Sci. Bull.
DOI 10.1007/s11434-016-1020-3

www.scibull.com
www.springer.com/scp

Article

Engineering Sciences

Determining the impact of rectangular grain aspect ratio on tortuosity–porosity correlations of two-dimensional stochastically generated porous media

A. Ebrahimi Khabbazi · J. Hinebaugh · A. Bazylak

Received: 21 October 2015 / Revised: 21 December 2015 / Accepted: 12 January 2016

Abstract Tortuosity is an important parameter for characterizing transport properties within porous materials and is of interest in a broad range of fields, such as energy storage and conversion materials. One of the parameters that impacts the tortuosity value is the geometry of the solid phase which, in this study, is considered as stochastically-placed rectangular particles. Through lattice Boltzmann modelling (LBM), we determined the impact of particle aspect ratio on the intrinsic tortuosity–porosity relationships of two-dimensional porous media composed of rectangular particles. These relationships were isolated for materials with grain (particle) aspect ratios of ∈ {1, 2, 3} and porosities from [0.55 – 0.95]. We determined that a minimum of 6, 8 and 10 stochastic simulations, respectively, were required to calculate these average tortuosity values in laminar flow ($Re \ll 1$). This novel application of the LBM to study the effects of porosity and aspect ratio of rectangular grains on tortuosity can be used in the tailoring of materials for clean energy.

SPECIAL TOPIC: Materials for Energy Conversion

A. Ebrahimi Khabbazi
Thermofluids for Energy and Advanced Materials (TEAM) Laboratory, University of Toronto, Toronto M5S 3G8, Canada

J. Hinebaugh
Department of Mechanical and Industrial Engineering, University of Toronto, Toronto M5S 3G8, Canada

A. Bazylak (✉)
Faculty of Applied Science and Engineering, University of Toronto, Toronto M5S 3G8, Canada
e-mail: abazylak@mie.utoronto.ca

Keywords Tortuosity · Porous media · Grain aspect ratio · Lattice-Boltzmann model · Stochastic simulation

1 Introduction

Permeability and effective diffusivity are valuable material properties for predictive continuum models of flow and mass transport through porous media. When empirical values for these properties are not available, estimates can be made based on porosity and tortuosity values. Tortuosity, τ, provides a means of measuring the complexity of fluid pathways through a porous material and has been strongly correlated to material porosity [1, 2]. Therefore, tortuosity has been applied in numerical models for science and engineering applications ranging from oil recovery and carbon sequestration to energy conversion and storage systems such as fuel cells and Li-ion batteries [3–7]. The significance of tortuosity for energy conversion and storage systems has been discussed previously [2, 8–15]. For instance, some studies have used tortuosity as an effective geometric parameter in models to describe ionic transport in porous electrodes [2, 9, 16].

There are several definitions of tortuosity in Refs. [17–22], depending on characterization needs, ranging from the determination of electrical conductivity to hydraulic conductivity. Several tortuosity definitions along with their variances and common applications are discussed below to emphasize the importance of implementing tortuosity definitions with care.

The geometrical tortuosity, τ_g, can be defined as the ratio of the average length of the geometric flow paths, $\langle L_g \rangle$, to the length of the medium in the direction of macroscopic flux, L_s, [17]:

$$\tau_g = \frac{\langle L_g \rangle}{L_s}, \quad (1)$$

while the hydraulic tortuosity, τ, is defined as the ratio of the average effective flow path length taken by the fluid, $\langle L_h \rangle$, to the straight-line length across the medium, L_s [23]:

$$\tau = \frac{\langle L_h \rangle}{L_s}. \quad (2)$$

Geometric pathways include the shortest paths consisting of straight lines touching and passing by grains with close tangents (Fig. 1a), whereas in reality, fluid particles are expected to travel through smoothed streamlines [17, 19]. Therefore, τ is always greater than τ_g. Furthermore, geometrical tortuosity is commonly based on geometric parameters, such as particle size, shape, and arrangement.

