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A simplistic model for the tortuosity in two-phase close-celled porous media

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Abstract

We present an analytical model capable of demonstrating the dependence of tortuosity of two-phase porous media upon two topological parameters: porosity and pore shape. Based on a generalized effective thermal conductivity model and a particular solution to the Laplace heat conduction equation for two-phase porous media having randomly distributed non-conducting circular pores, an analytical model of tortuosity is derived. For non-circular pores such as idealized polygonal pores, the circularity-based concept of pore shape factor is incorporated into the model, which is capable of analytically unifying existing models which are valid only for limited porosity ranges and circular pore shapes.

(Some figures may appear in colour only in the online journal)

1. Introduction

The understanding of transport phenomena in porous media paves the foundation for industrial and environmental processes covering a broad range of disciplines (e.g. geology, engineering, chemistry, and physics) and a variety of applications such as catalysis, separation and filtration, cement chemistry, and heat exchanger [1]. To describe such transport phenomena, conservation equations of energy, momentum and mass with boundary conditions are typically derived at the microscopic level (pore level). In common practice, their solutions are, however, sought at the macroscopic level using volume averaging, statistical averaging and homogenization due to difficulties in generalizing microscopic information (e.g. tortuosity) within porous media [2]. Such microscopic information is therefore often 'lumped' in macroscopic transport properties (e.g. porosity).

To better understand the mechanisms of transport phenomena in porous media, numerous attempts have been made to relate porosity with tortuosity [3–8], which, however, essentially require fitting factors based on experimental or numerical data. Although analytical models are preferable on a physical basis, the complex nature of tortuosity has hindered analytical modelling. Therefore, tortuosity in porous media is

determined conventionally by empirical correlations [3, 6] and numerical simulations (e.g. lattice gas cellular automaton [7, 9] and lattice Boltzmann model [10]).

Several analytical models have been developed for porous media with specific and well-defined pore topologies, requiring no adjustable factors but highly idealized topologies, such as spherical pores having monosize [11, 12] and ordered arrangement [13], which are far from the reality. Recently, analytical models relaxing some topological constraints such as randomization [14] and free overlapping [15] in terms of pore distribution have been proposed. However, all these models are invalid for non-spherical (non-circular) pores that are more realistic especially for high porosity close-celled foams (figure 1). Whilst most of the tortuosity models are built upon fitting factors that vary significantly amongst the models and have no physical basis, we demonstrate in this paper that the tortuosity in two-phase close-celled porous media can be analytically expressed as a function of porosity and pore shape.

2. Analytical model

Without adopting the analogy between heat conduction and mass diffusion, it can be directly established that an alternative

and general effective thermal conductivity model for two-phase close-celled porous media has the form [16]

$$\frac{k_e}{k_c} = \frac{(1 - \varepsilon)}{\tau}, \quad (1)$$

where it is assumed that the dispersed phase has negligible thermal conductivity, k_e is the effective thermal conductivity of the bulk material, k_c is the thermal conductivity of the continuous phase, τ is the average ‘tortuosity’ and ε is the volume fraction of the disperse phase (porosity).

Alternatively, solving the two-dimensional Laplace heat conduction equation, Bauer [17] presented a detailed expression of the effective thermal conductivity for such porous media, applicable over a full range of porosity. In this model, a particular solution to the Laplace heat conduction equation was obtained by perturbing the initially uniform temperature gradient in the parent (or continuous) medium as a result of the presence of the pores. The corresponding change in the effective thermal conductivity of the porous medium was calculated by solving the temperature profile, as [17]

$$\frac{dk_e}{k_e} = -\frac{1 - k_p/k_e}{2/3\beta + (1 - 2/3\beta)k_p/k_e} \frac{dV}{V}, \quad (2)$$

where k_p is the conductivity of the pores, k_e is the effective conductivity of the bulk material which is varied with the total pore volume V , and β is the pore ‘shape factor’. Integration of equation (2) from $V = 0$ to a given porosity yields

$$\frac{k_e - k_p}{k_c - k_p} \left(\frac{k_c}{k_e} \right)^{1-2/3\beta} = 1 - \varepsilon. \quad (3)$$

For non-conducting pores (i.e. $k_p = 0$), equation (3) reduces to

$$\frac{k_e}{k_c} = (1 - \varepsilon)^{3\beta/2}. \quad (4)$$

It follows from (1) and (4) that the tortuosity is related to the porosity and pore shape by

$$\tau = (1 - \varepsilon)^{1-3\beta/2}. \quad (5)$$

Upon comparing (4) with Bruggeman’s analysis [18], the shape factor β is found to be unity for spherical pores (or two-dimensional circular pores) [17].

