Tortuous flow in porous media

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The concept of tortuosity of fluid flow in porous media is discussed. A lattice-gas cellular automaton method is applied to solve the flow of a Newtonian uncompressible fluid in a two-dimensional porous substance constructed by randomly placed rectangles of equal size and with unrestricted overlap. A clear correlation between the average tortuosity of the flow paths and the porosity of the substance has been found. [S1063-651X(96)05006-4]

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I. INTRODUCTION

A common characteristic of any material transport in porous media, such as fluid flow or electric current, is that the actual path followed by the transported material is microscopically very complicated, or ''tortuous'' [1–4] (''microscopic'' here means the size scale of the average pore size of the substance). The concept of tortuosity is often introduced in the context of solving the closure problem for transport in porous media, i.e., in deriving the macroscopic transport equations in terms of averaged quantities alone. A usual method of deducing, e.g., the appropriate form of the drag force between fluid and the solid matrix, is to use some simplified model of the porous material, such as the capillary model, and to generalize the results for more realistic materials. This generalization may be attempted by introducing an additional parameter which is supposed to take care of the more complicated transport paths neglected in the model. In fact tortuosity is an example of such a parameter. As a physical quantity, it can be defined in various ways. Perhaps the most intuitive and straightforward definition is that of the ratio of the average length of true flow paths to the length of the system in the direction of the macroscopic flux. Notice that by this definition, tortuosity depends not only on the microscopic geometry of the pores, but also on the transport mechanism under consideration.

Tortuosity could also be defined without reference to a specific transport mechanism. This could be done, for example, by considering the shortest continuous paths between any two points within the pore space [5]. The advantage of this definition is that the tortuosity parameter thus defined will exclusively characterize the porous substance itself. When considering tortuosity in the context of transport phenomena, it seems quite more natural, however, to utilize the flux associated with the actual transport mechanism in the definition of tortuosity.

Moreover, it is possible to define tortuosity even without a direct reference to the lengths of the transport paths by considering the local deviations in the direction of the microscopic flux from the direction of the mean flux. (This approach will be discussed in some detail below.)

In what follows, we shall concentrate on the concept of tortuosity associated with the flow of a Newtonian fluid through a random porous medium at a low Reynolds number. In macroscopic terms, such a flow is governed by Darcy's law which states that the average flux $\mathbf{q}$ of fluid is proportional to the gradient of the phase averaged fluid pressure p,

$$\mathbf{q} = -\frac{k}{\mu}\nabla p. \tag{1}$$

Here, μ is the dynamic viscosity of the fluid and k is the flow permeability. In this paper, we shall first discuss the possible definitions of tortuosity which appear in deriving Darcy's law in the framework of capillary models. The definition is then generalized to random porous media. We then use a lattice-gas cellular automaton method [6–8] to find a numerical correlation between the tortuosity and the porosity for a two-dimensional porous material which consists of randomly positioned freely overlapping rectangles. The advantage of using the lattice-gas methods for this purpose is their geometric versatility, which makes them very useful in simulating flows in irregular geometries [9–11]. The results obtained can be applied, e.g., in inferring correlations between the permeability coefficient and the relevant macroscopic quantities that characterize the porous substance [12]. Finding such correlations is especially important in the case of flow through soft porous materials when flow can induce a strain to the solid matrix, and thereby locally affect the value of the permeability coefficient k [13].

II. TORTUOSITY OF FLOW IN POROUS MEDIA

Darcy's law Eq. (1) can easily be derived within the simple capillary theory by Kozeny, in which the porous medium is envisaged as a layer of solid material with straight parallel tubes of a fixed cross-sectional shape intersecting the sample. Within this model, the permeability is explicitly given as $k=\phi^3/cs^2$, where ϕ is the porosity, s is the specific surface area, i.e., the pore surface area per unit volume of porous material, and c is a structural parameter that depends on the cross section of the capillaries, for cylindrical capillaries $c=2$. The simplest way to introduce tortuosity in the capillary model is to allow the tubes to be inclined in such a way that the axes of the capillaries form a fixed angle θ with the normal of the surface of the material (while the azimuthal angle of the tubes is randomly distributed). In this case permeability becomes

$$k=\frac{\phi^3}{c\tau^2 s^2}, \tag{2}$$

where the tortuosity factor $\tau=1/\cos\theta$ can be given in terms of the tube length L_e and the thickness of the medium L as

$$\tau=L_e/L. \tag{3}$$

(Some authors prefer to define tortuosity as $\tau=(L_e/L)^2$ or as the inverses of these two definitions [3,4]. In this paper, we shall use definitions analogous to Eq. (3). Thus for the tortuosity defined here $\tau\geqslant 1$.)