Hydraulic tortuosity accounts for the hydrodynamics of the flow within porous formations (Fig. 1b). Hydraulic tortuosity is used to determine the permeability of porous media. For example, in the subsequent and often cited Kozeny–Carman relationship, the permeability is expressed as a function of tortuosity [1, 24]:

$$K = \frac{1}{C_{KC}} \cdot \frac{\phi^3}{S^2 \tau^2}, \quad (3)$$

where K, C_{KC}, ϕ, and S are permeability, Kozeny–Carman constant (shape factor), porosity, and specific surface area, respectively.

The electrical tortuosity is defined as [25–27]

$$\tau_e = \left(\frac{\langle L_e \rangle}{L_s} \right)^2, \quad (4)$$

where $\langle L_e \rangle$ is defined as the average path length for electronic flow. However, an alternate definition of the electrical tortuosity is the ratio of the conductivity of a porous medium saturated with an electrolyte to that of the free electrolyte [28]. Electrical tortuosity can play an important role in determining electrical resistivity of a given formation. Similar to the former definition of electrical tortuosity, diffusive tortuosity, τ_d, can be defined [22] as

$$\tau_d = \left(\frac{\langle L_d \rangle}{L_s} \right)^2, \quad (5)$$

where $\langle L_d \rangle$ is the average length of the diffusive pathway of a chemical species. Diffusive tortuosity can also be defined as the ratio of the diffusion coefficient of the given species in free fluid to its value in porous media [18, 19, 29–31]. Diffusive tortuosity is used when diffusion is the dominant transport mechanism in the porous media, such as in the case of gas diffusion layers in polymer electrolyte membrane fuel cells.

Hydraulic tortuosity calculations have been conducted using experimental [32–34], analytical [35, 36] and numerical methods [1, 20, 23, 37, 38]. Experimental-based parametric investigations pose challenges due to cost and time limitations as well as restrictions to probing in situ phenomena at the microscale. Analytical models, while highly insightful, are typically constrained to a particular class of structured domains. For example, Du Plessis and Masliyah [35] derived an analytical model particularly for isotropic granular media. Contrary to analytical and experimental methods, numerical models can be used to determine tortuosity values for wide ranges of porous media classes and with computational and temporal cost effectiveness.

Another advantage of pore-scale numerical modelling is the inherent high resolution representation of the pore-scale structure. A variety of numerical schemes are available for simulating flow in porous media at pore scales [39–42]. These include pore-network modelling (PNM), Navier–Stokes (NS) based computational fluid dynamics (CFD) techniques, and LBM. PNMs have attractive features (computational efficiency and capability of handling large domain sizes), but producing a topologically-equivalent network for certain classes of rocks can be challenging with this method [43]. Furthermore, PNM is not suited for resolving the velocity and concentration gradients within a

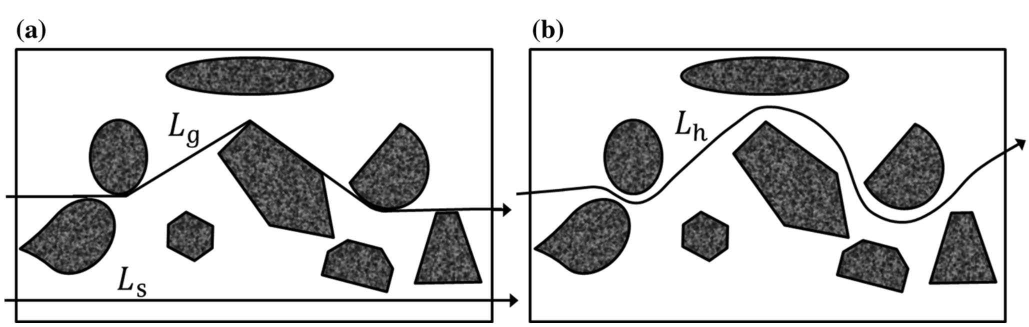

Fig. 1 Example schematic of a geometric (**a**) and hydraulic (**b**) flow path. Note that the hydraulic length (L_h) is greater than the geometric length (L_g)