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Direct evaluation of length scales and structural parameters associated with flow in porous media

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We directly evaluate the flow and structural properties of three-dimensional random porous media at a microscopic level via lattice gas automata. The length scale associated with the pore structure and the geometric factor accounting for pore shape, connectivity, and tortuosity used in empirical models are *independently* measured. It is shown that the empirical models greatly underestimate the effect of the structure of the medium on flow properties. The tortuosity, in particular, is shown to have a much larger effect than accounted for by empirical models.

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I. INTRODUCTION

The hydraulic conductivity of a porous medium for single-phase fluids is expressed, by analogy with electrical conductivity, by giving the permeability k defined by the phenomenological Darcy equation written here in differential form [1]:

$$\mathbf{v} = -\frac{k}{\mu}\boldsymbol{\nabla} P, \tag{1}$$

where $\mathbf{v}$ is the volumetric flow, P the hydrostatic pressure, and μ the fluid viscosity. While the physical basis underlying the Darcy equation is well understood [2], what remains unknown is how the permeability, which is dependent only on the structure of the porous medium, can be *predicted* from other porous media properties. It is clear that the property of permeability should be linked to other properties of the porous medium—internal surface area, porosity, pore size distribution, etc.—since all such properties are manifestations of the geometrical arrangement of the pores. However, to uncover the relationships is possible only if one is able to understand exactly how all these properties are conditioned by the geometrical properties of the pore system. To date the understanding of the relationship between media properties and the permeability has been poor. A direct approach to finding relationships between the various properties of random porous media has been limited to establishing empirical relationships, often aided by dimensional analysis and theoretical considerations. Of the many different empirical approaches for the treatment of single-phase flow, hydraulic radius models [1, 3] have resulted in excellent correlations.

In hydraulic radius models the porous medium is assumed to be equivalent to a conduit, the cross section of which has an extremely complicated shape, but, on average, a constant area. The theories all make use of the fundamental observation that the permeability, in absolute units, has the dimensions of length squared. It is argued that a length should be characteristic for the permeability of a porous medium. This length is called the "hydraulic radius" R_h. In analogy with laminar flow through tubes we define the average pore or seepage velocity v_p in the flow channels by

$$v_p = \frac{\Delta P}{L_e}\frac{c{R_h}^2}{\mu}, \tag{2}$$

where L_e is the average path length for flow and c is a shape factor associated with the channel cross section. The pore velocity and the macroscopic velocity v defined in Eq. (1) are related by $v_p = \frac{v}{\phi}\frac{L_e}{L}$. The division of v by ϕ is used to define an average interstitial velocity. The multiplication by $\frac{L_e}{L}$ is a correction for the fact that a hypothetical fluid particle used in the macroscopic flow equations and flowing with the macroscopic velocity v covers a length L in the same time as an actual fluid particle flowing at velocity v_p covers the effective length L_e [4].

Combination of Eqs. (1) and (2) and Darcy's law gives

$$k = \frac{c}{(\frac{L_e}{L})^2}R_h^2\phi. \tag{3}$$

This is the basic form of all hydraulic radius theories, differing only in the method of calculating the mean square hydraulic radius and in the definition of the geometric factor $\frac{c}{(\frac{L_e}{L})^2}$. It is useful to rewrite (3) as

$$k = k_0 l^2\phi, \tag{4}$$

where l is the length scale associated with the pore structure and k_0 is the geometric factor accounting for pore shape, tortuosity, connectivity, etc. and is a function of the pore geometry only.

The problem with the hydraulic radius approach is that the *substantiation* of the empirical equation is impossible. The length scale l and the geometrical parameter k_0 have to be determined by independent means in order to perform a valid check of the theory. In principle one requires a method to determine the macroscopic flow parameters, while providing information about the local flow configuration. Lattice gas methods have been shown to be capable of solving these problems [5, 6].

In this paper we determine the flow properties of three-dimensional random porous media over a large range of porosity using lattice gas automata (LGA) [7]. The LGA solution allows the *direct* evaluation of various flow and structural properties used in empirical models based on the hydraulic radius concept. We investigate the variation with porosity of the length scale parameter l defined by the pore structure and the geometrical parameter k_0 describing the pore shape, tortuosity, and connectivity. Comparing the hydraulic radius model predictions for these parameters with the simulation data shows that the models ignore a very strong effect that pore geometry has on flow in porous media. The tortuosity, in particular, is shown to have a much larger effect than accounted for by these models.

