Numerical evaluation of the permeability and the Kozeny constant for two types of porous media

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Using the lattice-Boltzmann method we have calculated the permeability of a random array of spheres and a clay soil. We have determined the structure of the clay soil by computed tomography imaging. As observed experimentally, the semiempirical Carman-Kozeny equation gives a good estimate for the permeability of the random array of spheres. For the soil sample, our calculated value of the permeability is consistent with experimental values. The Carman-Kozeny equation provides a much less successful estimate for the permeability of the soil than the random spheres.

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INTRODUCTION

The quantitative prediction of the flow of viscous fluids through microscopically disordered porous media is important for many problems in science and technology. For instance, knowledge of flow through a porous material is required for a good understanding of problems of oil recovery, the flow of groundwater, and the sedimentation of polymers. Here we present a study of another problem of considerable importance: the saturated flow of water in soil. To be suitable for agricultural use the soil must have sufficiently high permeability to prevent waterlogging. It must also have a sufficiently low permeability to retain moisture and thus permit plant growth. A starting point for studying these systems is Darcy's law [1], which says that as long as we consider saturated flow at a low Reynolds number, the mean flow rate $\langle u \rangle$ of a viscous fluid through a porous medium of length L is proportional to the applied pressure difference ΔP and inversely proportional to the viscosity η. The permeability k is the constant of proportionality, so

$$\langle u \rangle = \frac{k}{\eta} \frac{\Delta P}{L} . \tag{1}$$

For Darcy's law to be of quantitative value we need to know a value for the permeability. An examination of Eq. (1) shows that the permeability has units of length squared. On the reasonable assumption that this length will be something typical of the system under study, it is clear that permeability is a quantity that can vary hugely: from the order of millimeters squared for a gravel to values of order 10^{-14} mm^2 for a granite [2]. In principle, computing the permeability of a given medium is straightforward; if one knows the structure of the medium, it is possible to solve the Navier-Stokes equations, which describe fluid flow through the medium. Having determined the steady-state velocity field for a given pressure gradient one then has the mean flow velocity and hence the permeability. Unfortunately neither of these two steps is necessarily easy. Most porous media of practical interest have extremely complex three-dimensional geometries that are difficult to determine in detail. Given that some way can be found of determining the geometry of the solid matrix, solving the Navier-Stokes equations in the presence of highly irregular solid-fluid boundaries has proved to be a nontrivial problem. Our aim here is to describe the results of numerical evaluations of k obtained by solving directly for the flow in a realistic representation of a porous medium. To place this work in context we begin by discussing other approaches that have been applied to the problem, all of which fall short of a complete determination of the matrix geometry and flow fields.

One possible approach is to apply the simple Carman-Kozeny equation [3]. This equation is based on a simple scaling argument. It relates the permeability to the surface area per unit volume S and the solid volume fraction ϕ as

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$$k = \frac{1}{c_0} \frac{(1-\phi)^3}{S^2} , \quad (2)$$

where c_0 is a constant generally given the value $c_0 = 5$. The reason we refer to this equation as the "simple" Carman-Kozeny equation is because the quantity S could be considered to be some appropriate length scale, which we have then defined to be the specific surface area. This definition is of course neither unique nor necessarily the most appropriate [18]. It is, however, particularly convenient because the problem of calculating k now reduces to determining S and ϕ. Both of these quantities can be measured from an image of a porous media (or by other experimental methods). In principle this is very useful because it removes the necessity of solving for the fluid flow through the medium. Unfortunately Eq. (2) applies only under certain circumstances. Philipse *et al.* have shown that Eq. (2) is valid for random packings of spheres, both monodisperse [4] and bidisperse [5]. Equation (2) also predicts the permeability of periodic arrays of spheres to within 15% at high values of ϕ [6]. Lemaitre and Adler [7] compared values of the permeability calculated from the simple Carman-Kozeny equation with values they obtained by solving numerically for the flow through various fractal porous media. The porous media themselves were generated by computer. They again found that the simple Carman-Kozeny equation gave reasonable results at high values of ϕ.