Since the model presented by equation (3) is extended from circular pores, the shape factor represents a correctness factor for other pore shapes [19]. Here, we extend Wadell’s circularity (two-dimensional) concept [20] to relate circular pores with other shaped pores, as

$$\beta = C/C_{ref}, \quad (6)$$

where the shape factor β is defined as the ratio (circularity) of the perimeter (C) of a representative pore to the perimeter ($C_{ref} = 2\pi R$) of a reference circle with radius R , and it is assumed that the representative pore has an area equal to that of the reference circle. Once the shape factor is determined from equation (6), the tortuosity can be analytically estimated from equation (5).

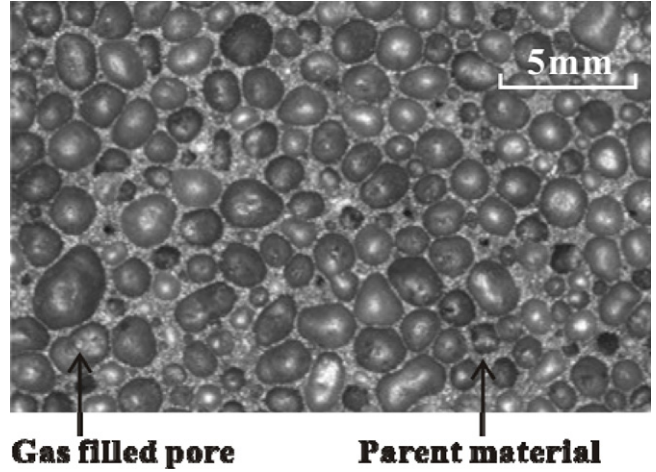


Figure 1. Typical two-phase close-celled porous medium (aluminum foam, porosity $\varepsilon = 0.76$) with non-spherical pores.

Table 1. Shape factors for selected pore shapes: comparison between present analysis and numerical simulation^a.

| Pore shape | Number of sides | Shape factor β | |
|------------|-----------------|-----------------------------------|---------------------------------|
| | | Numerical simulation ^a | Present analysis (equation (9)) |
| Square | 4 | 1.14 | 1.13 |
| Pentagon | 5 | 1.12 | 1.08 |
| Hexagon | 6 | 1.10 | 1.05 |
| Circle | Infinite | 1.01 | 1.00 |

^a See [21].

For close-celled metallic foams, the representative pore shape is known to vary with the porosity: spherical pores at relatively low porosities and polygonal pores at relatively high porosities [21]. Here, with focus placed upon high porosity metallic foams (figure 1), we assume that these foams are represented by randomly distributed regular polygonal pores, so that the area (A) and perimeter (C) of a representative polygon have the relationship as

$$A = \frac{C^2}{4n \tan(\pi/n)}, \quad (7)$$

where n is the number of sides for the polygon. Finally, upon setting A equal to the area of the reference circle of radius R

$$\frac{C^2}{4n \tan(\pi/n)} = \pi R^2 \quad (8)$$

we can express the shape factor as

$$\beta = \frac{C}{2\pi R} = \sqrt{\frac{n}{\pi} \tan\left(\frac{\pi}{n}\right)}. \quad (9)$$

With n taking separately the value of 4, 5, 6 and infinity, the polygon becomes a square, a pentagon, a hexagon and a circle; correspondingly, the shape factor is explicitly determined from (9) as summarized in table 1.

