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Fractal description of microstructures and properties of dynamically evolving porous media

A. Verma, R. Pitchumani *

Advanced Materials and Technologies Laboratory, Department of Mechanical Engineering, Virginia Tech, Blacksburg, Virginia 24061-0238, United States

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ABSTRACT

Transport through porous media is encountered in several engineering and biological applications. The porous media can be subjected to changes in structure owing to deposition, erosion, swelling or shrinkage which, in turn, affects the transport properties of the media. A dynamic fractal model (DFM) is developed to describe the evolution in pore structure undergoing deposition using fractal dimensions and to predict the changes in the effective diffusivity in terms of the dynamic fractal dimensions. Evolving microstructures undergoing deposition are analyzed at various saturation levels to determine the effective diffusivity using the dynamic fractal model. The effective diffusivity values of the evolving porous media are compared against existing data in the literature.

1. Introduction

The structure of porous media commonly undergoes changes over time as part of several physical processes such as flow in fuel cell layers, transport in batteries, fouling of membranes during filtration, percolation of minerals through rocks, contaminant transport and carbon-dioxide storage as seen in oil and gas industry, flow in biological tissue, and chemical vapor infiltration. Describing transport properties such as permeability, diffusivity and conductivity in these dynamically evolving porous media is critical to fundamental understanding, design and optimization of such systems and forms the focus of the proposed study.

Several experimental studies in the past have focused on measurement of transport properties in porous media by quantifying pressure drop, species concentration and flow. Recent literature has seen increase in numerical work involving reconstruction of porous media combined with pore scale modeling to predict transport properties [1–7]. Owing to their disordered nature, pore structures can be well described by fractal dimensions that, in turn, are used to predict transport properties such as permeability, conductivity and diffusivity [8–14]. Although the properties of porous media have been explored extensively, the study of changes in pore structure and, in turn, the corresponding properties owing to deposition, erosion swelling or shrinking remains a relatively unexplored area.

Previous theoretical and experimental studies have mainly focused on determining the properties for pore structures at the beginning of deposition or erosion, followed by use of analytical models or experimental correlations to describe changes in transport properties with deposition. The few studies relating to permeability reduction have used pore scale analysis of reconstructed pore structure to characterize the transport properties. Chen et al. [6] used X-ray computed microtomography (XCMT) to construct three-dimensional (3D) geometry of the pore structure before and after colloid deposition, followed by Lattice Boltzmann (LB) simulations to evaluate change in local permeability and tortuosity. It was found that the change in permeability followed a power law variation with respect to porosity and the results significantly differed from the predictions using Kozeny-Carman relationship. Similar studies involving XCMT and LB modeling were performed by Okabe et al. [7].

The most common practice is to use the Bruggeman equation [15] that relates the effective transport properties to the porosity of the medium and a constant term denoting the tortuosity. A limitation of this description is that any two geometries (pore structure) with same porosity would exhibit similar behavior irrespective of their morphology, which is inaccurate. In the absence of a comprehensive and accurate theoretical model, researchers use experimental data to obtain a correlation between tortuosity and porosity for different pore structures. The resulting models are, therefore, correlatory and not predictive. In the case of dynamic changes in pore structures, the number of experiments increases exponentially for a comprehensive description and, in some cases, the measurements require sophisticated tools and extensive effort to effectively determine the changes in pore structure. Moreover, the use of oversimplified models that are inaccurate, or the reliance on empirical expressions that involve tuning factors or post-facto correlations of experiments do not offer a truly predictive approach to describing evolving porous media and their properties.

In this communication, we address the challenge of predicting the evolution of pore structure as a function of deposition, saturation or erosion using a fractal model. A model to predict the changes in fractal dimensions for a pore structure undergoing deposition is developed and compared with the predictions obtained from image analysis. The

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* Corresponding author.
E-mail address: pitchu@vt.edu (R. Pitchumani).

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variation in effective diffusivity is predicted with the dynamic fractal model and compared with analytical solutions from other studies.

2. Fractal model

Fig. 1 shows the microstructural image of a disordered porous medium [12], where the black regions represent the pores and the white areas denote the solid matrix formed by the agglomeration of copper particles. Owing to the randomness and presence of multiple length scales, common to a wide range of porous media encountered in practical applications, the porous medium in Fig. 1 can be represented by fractal dimensions [1–10,14]. In a fractal representation, the pore architecture is usually quantified in terms of fractal dimensions d_T and d_N, corresponding to the tortuosity and area dimensions, respectively. The porous medium in this description can be envisioned to be a distribution of tortuous capillaries of various sizes, with the effective length, L_c, of a capillary of size λ given by [8–13]:

$$L_c(\lambda) = \lambda^{1-d_T} L_0^{d_T} \tag{1}$$

where L_0 is a representative length and d_T is the tortuosity fractal dimension, such that a value of $d_T = 1$ corresponds to a straight capillary and $d_T = 2$ corresponds to a highly tortuous medium. For a complete description of the pore structure, it is essential to also quantify the number of capillary pathways corresponding to every pore size, λ. The population of the intersecting pores in a cross section exhibits the general trend that $N(L \geq \lambda)$, which denotes the total number of pores of size exceeding or equal to a value λ, increases as the pore size decreases. Hence, the cumulative pore distribution in a cross section can be represented by [8–13]: The theory of fractal dimensions and representation of porous media using these dimensions is well established and is not discussed in detail here. Readers are referred to Refs. [8–14] for a more detailed explanation.