There is, then, evidence in the literature that Eq. (2) can be used to calculate k. The problem is that one can easily show that there are circumstances in which the simple Carman-Kozeny equation cannot be correct. For instance, it takes no account of connectivity. A porous medium that has no connected path of free space still has some permeability, according to Eq. (2). Of course its permeability is actually zero. A second objection one can raise is that the value of the specific surface area can be increased by making the solid surface progressively more complex. The simple Carman-Kozeny equation predicts a corresponding decrease in the permeability. However, if a second porous medium can be constructed from another, purely by the removal of some material, the permeability of this second medium cannot be lower than that of the first [8]. Again, in this respect the simple Carman-Kozeny equation is demonstrably wrong. This latter consideration has been discussed by Berryman and Blair [9]. The solid surface of a porous medium is typically complex, often fractal in nature [10,11]. If we analyze a high resolution image, they suggest that the measured value of S will be too high to use in Eq. (2). An appropriate value of S is derived from a more coarse grained image, which effectively blurs out unwanted surface detail and provides a value of S appropriate for use in Eq. (2). An alternative route for extracting the permeability of a porous medium from its image is that applied by Koplik and Lasseter [12]. They took serial sections of a sandstone and constructed an equivalent random network of the pore space. Using an effective-medium approximation they then calculated values of k. These, however, differed from measured values by an order of magnitude. A similar calculation performed by Doyen [13] gave results in better agreement with experiment.

An alternative approach to calculating the permeability is to approximate the geometry of the pore space as a collection of objects for which the solution to the Navier-Stokes equations is known, typically tubes. This approach has been applied by Bryant *et al.* [14,15]. They constructed a tube model of a random packing of ballbearings. Solving for the permeability of the resulting network they obtained good agreement with experimental values (and were also able to extend the calculation to the case of unsaturated flow). However, as we noted above, the simple Carman-Kozeny equation is valid for this type of system. The pore space is connected and the surface of the spheres is smooth, so neither of the two principal objections apply. Thus obtaining the correct value of k only involves specifying S and ϕ correctly. There is no guarantee that the flow itself is accurately reproduced or that the method will apply to more complex geometries. The most extensive calculations of permeability obtained by solving the Navier-Stokes equations for a statistically representative porous medium have been performed by Adler *et al.* [16,17]. They calculated k values for computer generated fractal porous media and model sandstones. As mentioned above, they showed, somewhat surprisingly, that the simple Carman-Kozeny equation yielded good agreement with numerical values for the fractal medium. For their model sandstone the results differed from experimental values by a factor of 5. Schwartz *et al.* [18] solved directly for the flow in a number of model sphere packings. They compared their numerical values for the permeability with values obtained from the simple Carman-Kozeny equation. They also compared their results with theoretical predictions obtained using other definitions of the length scale proposed in the literature. The simple Carman-Kozeny equation, where the length scale is the specific surface area, was found to perform rather poorly when compared to other methods.

In conclusion, there are several methods of attempting to calculate the permeability of porous media that fall short of determining the detailed structure and then solving for the flow. These basically fall into two categories: either simplifying the geometry and then solving for the flow of the fluid or taking a realistic geometry and then using a simplified technique for solving for the flow. These approaches have been applied with varying degrees of success. However, it is not obvious that any of these approaches will work under all circumstances. Using modern techniques it is possible to use the more direct approach of solving directly for the flow in a realistic representation of the geometry [19,18] and thus avoid some of the uncertainty associated with other approaches. We illustrate this by presenting values of k determined numerically for random arrays of spheres and a sample of a clay soil. We also wish to establish the validity, or otherwise, of the simple Carman-Kozeny equation for the two random media. For the random spheres we may expect that the equation does rather well, but for the soil sample with its much more complex topology, it is not clear that the simple Carman-Kozeny approach is valid.