For flow in random porous media, one can replace the ''tube length'' L_e by the average length of the flow paths of a fluid particle through the sample. At least two possible alternatives for taking this average can be considered [3]. One may average over the actual lengths of the *flow lines themselves*, disregarding thereby the fact that fluid particles move along these flow lines at different velocities. Another way of averaging is over the lengths of the *flow lines of all fluid particles* passing through a given cross section during a given period of time. This leads to flux weighted averaging. The first alternative is suitable at least for pistonlike flows, such as molecular diffusion and electric current [3]. The latter alternative appears more natural when fluid flow in porous media is considered.

In order to gain more insight into the definition (or definitions) of tortuosity of flow in porous media, we shall also consider a solid material of thickness L, intersected by N cylindrical capillaries per unit transverse area. We assume the capillaries are straight and of equal radius R, but allow for a randomly varying angle between them and the x axis, which is perpendicular to the surfaces of the material. For the ith capillary of length L_i we define, in accordance with Eq. (3), $\tilde{\tau}_i=L_i/L$. Next, flow through the capillaries is induced by applying a pressure difference Δp across the sample. Solving the Navier-Stokes equation for each capillary separately, we can determine the average flux through the sample, with the result

$$\mathbf{q}=-\frac{\phi^3}{2s^2}\frac{\nabla p}{\mu}\frac{\frac{1}{N}\sum_{i=1}^{N}1/\tilde{\tau}_i}{\frac{1}{N}\sum_{i=1}^{N}\tilde{\tau}_i}, \tag{4}$$

where $\nabla p=(\Delta p/L)\hat{\mathbf{e}}_x$ is the phase averaged pressure gradient.

Comparison of Eq. (4) with Eqs. (1) and (2) suggests a definition for the tortuosity within this capillary model in the form

$$\tau^2=\frac{\frac{1}{N}\sum_{i=1}^{N}\tilde{\tau}_i}{\frac{1}{N}\sum_{i=1}^{N}1/\tilde{\tau}_i}. \tag{5}$$

This definition can be expressed in a form that is more suitable for generalization for random porous media by converting the sums into integrals over an arbitrary plane A which is perpendicular to the x axis (direction of the average flux). Notice first that, within the capillary model, the product of A_i, the area of the intersection of the ith tube with plane A, and the average flow velocity in the ith capillary v_i is independent of i ($v_iA_i=\pi R^4|\nabla p|/8\mu$). Using this result we find that

$$\frac{1}{N}\sum_{i=1}^{N}\tilde{\tau}_i=\frac{\sum_{i=1}^{N}\tilde{\tau}_i v_i A_i}{\sum_{i=1}^{N}v_i A_i}=\frac{\int_A\tilde{\tau}v\,dA}{\int_A v\,dA}. \tag{6}$$

Here, $v=|\mathbf{v}(\mathbf{r})|$ is the tangential velocity of the fluid at point $\mathbf{r}$, and $\tilde{\tau}=\tilde{\tau}(\mathbf{r})$ is the ratio of the length of the flow line passing through the point $\mathbf{r}$ to the thickness of the sample [$\tilde{\tau}(\mathbf{r})$ and v are defined to be zero inside the solid phase]. A similar result is valid for the sum containing $1/\tilde{\tau}_i$. This suggests the following definitions,

$$\tau_1=\frac{\int_A\tilde{\tau}v\,dA}{\int_A v\,dA}=\frac{\int_V\tilde{\tau}v\,dV}{\int_V v\,dV}, \tag{7}$$

