of Sierpinski carpet. Therefore, for a certain tolerance one can consider that the tortuosity is independent of Re and consequently the pressure gradient for the different orders of the Sierpinski carpet.

Table 2. Tortuosity of different Sierpinski carpet iterations (n) varying Re.

Re		n				
	Grid	81x81	162x162	324x324	648x648	1296x1296
	r	2^7	2^8	2^9	2^{10}	2^{11}
		1	2	3	4	5
0.1		1.0340	1.0788	1.1269	1.1682	1.2021
1		1.0340	1.0794	1.1284	1.1678	1.2078
10		1.0339	1.0803	1.1291	1.1686	1.2081
100		1.0302	1.0795	1.1293	1.1683	1.2079
$\frac{\tau_{max} - \tau_{min}}{\tau_{min}} \times 100\%$		0.3672%	0.1363%	0.1965%	0.0685%	0.4966%

In Figure 3 the velocity magnitude of steady-state flow is shown for the 5 iterations of the Sierpinski carpet and an increase of the velocity magnitude at the points where a reduced pore throats are observed.

4.2 Relation between tortuosity and order of Sierpinski carpet

The approach employed by Luo *et al.* (2014) applying a linear fit to the points of tortuosity by the orders of Sierpinski carpet iteration, is shown in Figure 4 for the tortuosity values of $Re = 100$. Therefore, the present numerical correlation obtained with the lattice-Boltzmann method is given by

$$\tau = 0.041749n + 0.997295, \tag{26}$$

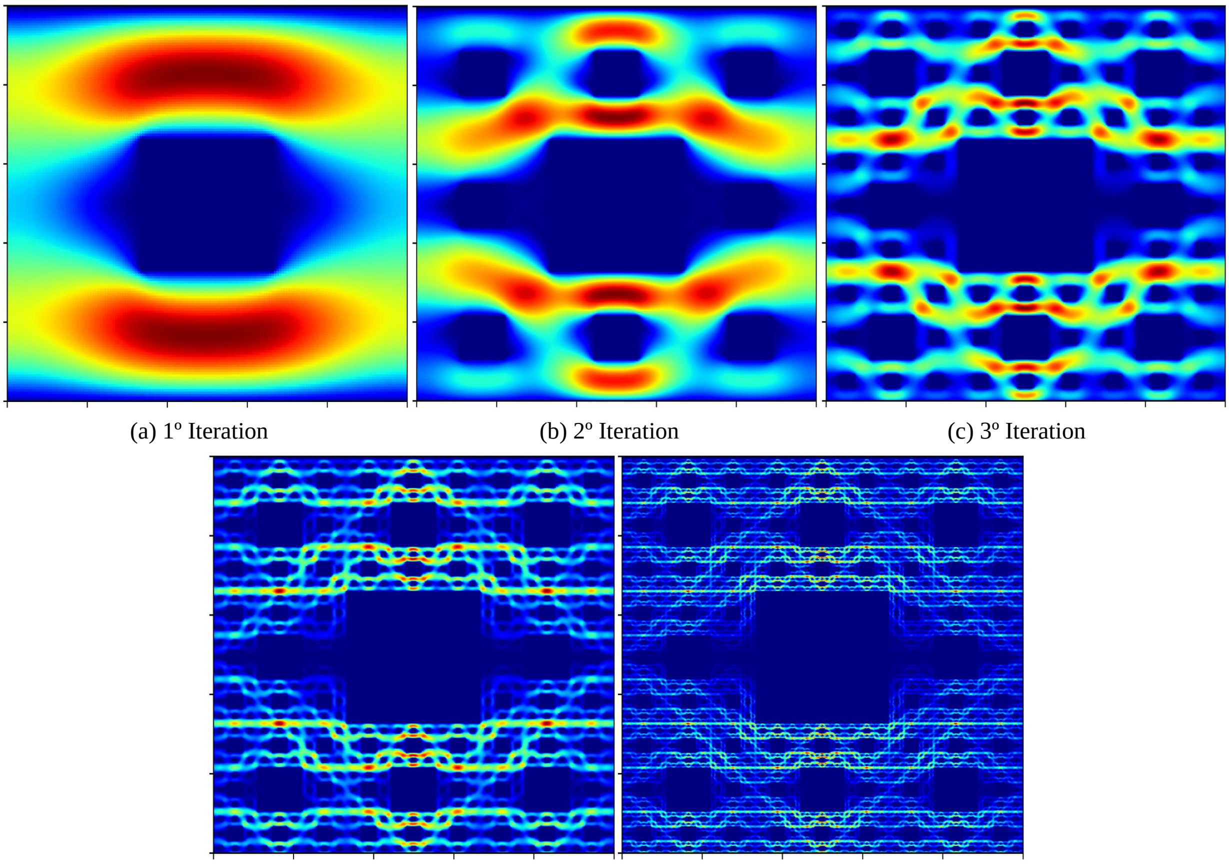
replacing the order n of Sierpinski carpet iteration by the term of porosity

