Numerical simulation of creeping fluid flow in reconstruction models of porous media

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Abstract

In this paper we examine representative examples of realistic three-dimensional models for porous media by comparing their geometry and permeability with those of the original experimental specimen. The comparison is based on numerically exact evaluations of permeability, porosity, specific internal surface, mean curvature, Euler number and local percolation probabilities. The experimental specimen is a three-dimensional computer tomographic image of Fontainebleau sandstone. The three models are stochastic reconstructions for which many of the geometrical characteristics coincide with those of the experimental specimen. We find that in spite of the similarity in the geometrical properties the permeability and formation factor can differ greatly between models and the experiment.
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A better understanding of fluid flow in porous media underlies many unsolved problems in the applied and engineering sciences ranging from geosciences [1,2] and petroleum engineering [3,4] to contaminant transport [5,6] and paper manufacturing [7]. Despite many years of research there is still no agreement on the basic question namely which macroscopic geometrical observables besides porosity are needed to predict macroscopic transport parameters such as the permeability of a given porous microstructure [8–10].

Most works on transport through porous media assert the validity of a specific model for the porous microstructure and proceed by calculating physical properties

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for the model rather than for the original microstructure itself [11–13,3]. A multi-tude of porous media models have been proposed that may be roughly divided into reconstruction models, that attempt to reconstruct a realistic three-dimensional pore structure [14], and non-reconstruction models, such as the classical capillary tube model [1] or network models [11,15], that postulate an artificial model geometry. In this work, we report the comparison of exact geometrical and transport properties of three stochas-tic reconstruction models for Fontainebleau sandstone with those of an experimental specimen. One of our motivations has been to test the reliability of reconstruction models that have recently found much attention [16–18]. Reconstruction models are models that attempt to reconstruct the experimental porous microstructure usually in a statistical sense [14,10]. Equally important has been our second motivation, namely to improve the simulated annealing models by including special characteristics of the porous medium into its geometrical reconstruction process. Motivated by the attempt to improve the model we present a new reconstruction model.

Direct comparisons between different reconstruction models have, to the best of our knowledge, not been carried out in the literature. Establishing such direct comparisons between different models is needed not only for academic research purposes but also for applications in hydrology or petroleum engineering. In this paper we explore models for the popular and well-studied example of Fontainebleau sandstone.

Given a porous sample $\mathbb{S} \subset \mathbb{R}^3$, such as a piece of Fontainebleau sandstone, with pore space $\mathbb{P}$ and matrix space $\mathbb{M}$ with $\mathbb{P} \cup \mathbb{M} = \mathbb{S}$ and $\mathbb{P} \cap \mathbb{M} = \emptyset$ we assume that the internal boundaries (i.e., the difference between the closure and the interior) coincide, i.e., $\partial\mathbb{P} = \partial\mathbb{M}$. Let the porous sample $\mathbb{S}$ have the shape of a cube or rectangular par-allelepiped with sidelengths $L_i \, (i = x, y, z)$, and let it be discretized into cubic voxels of side length a such that $L_i = M_i a$. On the microscopic (pore) scale, the boundary value problem for stationary creeping fluid flow of an incompressible Newtonian fluid reads

$$\eta \Delta \mathbf{v}(\mathbf{r}) - \nabla p(\mathbf{r}) = 0, \quad \mathbf{r} \in \mathbb{P} \,, \tag{1a}$$

$$\nabla \cdot \mathbf{v}(\mathbf{r}) = 0, \quad \mathbf{r} \in \mathbb{P} \,, \tag{1b}$$

$$\mathbf{v}(\mathbf{r}) = 0, \quad \mathbf{r} \in \partial\mathbb{P} \,, \tag{1c}$$

where $\mathbf{v}(\mathbf{r})$ and $p(\mathbf{r})$ denote the microscopic velocity and pressure fields that may be extended to all of $\mathbb{S}$ by setting them to zero on $\mathbb{M}$.