$$1/\tau_{-1}=\frac{\int_A\frac{1}{\tilde{\tau}}v\,dA}{\int_A v\,dA}=\frac{\int_V\frac{1}{\tilde{\tau}}v\,dV}{\int_V v\,dV}, \tag{8}$$

where V is the volume of the porous sample. The latter forms of Eqs. (7) and (8) follow from the fact that surface integrals do not depend on the position (x coordinate) of surface A inside the sample. The tortuosity factor as determined from Eq. (7) can be interpreted as the average of the relative lengths of the flow lines of all fluid elements (with a fixed volume) passing through a given cross section during a given period of time. The latter definition Eq. (8) corresponds to the average of inverse lengths of the same flow lines. The tortuosity factor (5) appearing in Darcy's law Eq. (4) can now be expressed in a generalized form which is applicable in random porous materials,

$$\tau^2=\tau_1\tau_{-1}. \tag{9}$$

Equations (7) through (9) do not, however, provide the only way of generalizing the results of the capillary model to the random media. For example, in the case of capillary systems, the tortuosity factor τ_{-1} of Eq. (8) is in fact equal to the ratio

$$\tau_v\equiv\frac{\langle|\mathbf{v}|\rangle}{\langle v_x\rangle}, \tag{10}$$

where $|\mathbf{v}|$ is the absolute value of the local flow velocity, v_x is the x component of that velocity, and $\langle\ \rangle$ denotes the spatial average over the pore space. Notice that Eq. (10) is reminiscent of the hypothesis made by Carman in Ref. [1] that $L_e/L=V/\overline{u_e}$, where V is the average tangential velocity in a tortuous capillary, L_e is the length of that capillary, $\overline{u_e}$ is the mean value of the projection of flow velocity on the straight line connecting the two ends of the capillary, and L is the length of that line. According to Eq. (10), τ_v is solely determined by fluctuations of the local flow field around the direction of the average flux, and has no direct connection with the length of the actual flow paths. In deriving the above results, we have assumed that the radius of the capil-

laries is fixed while their lengths may vary. The results are, however, valid also in the case of varying capillary radii, provided that these and the lengths of the capillaries are uncorrelated.

Yet another possibility, which may be encountered in other kinds of models, is to define the tortuosity as an average of the lengths of flow lines squared [3,4]. Analogously to Eqs. (7) and (8), we may then define

$$(\tau_2)^2=\frac{\int_V v\,\tilde{\tau}^{\,2}dV}{\int_V v\,dV}, \tag{11}$$

$$\frac{1}{(\tau_{-2})^2}=\frac{\int_V v\,\frac{1}{\tilde{\tau}^{\,2}}\,dV}{\int_V v\,dV}. \tag{12}$$

At this point, we shall not try to select a preferred definition of tortuosity among the ones discussed above. Instead, we will use the lattice-gas word-cellular automaton method to find numerical correlations between these tortuosity factors and the porosity of a two-dimensional random porous medium. In a forthcoming publication, these results will be used to find correlations between the flow permeability and the macroscopic characteristics of the medium [12].

III. LATTICE-GAS SIMULATIONS

We solved numerically the two-dimensional flow in a random porous medium using the FHP-III lattice-gas model [6] in a discrete triangular mesh of 100×100 lattice sites. The two-dimensional porous medium was constructed by random positioning of rectangles of an equal size of 10×10 lattice sites and with unrestricted overlap. The porosity ϕ of the medium was defined as the ratio of the number of unoccupied sites to the number of all lattice sites. The number of rectangles K in the lattice varied between 10 and 68, which corresponds to porosities ranging from 0.9 to 0.5. (It is straightforward to show that, with the numbers given above, the expectation value of the porosity for a given K is $\langle\phi\rangle=0.99^K$.) The number of fluid particles per lattice site was 3.5 which provides the best approximation for the solution of the linearized Navier-Stokes equation (creeping flow) within the present method [6]. The fluid was forced to move in the positive x direction by applying an external force on the particles [7]. Periodic boundary conditions were imposed on the lattice in both directions.