II. IMPLEMENTATION OF THREE-DIMENSIONAL LATTICE GAS AUTOMATA

LGA are discrete analogs of molecular dynamics, in which particles with discrete velocities populate the links of a fixed array of lattice sites. The lattice gas model we use in this paper was originally proposed by D'Humières, Lallemand, and Frisch [7]. In this method a four-dimensional face-centered hypercubic lattice (FCHC) is used. A four-dimensional single-speed model is required because no three-dimensional single-speed lattice model yields a stress tensor which is isotropic to fourth order in the velocity. The FCHC is the simplest lattice to meet the required symmetry conditions. The FCHC lattice is the set of all points in the four-dimensional lattice for which the sum of coordinates is even. Each lattice site has 12 nearest neighbors a distance $\sqrt{2}$ away.

An exclusion principle is imposed so that no more than one particle at a given site can have a given momentum state. The configuration of sites evolves in a sequence of discrete time steps. There are two microscopic updating processes at each step—advection and collision. In the advection step every particle moves from its present site $\vec{x}$ to a nearest neighbor site at $\vec{x} + \vec{e}_a, a = (1,2,...,24)$. In the collision process the particles at each site are rearranged subject to the constraint of local mass and momentum conservation.

From the macroscopic transport equations for the particle distribution functions, the Navier-Stokes equation can be obtained using a Chapman-Enskog expansion [8]. The continuum fluid properties are derived from large scale averaging of the LGA solution of the transport equations. Despite the discrete nature of the method, this model is capable of exhibiting rich macroscopic complexity such as turbulence [9]. Moreover rigorous comparisons between theoretical predictions and lattice gas simulations have been reported with impressive results [10].

An important feature of the lattice gas method is that all operations are purely discrete, local, and logical—ideal for high speed simulation on parallel computers. A second feature of the method is its flexibility. In lattice gas models boundary conditions are very easy to implement. Total reflection of particles at a solid boundary simulates a macroscopic "no-slip" boundary condition; specular reflection of particles gives a macroscopic "free-slip" boundary condition. Arbitrary complex solid boundaries can be modeled by appropriate arrangements of boundary cells. The application of lattice gas method to the study of fluid flow in porous media is particularly promising because of the relative ease with which complicated boundary conditions can be implemented.

As described above, the basic operation of the lattice gas algorithm involves the two steps of collision and propagation. In the collision step, table lookup into predefined collision tables is employed to replace the bit configurations at each node on the lattice with its corresponding after-collision configuration. In the propagation step the particles at every node propagate to their corresponding nearest neighbor node. The first step, the collision phase, is implemented using table lookup. We use the table reduction algorithm of Somers and Rem [11] and implement the code on a 16K Connection Machine 2. The flow channel dimensions are 128 sites along the flow direction with a cross-sectional area 64×64. A minimum of four simulations are performed for each porosity. In each simulation the system equilibrates for 8000 steps and measurements are taken from 8000 to 10 000 steps. Local flow information (e.g., local drag measurements on obstacles) is consistently obtained within 2000 steps of measurement in the lattice gas scheme with small relative errors. To create a pressure gradient across the channel, we use a uniform forcing condition at the inlet of the channel.

A crucial consideration in the lattice gas technique is the assessment of the range of parameters in which the lattice gas solution gives a faithful representation of the hydrodynamic equations. In this respect, a crucial parameter is the size of the open pores. If the pore size is too small, then it can become comparable to the mean free path of the particles and true fluid behavior will not be obtained within the pores. The average density for our lattice gas runs was $\frac{1}{8}$, which gives a mean free path of approximately 1.4 lattice units [6]. In order that the LGA results approach the continuum limit, the mean size of obstacles must be at least twice the mean free path of the simulation [12]. We ensure therefore that the smallest cross-section area of the pores is 4×4. The random media are constructed by randomly depositing cubic obstacles with a side length of 4 lattice units within the channel. We systematically step through the lattice, randomly placing obstacles of size 4^3 with probability $1 - \phi$ within the lattice, i.e., no overlapping is allowed.