$$N(L \geq \lambda) = \left(\frac{\lambda_{max}}{\lambda}\right)^{d_N} \tag{2}$$

The area and tortuosity dimensions can be obtained from a box-counting analysis [9,10] of the area and the perimeter of the pores, respectively, in a microstructural image of the porous structure. The results of box-counting analysis of the microstructure in Fig. 1 are presented in Fig. 2, where Fig. 2(a) describes the log-log variation of the cumulative pore distribution as a function of pore size. The negative of slope of a linear fit through the data gives the area fractal dimension, d_N (=1.76 for Fig. 1), which is representative of the cumulative pore distribution as given by Eq. (2). The value calculated by Yu and Cheng [12] for the above geometry was 1.79 considering a bi-dispersed porous media, which is very close to the value obtained here, while treating the media as mono-dispersed. Similarly, by using the box-counting method on the perimeter of the pores [9,10], the tortuosity dimension, d_T, can be obtained from the slope of a linear fit through data on a log-log plot to be d_T (=1.18 for Fig. 1), as seen in Fig. 2(b).

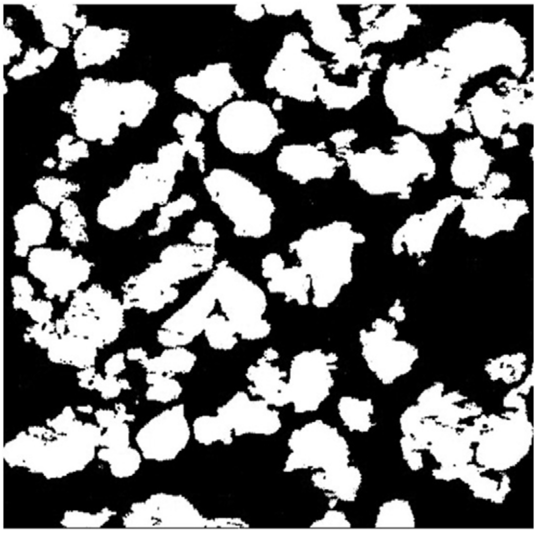

Fig. 1. Microstructure image of a disordered porous media [12].

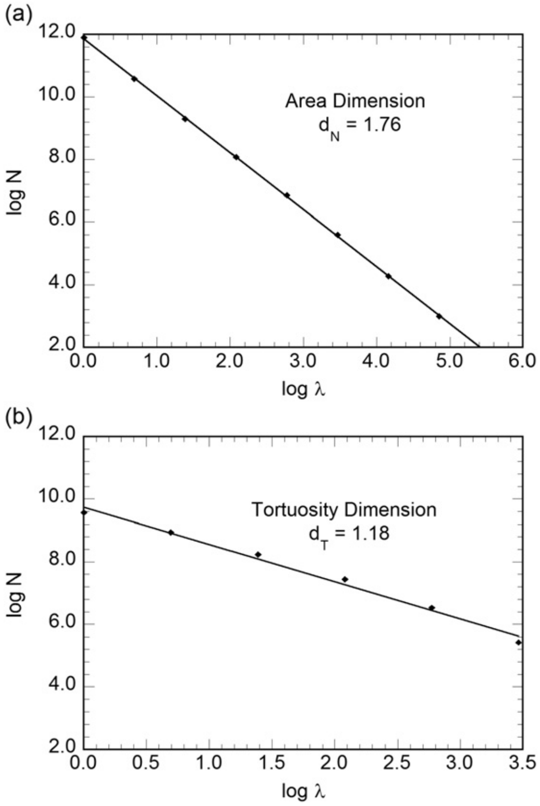

Fig. 2. Box-counting analysis for (a) area flow dimension, d_N and (b) tortuosity dimension, d_T.

3. Deposition in porous media

Based on the fractal description discussed above, the changes in pore structure as a function of saturation or deposition is modeled. Deposition (or saturation) is simulated in porous media by numerically dilating [16] the solid boundaries in the pore structure image to mimic a physical deposition in pores. Fig. 3 shows the pore structure images with different saturation values, where saturation is defined as, $s = 1 - \varepsilon^{new}/\varepsilon^0$, with ε^0 and ε^{new} as the porosity of the medium before and after deposition, respectively. The porosity and saturation values for Fig. 3(a), (b), (c) are s = 0, 0.116, 0.208 and ε = 0.575, 0.508, 0.456, respectively. The methodology to quantify changes in fractal dimensions with changes in saturation levels is discussed next.

3.1. Evaluating changes in d_N

According to Yu and Cheng [12], the area fractal dimension, d_N, can be expressed as:

$$d_N = k - \frac{\ln \varepsilon}{\ln \frac{\lambda_{min}}{\lambda_{max}}} \tag{3}$$