$$\tau = 0.997295 - 0.35445 \ln(\phi). \tag{27}$$

In Figure 5 a graphical comparison between the correlation here proposed - Equation (27) - and the cited correlations, which do not consider specifically the Sierpinski carpet geometry, is presented. As porosity tends to zero, one can observe that the Equations (3), (5), (6) and (27) tends to infinity and the Equation (4), tends to fixed value. However, Koponen *et al.* (1996) and Koponen *et al.* (1997) make it clear that the equations (4) and (5), are for the porosity ranges $[0.5, 1]$ and $[0.4, 1]$, respectively.

In Figure 6 a comparison between the present work correlation - Equation (27) - and those based on the Sierpinski carpet are performed. As in the Figure 5, one can observe a trend for tortuosity to infinity in the Equations (9), (10) and (27), when the porosity tends to zero. As for the Equation (11) tortuosity goes to 1.5 when the porosity tends to zero.

Therefore, the correlation obtained in the present work - Equation (27) - in comparison with those of Comiti and Renaud (1989), Koponen *et al.* (1996), Koponen *et al.* (1997) and Yu and Li (2004), for tortuosity in flows around rectangles, presents a great difference due to its formulations, as for example the considerations of random pore distribution. Concerning to the analytical correlations of Yu and Li (2004), Li and Yu (2011) and Khabbazi *et al.* (2015), the difference presented is probably due to the fact that such models neglect some flow geometric aspects such as recirculations, which are considered in the numerical and experimental models. Notice that the correlation of Luo *et al.* (2014) displayed good approximate, since it follows the same methodology of the present work. However, in cases where the porosity is close to



(a) 1º Iteration (b) 2º Iteration (c) 3º Iteration

(d) 4º Iteration (e) 5º Iteration

Figure 3. Flow velocity magnitude considering 5 Sierpinski carpet iterations.

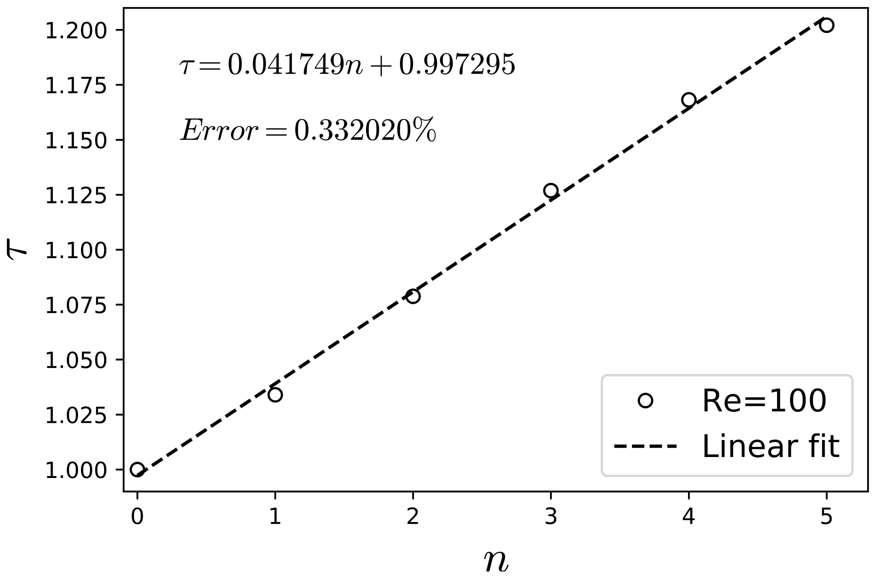


Figure 4. Relation between tortusity and orders of Sierpinski carpet iteration.

one, the obtained results present better adjustment, whereas for the first iteration of the Sierpinski carpet the correlation of Luo *et al.* (2014) presents a tortuosity smaller than one, which is physically impracticable.