III. EVALUATION OF LENGTH SCALES AND COMPARISON WITH HYDRAULIC RADIUS THEORY

Among the hydraulic radius theories, the Kozeny theory has had much success [1]. The permeability is expressed in terms of the specific surface S_0 of the porous medium, defined as the wetted pore surface per solid (nonporous) volume of the bed, and the porosity ϕ by

$$k = (c)\left(\frac{\phi}{S_0(1-\phi)}\right)^2 \phi, \tag{5}$$

where c, the Kozeny constant, a dimensionless number approximately equal to $\frac{1}{2}$, is dependent only on the flow cross section. In the Kozeny theory, by analogy to Eq. (4), the length scale l is equivalent to the hydraulic radius, defined as $l = R_h = \frac{\phi}{S_0(1-\phi)}$, and the geometrical factor is given by $k_0 = c$. The LGA solution to the porous flow problem allows us to directly evaluate the surface property S_0. In Fig. 1 we compare the prediction of the Kozeny theory with our data. As one can see the prediction of the theory is not satisfactory.

Empirical attempts to establish correlations between properties of porous media are futile unless additional parameters are introduced. A parameter often invoked is the "tortuosity." Tortuosity is related to the fact that the actual flow path of the fluid is greater than the apparent path length across the medium. As the Kozeny equation neglects the tangential component of the velocity, the equation is extended by introducing the tortuosity Υ as an undetermined factor. This leads to the expression

$$k = (\frac{c}{\Upsilon})\left(\frac{\phi}{S_0(1-\phi)}\right)^2 \phi. \tag{6}$$

To date the tortuosity could not be directly measured. It has therefore been largely used as an additional arbitrary parameter relating the theoretically predicted permeability to the measured permeability.

Carman [4] first realized the need to introduce a geometrical parameter similar to the tortousity into the Kozeny theory. By fitting experimental data on packed beds he determined the best value of the tortuosity $\Upsilon \simeq \frac{5}{2}$. The Kozeny-Carman relation is thus given by

$$k = \left(\frac{1}{5}\right)\left(\frac{\phi}{S_0(1-\phi)}\right)^2 \phi. \tag{7}$$

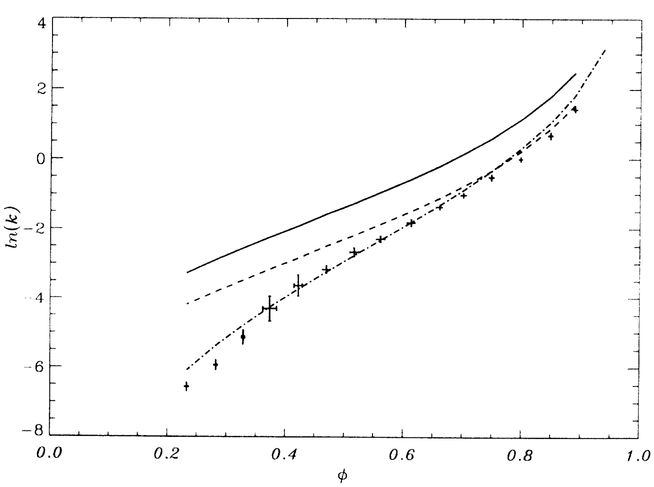

FIG. 1. The log of the permeability k of the porous media as a function of the porosity ϕ. The curves are the prediction of the empirical equations: Kozeny (——), Kozeny-Carman (- - -), and Blake-Kozeny (– · – · –).

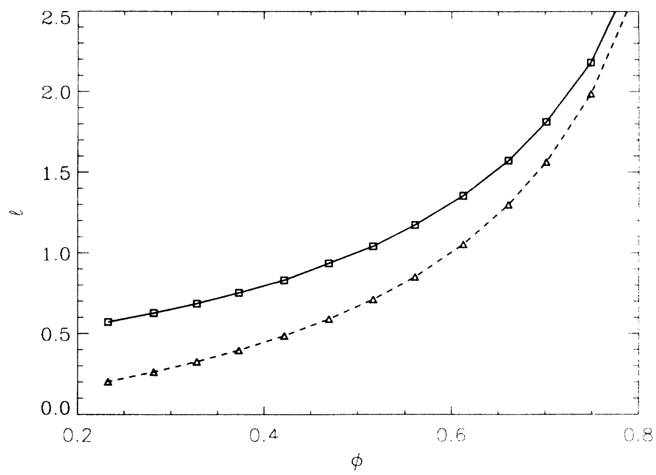

FIG. 2. Comparison of the length scale l (in lattice gas units) defined by the different empirical models plotted as a function of porosity. (□) Hydraulic radius, $l = \frac{\phi}{S_0(1-\phi)}$ and (△) $l = \frac{\phi D_p}{6(1-\phi)}$.