Simulations were carried out for about 35 configurations for each K, and the total number of different configurations was 1080. A single configuration used about 2.2 hours CPU time on a Dec 3000 workstation. For each configuration the system was first allowed to saturate for 40 000 time steps which was found to yield a stationary flow pattern. The local velocities of particles were then averaged over 400 000 time steps in order to ensure an undisturbed and smooth flow velocity field. Flow lines starting from randomly chosen places $\mathbf{r}_i$ in the pore space were found by interpolating the time-averaged flow velocity field. The length $L(\mathbf{r}_i)$ of each flow line (within one length period in the direction x) was then computed and the tortuosity τ_1, e.g., was calculated using the following approximation for the volume integral of Eq. (7),

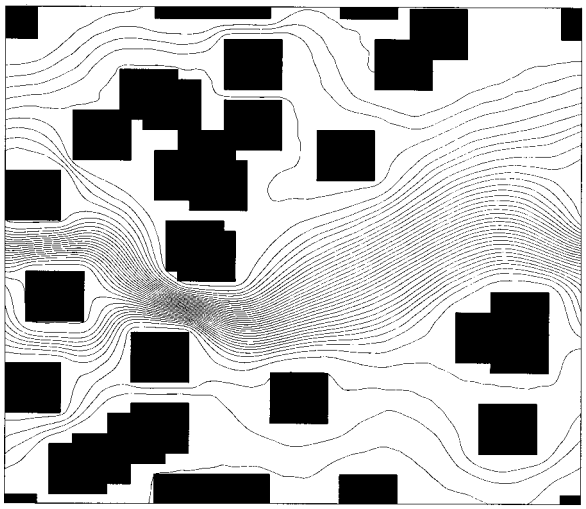

FIG. 1. Flow lines through a two-dimensional random porous medium.

$$\tau_1\approx\frac{\sum_{i=1}^{N}\tilde{\tau}(\mathbf{r}_i)v(\mathbf{r}_i)}{\sum_{i=1}^{N}v(\mathbf{r}_i)}. \tag{13}$$

Here, $N=1000$ is the number of flow lines found for each configuration, $\tilde{\tau}(\mathbf{r}_i)=L(\mathbf{r}_i)/L_x$ is the tortuosity of the ith flow line, L_x is the length of the lattice in the x direction, and $v(\mathbf{r}_i)$ is the averaged tangential velocity of the fluid at the starting point. Tortuosities τ_{-1}, τ_2 and τ_{-2} were determined using expressions similar to Eq. (13), while τ_v was determined directly from the averaged velocity field according to Eq. (10).

In Fig. 1 we show an example of the flow line fields for a configuration of 30 rectangles corresponding to a porosity $\phi=0.74$. The vertical distances between the flow lines of this figure are determined such that the flux between neighboring flow lines is constant. The tortuosity τ, as determined from Eq. (9), is $\tau=1.2$ for this particular configuration. The values of tortuosities τ_1 and τ_{-1} [see Eqs. (7) and (8)] were found to be very close to each other (see Fig. 3). In Fig. 2 we show the calculated tortuosity $\tau=\sqrt{\tau_1\tau_{-1}}$ as a function of porosity ϕ. The small dots give the values of ϕ and τ for the 1080 individual configurations. The large dots with error bars show the mean value and the standard deviation of τ and ϕ at each value of K. Within the porosity range covered by these simulations, the dependence on porosity of tortuosity τ is approximately linear. The solid line shown in Fig. 2 is a fit by

$$\tau=0.8(1-\phi)+1. \tag{14}$$

In Fig. 3 we compare the simulated values of the tortuosities defined by Eqs. (7)–(12). The curves shown in this figure are fits to the determined points which are not shown. For τ_v the fit is parabolic while for the other tortuosities it is linear. It is evident that the different definitions give approximately the same qualitative dependence on porosity, and that the numerical values do not dramatically differ from each