NUMERICAL EVALUATION OF THE PERMEABILITY

In order to solve the Navier-Stokes equations we use a technique based on the lattice-Boltzmann equation. The details of this approach are well documented elsewhere [20,23]. Here we offer a brief summary in which we focus on what we consider to be the advantages of applying this technique to our problem. The basic idea of the lattice-Boltzmann scheme is to simulate a lattice gas [24] at the ensemble averaged level. A lattice gas consists of a system of particles confined to move on a lattice. In the Boltzmann approximation, the motion of individual particles in the lattice gas is regarded as uncorrelated and the quantity propagated is the ensemble averaged occupancy $f_i(\mathbf{r},t)$. The following equation governs the time evolution of $f_i(\mathbf{r},t)$:

$$f_i(\mathbf{r},t+1) = f_i(\mathbf{r},t) + \Delta_i(f(\mathbf{r},t)) \ , \tag{3}$$

where the collision term Δ_i is a function of only the input state. If the collision term is specified correctly then the local fluid velocity $\mathbf{u}(\mathbf{r})$ and the density $\rho(\mathbf{r})$ are solutions of the Navier-Stokes equations. These quantities are moments of the distribution, defined as

$$\rho(\mathbf{r},t) = \sum_i f_i(\mathbf{r},t) \ , \tag{4}$$

$$\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) = \sum_i f_i(\mathbf{r},t)\mathbf{c}_i \ , \tag{5}$$

where $\mathbf{c}_i$ is the particle velocity. The specific form of the collision term used in this work has been given by Ladd [20]. Stick boundary conditions at the solid-fluid interface are imposed by a simple bounce-back rule; for any boundary link f_i is reflected at half integer times. A boundary link is defined as being a link connecting a node inside the solid matrix to a node in the fluid. Using this procedure we nominally locate the boundary as being halfway along a lattice link.

The suggestion has often been made in the literature that lattice-gas and lattice-Boltzmann equation techniques should be powerful tools for studying flow in porous media [21,22] because the complexity of the calculation is effectively independent of the complexity of the matrix. As with all numerical techniques, the accuracy of the solution that we obtain is limited by the resolution of the grid used. However, the lattice-Boltzmann scheme is also advantageous in that even with a very crude lattice, where some areas of free space in the system consist of only a handful of lattice nodes, quantitatively significant numbers are still produced. We illustrate this in Table I, where we have tabulated the mean flow velocity in a tube, calculated using the lattice Boltzmann method, as a function of the number of lattice nodes making up a tube radius R. To get good accuracy the free space in the system must indeed be represented by several nodes ($R \approx 2.5$). However, even with just one node we reproduce the Poiseuille result to within 35%.

TABLE I. Ratio of the calculated mean flow velocity $\langle u \rangle$ and the Poiseuille result $\langle u \rangle_P$ for cylindrical tubes of radius R (in lattice units).

R	$\langle u \rangle / \langle u \rangle_P$
0.5	1.35
1.5	1.42
2.5	1.05
3.5	0.98
4.5	1.04
5.5	1.02

In order to perform the calculation we need a map of free space and solid matrix from which to compile a list of boundary links. For the random array of spheres we have used configurations generated by an isobaric Monte Carlo simulation of an initially random configuration of hard spheres, using periodic boundary conditions. For the soil sample we read the solid-matrix map directly from a segmented computed tomography (CT) image. The image is that of a cylindrical sample, with radius 12.3 cm, of a young marine clay soil, sampled in the field at a depth of 15–40 cm. 150 adjacent scans were taken, starting 5 cm below the top and finishing 5 cm above the bottom. The spacial resolution was $0.27 \times 0.27 \times 1.0$ mm^3 and the images were reduced in size from 512^2 to 452^2 pixels so as to only contain the soil region. Before the image segmentation a 3×3 uniform filter per slice was used, to remove noise, followed by a Sobel filter for edge enhancement. The image was segmented into regions of free space and solid, based on the gray values in the original CT image. The high contrast difference between air and clay allowed us to work directly with the bimodal gray value distribution and segmentation was done by a global thresholding technique. The bimodal gray value distribution of the object and background densities were approximated by two Gaussian distributions. A threshold value equal to the mean gray value of the pore network minus three standard deviations (of the pore network) was used. Full details of the experiment and image processing are given by Heijs *et al.* [25]. Having obtained the segmented image, a cluster analysis was performed to identify connected clusters, which we then consider to make up the pore network. The data were found to contain only one continuous pore network connecting the top and bottom of the sample. It is on this single connected pore that we perform the flow calculation. This type of soil typically has a free volume fraction of about 40%. The segmented CT image, however, has a free volume fraction of only 12%. We can therefore estimate that $\approx$ 28% of the total free space consists of pores with a length scale smaller than our spacial resolution. Of the $\approx$ 12% of free space that we do identify, about one-quarter belongs to the connected pore. So, for the purposes of our calculation, the fluid flow through the sample occurs in only $\approx$ 4% of the total volume. We assume that the remainder does not contribute to the permeability either because it is disconnected or because the local perme-