The prediction of the model is shown in Fig. 1. The theory is in reasonable agreement with the data at higher porosities.

An empirical equation that has resulted in excellent correlations for flow in random porous media, particularly at lower porosities, is the Blake-Kozeny equation [13]. In this model, the specific surface of the porous medium is related to the average particle size within the medium. Defining the mean particle diameter D_p as the diameter of the hypothetical sphere with the same S_0 as the medium, one can express $D_p = \frac{6}{S_0}$ [14]. This approximation, coupled with a slight change in the geometric factor k_0 to $\frac{6}{25}$ ($\Upsilon = \frac{25}{12}$), gives

$$k = \left(\frac{6}{25}\right)\left(\frac{\phi D_p}{6(1-\phi)}\right)^2 \phi. \tag{8}$$

The comparison of the prediction of the Blake-Kozeny equation with the experimental data is shown also in Fig. 1. The Blake-Kozeny equation is in *remarkable* agreement with the lattice gas results for the full range of the porosity. Only at the lowest porosities do we note a significant difference between the Blake-Kozeny model and our simulation data. The length scale l in the Blake-Kozeny model is given by $l = \frac{\phi D_p}{6(1-\phi)}$. It is difficult to justify that the length scale based on the mean particle size D_p is a more meaningful measure of the length scale of a porous media than the hydraulic radius [15]. A plot of the magnitude of the length scales defined by (5) and (8) is given in Fig. 2.

IV. DIRECT EVALUATION OF STRUCTURAL PARAMETER

The parameter k_0 in Eq. (4) accounts for the connectedness, pore shape, coordination, and tortuosity of the flow paths. The lattice gas method enables one to determine the tortuosity of a random media and thus directly measure the structure factor k_0 of the medium.

From the LGA simulations, the volumetric flow speed at each node within the pore space of the medium is known. To determine the tortuosity of the medium we record all streamlines (> 2000) crossing every lattice node along an inlet plane. We then trace the streamlines through the medium until they pass across a chosen outlet plane. The integral length L_i of the ith streamline is measured. The streamline tortuosity T_i is then defined by $T_i = \frac{L_i}{L_f}$, where L_f is the macroscopic distance between the upstream and downstream planes. The number of steps it takes to move along the streamline is recorded as t_i. As the overall *volumetric* flow varies greatly from one streamline to another, we do not define the tortuosity factor by simply averaging over the N streamlines $\sum_{i=1}^{N} T_i/N$. We choose instead to weight the streamline tortuosities by the overall volumetric flow associated with the streamline, which is proportional to t_i^{-1}. We therefore define a macroscopic tortuosity factor $T \equiv \frac{L_e}{L}$ of our random media as $T = \sum_{i=1}^{N} t_i^{-1} T_i / \sum_{i=1}^{N} t_i^{-1}$.

All of the popular hydraulic radius theories assume that the structure factor k_0 is approximately *constant* over a wide porosity range. For example, Carman determined experimentally that the *best* value for the tortuosity factor is $\frac{5}{2}$ for the range of porosity $0.90 \leq \phi \leq 0.25$ [4]. Our determination of the tortuosity factor T as a function of porosity is shown in Fig. 3. According to the definition of k_0, the tortuosity Υ of the medium should be given by T^2. We find that Υ varies from 1.0 at porosities near 0.90 up to values greater than 50 at porosities less than 0.40. Clearly the models do not correctly account for the strong effect of the structure of the medium. The quantities T and T^2 have been defined by various authors as the true tortuosity of the medium. We believe that the actual value will lie somewhere between these values [16]. We show in Fig. 4 the Kozeny theory prediction (6) with our direct determination of Υ. The introduction of either definition of Υ greatly improves the prediction of the Kozeny theory.