3. Discussion of results

The inclusion of randomly distributed spherical (or circular if the symmetry condition is assumed) pores with negligible

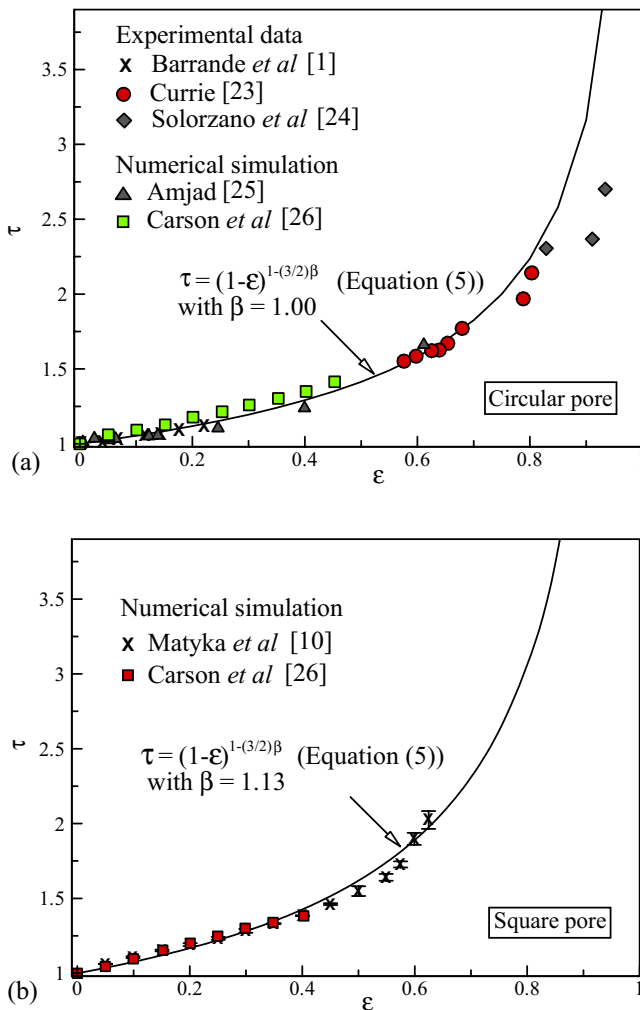


Figure 2. Tortuosity (τ) obtained from the present analysis (equations (5) and (9)) plotted as a function of porosity (ϵ): (a) randomly distributed circular pores (electrical, thermal and diffusive tortuosity data from experiments and numerical simulations [1, 23–26]); (b) randomly distributed, freely overlapped square pores (hydraulic and thermal tortuosity data from numerical simulations [10, 26]).

conductivity ($k_p = 0$) into the parent material, e.g. close-celled aluminum foams as shown in figure 1, decreases the effective thermal conductivity as a result of the increased tortuosity (figure 2(a), solid line). As the porosity is increased, the tortuosity is increased monotonically, the extent of which becomes substantial at high porosities. To validate the present analytical model prediction, three separate sets of experimental measurement data and two separate sets of numerical simulation data are also plotted in figure 2(a). The present model predicts accurately the dependence of tortuosity on porosity for both low and high porosity ranges. Given that both the diffusion and conduction phenomena are governed by the Laplace equation, the observed good agreement between the diffusive tortuosity and the thermal tortuosity is anticipated and both behave in a similar manner as the porosity is varied.

For relatively low porosity porous media having randomly and freely overlapped ‘square’ pores, the dependence of tortuosity upon porosity previously predicted numerically

[10, 26] is also well estimated by the present analytical model (figure 2(b), solid line). For both circular and square pores, the corresponding shape factors calculated by equation (9) are substituted into equation (5) to calculate the tortuosity. For a given porosity, non-circular (or non-spherical) pores lead to elongated heat conduction distances (tortuosity) in comparison with circular pores, reducing therefore the effective thermal conductivity as shown in equation (1).

4. Conclusions

A simple yet accurate model for the tortuosity in two-phase porous media having two-dimensional closed-cells has been presented. The present model analytically lays the physical basis for the widely accepted power-law dependence of tortuosity (both diffusion and heat conduction) upon porosity, and provides the physical evidence of the empirical coefficient n being 0.5 for spherical (or circular) pores. Further, the inclusion of shape factor enables the extension of existing tortuosity model for porous media with randomly distributed circular pores to porous media containing randomly distributed non-circular pores (e.g. polygons) without requiring any empirical or numerical fitting factor. The present model is, however, only applicable to porous media having two-dimensional pores. Practically, the majority of natural and engineered porous media is three-dimensional, resulting in increased tortuosity, which requires further study to account for such three-dimensionality in the present model.

Acknowledgments

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