ability is negligible. In order to mimic a pore structure percolating through an infinite medium, the simulation box is repeated periodically using *anti*periodic boundary conditions. Antiperiodic (rather than periodic) boundary conditions are needed to ensure that a pore is always continued in the adjacent box.

In order to vary the image resolution we form larger volume elements from the image by computing the free volume present in N^3 cubes. If this quantity exceeds one-half of the volume of the new cube it is treated as free space. Using this procedure we can lower the resolution to $N = 4$ before we lose the connectivity of the pore network. We also define a second resolution n, which indicates that an $n \times n \times n$ cube of nodes is used in the lattice-Boltzmann simulation to represent each cube of merged volume elements. While changing the value of N effectively changes the detailed representation of the medium, changing the value of n leaves the structure unchanged, but affects the accuracy of the permeability calculation.

RESULTS FOR THE RANDOM PACKING OF SPHERES

The random packing of spheres we used consists of 1000 spheres at a solid volume fraction $\phi = 0.6$. This system size is large enough to effectively eliminate the effects of the periodic boundary conditions [26]. We have calculated the permeability as a function of the number of lattice nodes making up a sphere radius. If we substitute the value of S for an assembly of nonoverlapping spheres with radius r into Eq. (2) we have

$$k(\phi) = \frac{(1-\phi)^3}{9c_0\phi^2} r^2 \ . \tag{6}$$

In Table II we tabulate the values of the Kozeny-constant c_0, which we have calculated using Eq. (6). The values for k were determined using spheres of radii 2.5, 3.5, and 4.5 lattice units. There are two points to note from these results. First, the result for the smallest representation of the sphere only differs from the result for the largest by some 30%. The values that we obtain for sphere radii of 3.5 and 4.5 differ only 5%. We therefore estimate that the result for the sphere of radius 4.5 lies within approximately 5% of the true value. As was the case for Poiseuille flow, unless a high accuracy is required, a relatively crude representation of the solid-fluid interface appears to suffice. Second, the best value we obtain is consistent with the experimental observation of Philipse and Pathmamanoharan [4], who found that the permeability of a dense colloidal hard sphere packing was given, to within the experimental errors, by the simple Carman-Kozeny equation with $c_0 = 5$. In a further (more accurate) study of bidisperse packings of spheres Thies-Weesie and Philipse calculated a value of $c_0 = 3.9 \pm 0.4$, independent of the fraction of small spheres [5]. Our result $c_0 = 3.8$ is consistent with this value, so both experiment and simulation suggest a small, but statistically significant, deviation of the Kozeny constant from a value of 5.

TABLE II. Values of the Kozeny constant c_0 for the random pack of spheres, as a function of the sphere radius (in lattice units).