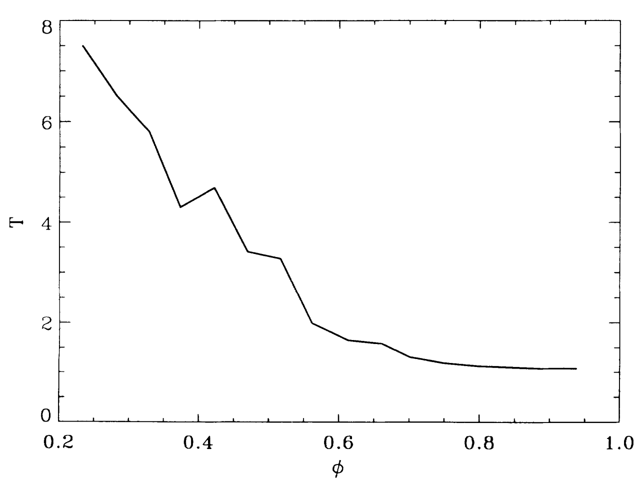

FIG. 3. The tortuosity factor $T \equiv \frac{L_e}{L}$ as a function of porosity.

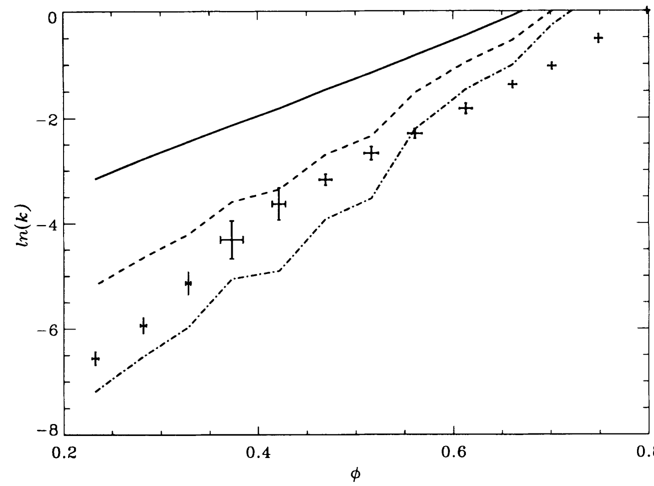

FIG. 4. Kozeny theory prediction with the two definitions of the tortuosity Υ defined in the literature. (——) The prediction of the original Kozeny theory ($\Upsilon = 1$). The two other curves show the prediction of Eq. (6) with the tortuosity Υ given by $\Upsilon = T$ (- - -) and $\Upsilon = T^2$ (- · · - · -).

In the literature there is frequent disagreement between the experimentally measured permeability of a porous sample and the permeability as predicted by the Kozeny-Carman equation. Authors often make a controversial claim that higher sample tortuosities are experienced in the experimental samples than are accounted for by theory [17]. Our results support these claims, particularly at lower porosities.

V. CONCLUSION

That the hydraulic radius concept gives a good match to the data with a correct evaluation of the tortuosity is a confirmation that this remarkably simple concept known to be a good approximation under turbulent flow conditions accurately describes creeping flow in porous media. The results of our study show, however, that the approximation used in most hydraulic radius theories, that the tortuosity can be considered approximately constant over a wide range of the porosity, is incorrect. The geometrical parameter associated with the tortuosity of the medium has a marked effect on the flow properties of porous media. The Blake-Kozeny equation, which matches the data very well, does not predict a change in the structural factor k_0 over all porosities, in clear contradiction to the results of this study. The fit of the Blake-Kozeny equation [Eq. (8)] to the data is simply fortuitous and is not due to a better understanding of the flow properties. The success of this model is due to the circumstance that the approximation $S_0 = 6/D_p$ "corrects" in the same manner as an increasing tortuosity for lower porosities and is not based on a more meaningful measure of the length scale associated with the pore structure.

Relating the permeability to other macroscopic properties of a porous medium has to date been chiefly empirical. The lattice gas method allows one to describe macroscopic flow phenomena using large-scale averaging, but, more importantly, provides microscopic detail crucial to the understanding of relationships between the volume-averaged parameters. In future work we will attempt to ascertain which parameters in the determination of macroscopic flow properties in more general porous media are most meaningful. In particular, in an extension of this work we will study the effect of particle shape and size on the permeability of unconsolidated media. In these cases the empirical models have difficulty defining meaningful parameters to characterize shape and packing structure. Finally, a critical study of the relationship between the permeability (hydraulic conductivity) of a porous medium and the electrical conductivity is currently underway.

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