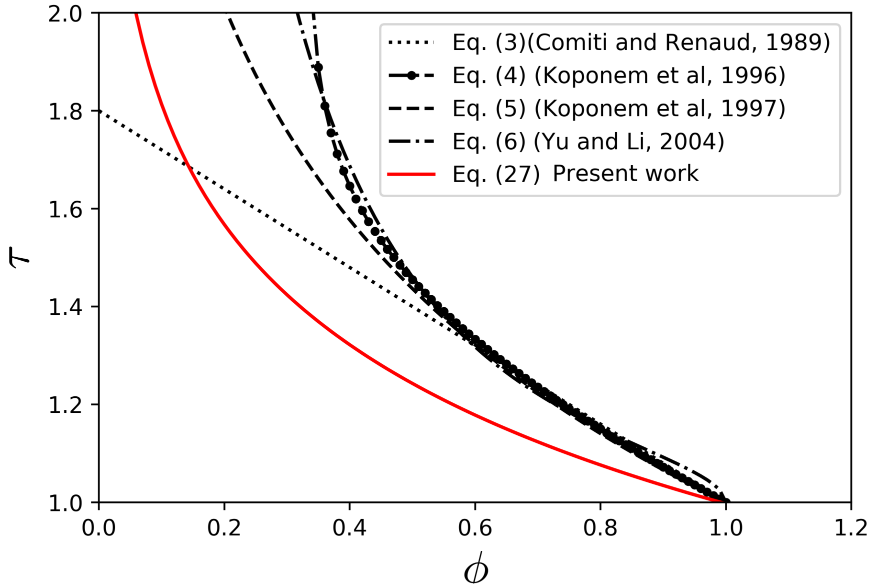


Figure 5. Comparison between the present correlation Eq.(27) and the correlations of Comiti and Renaud (1989), Koponen *et al.* (1996), Koponen *et al.* (1997) and Yu and Li (2004).

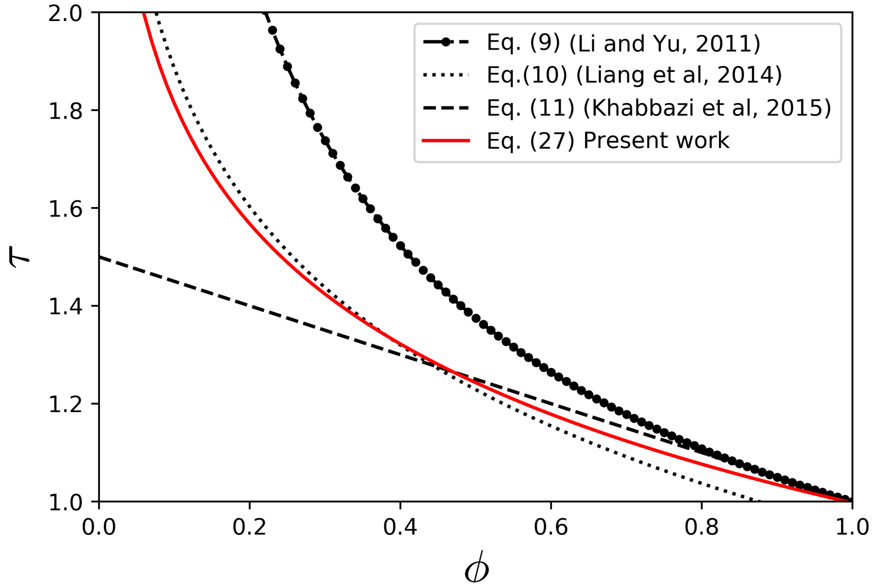


Figure 6. Comparison between the present correlation Eq.(27) and the correlations of Li and Yu (2011), Luo *et al.* (2014) e Khabbazi *et al.* (2015).

5. CONCLUSIONS

In the literature, there are several models that attempt to predict the tortuosity of porous media. Some of them are based on analytical, experimental and numerical approaches. The correlation proposed in the present work is based on the numerical methodology made by Luo *et al.* (2014), using as a differential the lattice-Boltzmann method that is reference in the simulation of flow in porous media.

Comparing the correlation obtained with the correlation of Luo *et al.* (2014) a proximity was observed. Nevertheless the present correlation better adjusts the results for porosities close to one. In relation to the other mentioned correlations a non-proximity is observed, a behavior already expected due to the different approaches used to deduce the respective correlations.

Therefore, the present work demonstrates the good applicability of the lattice-Boltzmann method to solve flow around specific geometries, such as porous media, allowing the determination of flow properties such as tortuosity.

6. ACKNOWLEDGEMENTS

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