R	c_0
2.5	2.79
3.5	3.62
4.5	3.80

RESULTS FOR THE SOIL SAMPLE

A visualization of the connected pore, present in the soil sample, is shown in Fig. 1. The soil sample is interesting not just because it is of practical importance, but also in that it represents a rather different type of porous medium than the random spheres. Whereas the free space in the random spheres can be thought of as a set of simple connected void spaces (a fact exploited in many of the techniques for calculating the permeability described earlier), here we have a single, but highly complex, void space. The values of k that we have calculated for the soil sample, using various values of N and n, are tabulated in Table III. Doubling the resolution of the lattice (indicated by the value $n = 2$), while leaving the image resolution unchanged, produces a change in the calculated value of k of about 20% (see Table III). For the higher resolution values (smaller N) the error should be smaller because, by definition, we have more nodes representing the areas of free space in the system. We therefore estimate an upper limit of 20% on the errors associated with the k values calculated at $N = 2$ and $N = 1$. We wish to stress that these are estimates of the error associated with the calculation of k for a particular representation of the pore structure. There is also an error in our calculated value of k that is due to the fact that the CT image itself is an approximate representation of the true pore structure. This error is more difficult to estimate and we have to assume that the resolution of the CT image is sufficiently high for this error to be small. In addition, it has not proved possible to perform the calculation on the full image at a resolution of $N = 1$. Instead we have calculated k separately for four sections, each consisting of one-quarter of the full data set. We have also performed this procedure for the $N = 2$ case, where we can perform the calculation on the entire data set for comparison. We see from the $N = 2$ data that the permeability of the entire sample differs by less than 30% from the average of the values for the four separate sections. Although there is no reason to assume that this is the case in general, it appears to be a reasonable approximation here. We believe our best estimate for the permeability to be the value we obtain by averaging the four values obtained for $N = 1$, that is, $k = 1.5 \times 10^{-4}$ mm^2. This compares with an experimental value [27] for this type of soil of $k = 0.7 \times 10^{-4}$ mm^2. There is, however, a considerable experimental uncertainty associated with this value [28]. We note from the fact that the calculated permeability decreases as we go from the $N = 2$ to the

TABLE III. Values for the permeability of the soil sample (mm^2). The value of N indicates the size of the N^3 cube of volume elements merged. The value of n indicates that an $n \times n \times n$ cube was used in the lattice-Boltzmann calculation to represent each (merged) volume element in the image. The subscript z_{all} indicates that the calculation was performed on the full data set. The subscripts z_1 (top), z_2, z_3, and z_4 (bottom) indicate results obtained for subsamples consisting of successive slabs of one-quarter of the full data set. $k_{\langle z \rangle}$ is the average of the permeability obtained for these four slabs.

N	$k_{z_{all}}$ n=1	$k_{z_{all}}$ n=2	k_{z_1} n=1	k_{z_2} n=1	k_{z_3} n=1	k_{z_4} n=1	$k_{\langle z \rangle}$ n=1
4	4.6×10^{-4}	3.8×10^{-4}					
2	2.0×10^{-4}		1.8×10^{-4}	1.6×10^{-4}	1.0×10^{-4}	4.5×10^{-4}	2.2×10^{-4}
1			1.3×10^{-4}	1.0×10^{-4}	0.5×10^{-5}	3.2×10^{-4}	1.5×10^{-4}

$N = 1$ resolution that if we could solve for the flow in an even higher resolution image, we would be likely to see a further decrease in the permeability. This suggests that our calculated value lies on the high side of the true value. On the other hand, our assumption that flow only occurs in the connected pore, when in reality there is also a contribution due to flow in pores that is too small to be detected in the CT scan, would result in an underestimate of the permeability. Despite this uncertainty, we can at least conclude that our value for the permeability is in general terms consistent with the experimental value. In Fig. 1 we illustrate the flow fields, along with the pore structure. The figure illustrates the complexity of the pore structure and gives an indication of the principal path by which the fluid flows through the pore (red vectors). In areas of the pore that lie away from this path there is very little flow, indicated by the blue and purple vectors.