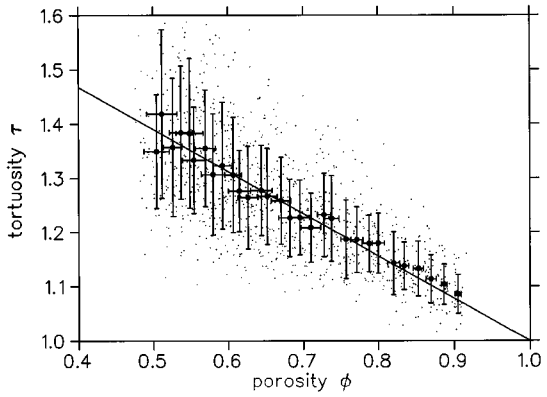

FIG. 2. The calculated tortuosity τ [see Eq. (9)] as a function of porosity ϕ. Small dots are the results of numerical solutions for 1080 individual configurations equivalent to that shown in Fig. 1. Large symbols with error bars indicate the mean values and standard deviations of porosity and tortuosity for each fixed number of solid blocks.

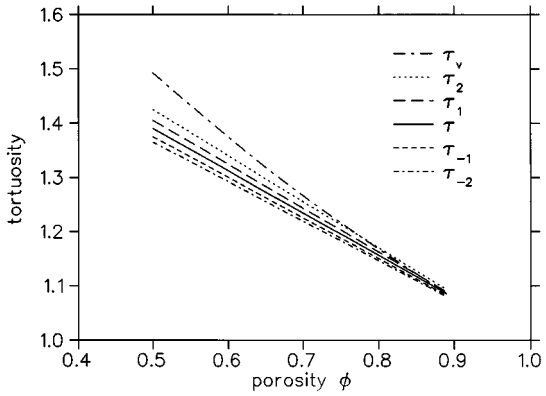

FIG. 3. Comparison of tortuosity factors defined by Eqs. (7)–(12).

other in this porosity range. Notice finally that the presented results are in full agreement with an approximate upper limit of tortuosity 1.6 which follows from a model of randomly oriented connected straight tubes [3,4] in two dimensions.

IV. DISCUSSION

We have used the lattice-gas simulation method for solving a low Reynolds number flow in a two-dimensional matrix formed by randomly placed fully overlapping rectangles. Numerical uncertainties were found to be reasonably small provided that long enough simulation and averaging times were used to ensure stationary states and smooth velocity profiles. For a given obstacle configuration the tortuosities calculated with different lattice resolutions were always found to be close to each other, and no systematic resolution effects were seen.

In some cases the procedure for finding a flow line passing a given starting point failed since the flow line hit a solid wall. The contribution from such flow lines was neglected. (See, e.g., the second flow line from the top in Fig. 1). Such cases were most frequently found in blocked areas where the residual fluctuating component of the velocity was relatively large as compared to the averaged flow velocity. The total flux associated with the failed flow lines and thus their total weight in the tortuosity equations was however small. Making a conservative assumption that the true lengths of the failed flow lines would differ by at most 30% from those of the successful flow lines, the error caused by this and other numerical uncertainties was estimated to be below 5%, even at the lowest porosities where failing of flow lines was most pronounced.

It is evident that, as a physical quantity, tortuosity is not uniquely defined. The preferred definition depends on the context and on the model being used. Our simulations suggest, however, that the model dependence is quite small, at least for a two-dimensional flow at relatively high porosities. Usually the purpose of introducing tortuosity, as a parameter in macroscopic theories dealing with transport in porous media, is to add an additional degree of freedom to account for the rather complex structure of real porous materials. As such, tortuosity can hardly be expected to provide more than a qualitative description of the true transport dynamics in these complex structures. The smallness of the differences between the numerical values of this quantity, arising from its various plausible definitions, seems to indicate that tortuosity indeed is a useful concept.

The determined interrelation Eq. (14) of porosity and tortuosity can be applied, e.g., in inferring relations between permeability and porosity [12]. The basic limitation in doing this is that the present simulations are two dimensional. For a three-dimensional flow around nonelongated particles, the relation between tortuosity and porosity may not be of the same form as for two-dimensional objects considered here. Also, two dimensionality restricts the useful configurations to those with quite a high porosity. This is due to the percolation threshold, which is approximately at $\phi=0.33$ for randomly placed and freely overlapping obstacles (whose length to width ratio is approximately 1) in two dimensions [14]. Close to this porosity, simulations with the present method fail. We therefore expect that the results shown here will be most directly applicable to flow in fibrous porous media with a high porosity.

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