In Table IV we list values of the Kozeny constant. These are calculated by using the values of k calculated from the lattice Boltzmann simulation (Table III) and values of ϕ and S calculated from the image. We see that, unlike the case of the random spheres, the value of the Kozeny constant is nowhere near the commonly assigned value of 5. It is much smaller and a strong function of the image resolution. We believe that this behavior illustrates the point raised by Berryman and Blair [9], namely, that the specific surface area obtained from a high resolution image is not valid input to the simple Carman-Kozeny equation. We would also like to point out that our Carman-Kozeny calculation is more sophisticated than may be typical. By this we mean that we have already corrected for problems associated with the connectivity. We have applied the simple Carman-Kozeny equation only to the connected pore. If we did not do this (as would be the case if, for instance, we had analyzed a series of two-dimensional images) the values of the Kozeny constant would have been even lower by another factor of 4. As we discussed above, at any given value of the image resolution N we estimate an upper limit on the error in k of 20%. This then suggests that the variation in the value of k that we observe at different image resolutions is primarily a consequence of small differences in the detailed representation of the medium. It appears that the detailed structure of the pore, which we include at the higher resolutions, is still influencing the value of the permeability. The fact that the detailed structure of the pore is still affecting the permeability, but that the simple Carman-Kozeny equation is already incorrect, suggests that for this type of structure the idea of an "appropriate resolution" is not valid. From this we conclude that the specific surface area cannot be considered to be an appropriate length scale, regardless of the resolution, and that the simple Carman-Kozeny equation is inappropriate for this type of porous medium.

TABLE IV. Values of the Kozeny constant as a function of the image resolution. For $N = 4$ and $N = 2$ the k value obtained for the full data has been used. For $N = 1$ we have used a value of k obtained by averaging the results for the four successive slabs. We also tabulate the values of the free volume fraction $1 - \phi$ and the specific surface area S (mm) calculated from the image.

N	$1 - \phi$	S	c_0
4	0.038	0.28	1.46
2	0.038	0.61	0.74
1	0.038	1.07	0.32

DISCUSSION

We have used the lattice-Boltzmann equation technique to calculate the the permeability of a random array of spheres. For this relatively simple system, good experimental values of the permeability are available and our calculation reproduces these results satisfactorally. Both numerical and experimental results show that the simple Carman-Kozeny equation gives a good estimate of the permeability, although a statistically significant difference exists.

Having determined the structure of a soil sample by CT imaging, we have applied the same technique to calculate the permeability of the soil. We made the additional assumption that fluid flow occurs through the only continuous connected pore found in the sample and that flow occurring at a smaller scale is negligible. This meant that we only allowed the fluid to flow in a small fraction of the total amount of the free space identified in the sample. By varying the resolution of the image we found that the permeability depended on the detailed structure of the pore. Our best estimate of the permeability (ob-

tained at the highest resolution) was, however, consistent with an experimental value for this type of soil. When we applied the simple Carman-Kozeny equation to the pore image we found that it gave rather poor agreement with the numerical values for the permeability and that this discrepancy increased with increasing image resolution. The fact that the resolution was affecting the numerical value for the permeability, but that the simple Carman-

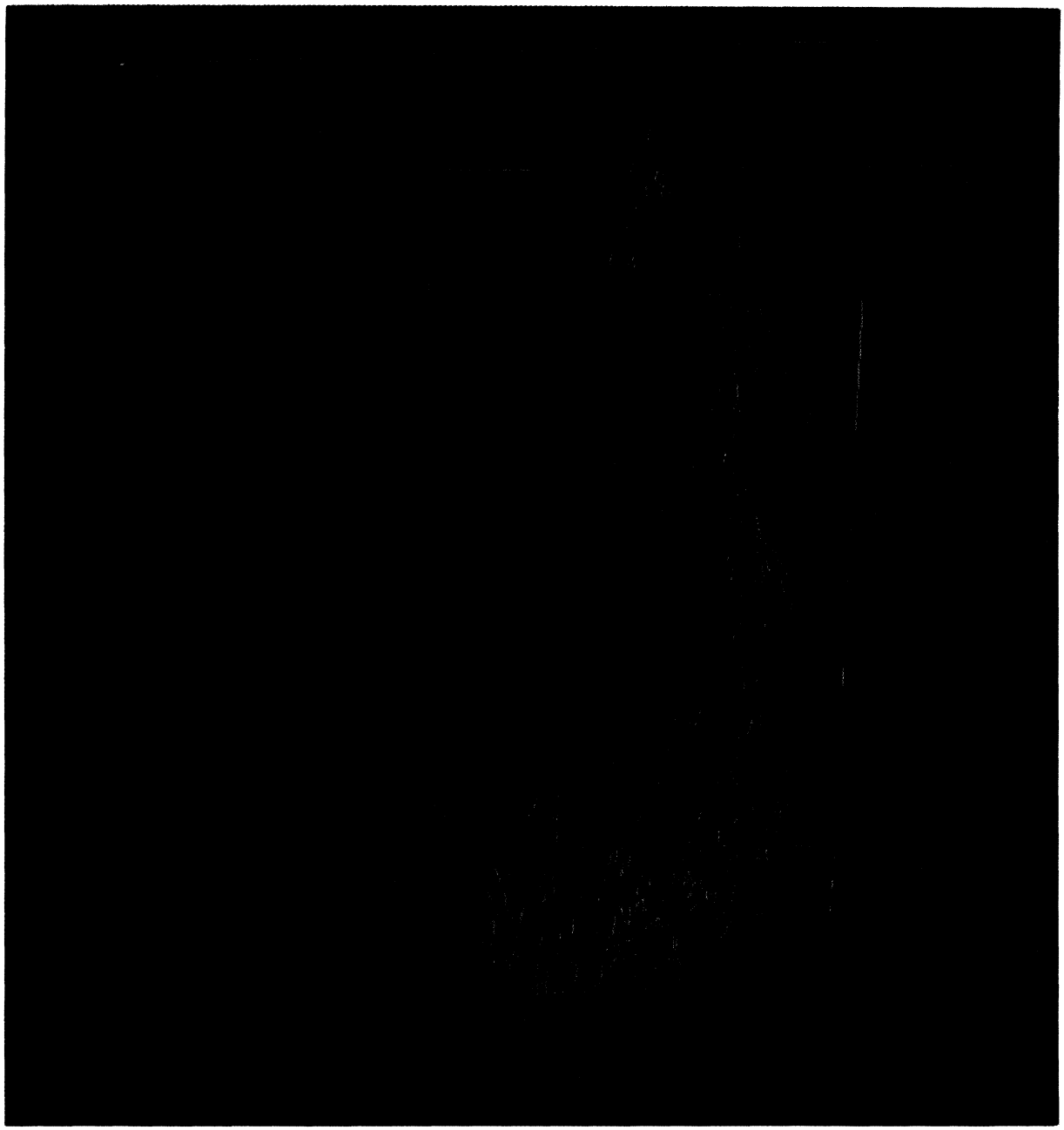

FIG. 1. Visualization of the pore structure in the clay soil (transparent gray). The vectors representing the velocity field are color coded on the basis of their velocity component parallel to the mean flow direction u_z. The mean flow direction is from top to bottom, parallel to the bounding box. Positive components are color coded from light blue ($u_z = 0$) to red ($u_z = U_{\max}$). Negative values of u_z are colored purple. In order to give a clear representation of the flow field, the data have been subsampled. The apparent lack of connectivity in the pore structure is merely a consequence of the subsampling.

Kozeny equation was giving increasingly poor estimates for the permeability, led us to conclude that, for this type of porous medium, the specific surface area is an inappropriate length scale at any resolution.

There are several ways in which we should extend this work. First, although we have applied the lattice-Boltzmann-equation technique with apparent success, there are other methods, such as those applied by Spanne *et al.* [19] and Schwartz *et al.* [18], which have also been used on similar problems. A direct comparison between these methods would be useful—to determine whether the lattice-Boltzmann-equation method is, or is not, the most appropriate. Second, we have compared our numerical results with only theoretical values obtained from the simple Carman-Kozeny equation. It would be useful to follow the example of Schwartz *et al.* [18] and Spanne *et al.* [19] and test theoretical predictions that utilize a length scale other than just the specific surface area.

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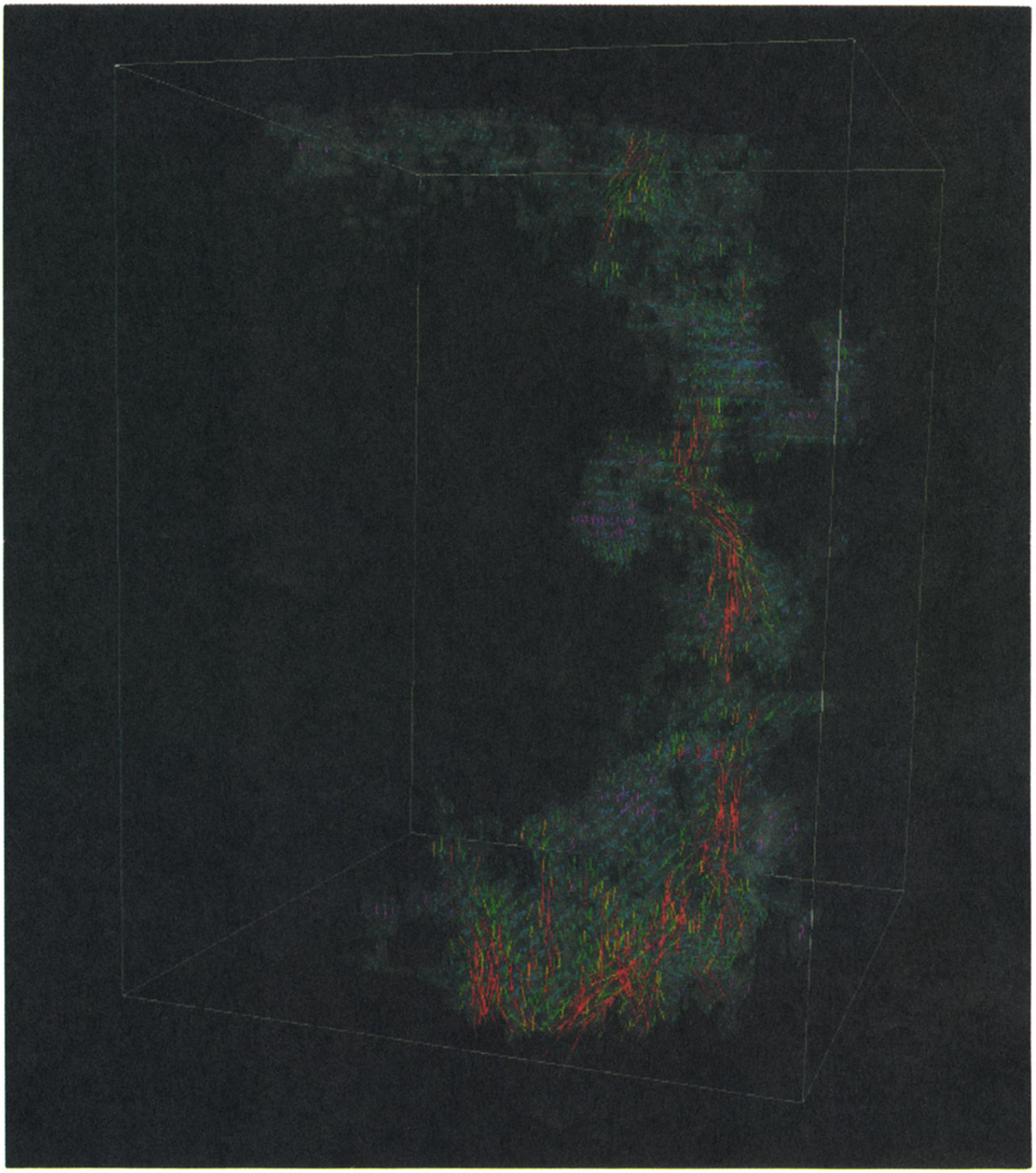

FIG. 1. Visualization of the pore structure in the clay soil (transparent gray). The vectors representing the velocity field are color coded on the basis of their velocity component parallel to the mean flow direction u_z. The mean flow direction is from top to bottom, parallel to the bounding box. Positive components are color coded from light blue ($u_z = 0$) to red ($u_z = U_{\max}$). Negative values of u_z are colored purple. In order to give a clear representation of the flow field, the data have been subsampled. The apparent lack of connectivity in the pore structure is merely a consequence of the subsampling.