We have implemented a standard pressure correction algorithm [19] to solve the Stokes equations in a three-dimensional geometry numerically. For details we refer to Ref. [20]. The time-consuming step is to solve the Poisson equation for the pressure correction. We use a successive overrelaxation method for this step. Of course it would be desirable to use more sophisticated methods as e.g. a multigrid method. But we could not find a general procedure to restrict the microstructure of the porous medium to a coarser grid without changing the topology of the pore space. We find that the speed of the algorithm is comparable to that of lattice Boltzmann methods [21]. Our spatial discretization uses a marker-and-cell (MAC) grid. The pressure values are placed in the center of the grid cells. On each face of a grid cell the velocity component perpendicular

Table 1
Geometric properties of the four porous samples

	EX	GF	SA	SK
ϕ	0.1355	0.1421	0.1354	0.1355
S_G (mm^{-1})	10.42	16.71	11.07	10.42
S (mm^{-1})	9.99	14.53	11.04	10.21
κ (mm^{-2})	-151	-449	-222	-118
E (mm^{-3})	-172	4334	1153	776
$p_3\,(60a)$	0.9561	0.3255	0.1695	0.4850

ϕ is the porosity, S is the specific surface, κ is the mean curvature and E is the Euler number, all calculated according to the methods in Ref. [30]. S_G is the specific surface calculated from the slope of the correlation function. The last row, $p_3(60a)$, is the total fraction of subblocks of sidelength $L = 60a$ that are percolating in all three coordinate directions from local porosity theory [9]. "Percolating in x, y- or z-direction" means that the subblock contains a path inside the pore space that connects opposite faces perpendicular to the x, y- or z-direction. The experimentally measured porosity was $\phi^* = 0.1484$ (see text).

to this face is located. The pore-matrix-interface $\partial\mathbb{P}$ is assumed to coincide with the surface of the cubic grid cells.

The macroscopic permeability tensor is evaluated as follows. First, the microscopic pressure and velocity fields are obtained by solving the boundary value problem (1) with a pressure gradient applied along the x-direction. Let $\bar{p}_{x0}$ denote the inlet pressure, i.e., the pressure applied to the plane $x = 0$, and let $\bar{p}_{xL}$ denote the outlet pressure, i.e., the fluid pressure applied at the plane $x = L_x$, where $L_x = M_x a$ denotes the distance between the inlet and the outlet. Then the first row of the macroscopic permeability tensor is obtained from Darcys law as

$$\mathbf{k}_x = (k_{xx}, k_{xy}, k_{xz}) = \frac{\eta L_x}{\bar{p}_{x0} - \bar{p}_{xL}}\bar{\mathbf{v}}\,,\tag{2}$$

where the macroscopically averaged velocity is defined as

$$\bar{\mathbf{v}} = \frac{1}{|\mathbb{S}|}\int_{\mathbb{S}} \mathbf{v}(\mathbf{r})\,d\mathbf{r}\tag{3}$$

and $|\mathbb{S}|$ denotes the volume of the set $\mathbb{S}$. The second and third rows of the permeability tensor are obtained analogously by applying a pressure gradient along the y- or z-direction.

We consider the above boundary value problem for four particular porous samples EX, GF, SA and SK. The sample EX is a three-dimensional computer tomographic image of a Fontainebleau sandstone with resolution $a = 7.5\,\mu$m and sidelengths $M_x = 299$, $M_y = 300$, and $M_z = 300$. This sandstone is a popular reference standard because of its exceptional chemical, crystallographic and microstructural simplicity [22,23]. The computer-assisted microtomography was carried out on a micro-plug drilled from a larger original core. The original core from which the micro-plug was taken had a porosity of $\phi^* = 0.1484$, a permeability of $k^* = 1.3D$ and a formation factor of $F^* = 22.1$. The porosity $\phi(\mathbb{S}_{EX})$, of our microtomographic data set (representing a subsample of the core) is only 0.1355 (see Table 1). The difference between the porosity of the original core and that of the final data set is due to the heterogeneity of the sandstone

and to the difference in sample size. The experimental sample is referred to as EX in the following.

The three other samples are fully three-dimensional stochastic reconstruction models for the experimental sample EX. The resolution of all models is again $a = 7.5 \, \mu m$, and their size is $M_x = M_y = M_z = 256$.

The Gaussian field (GF) reconstruction model provides a random pore space configuration in such a way that its correlation function equals the prescribed reference correlation function of EX. The method of Gaussian field reconstruction is well documented in the literature [24,25,14,26,27]. Given the reference correlation function $G_{EX}(\mathbf{r})$ and porosity $\phi(\mathbb{S}_{EX})$ of the experimental sample, the three main steps of constructing the sample $\mathbb{S}_{GF}$ with correlation function $G_{GF}(\mathbf{r}) = G_{EX}(\mathbf{r})$ are as follows. First a standard Gaussian field $X(\mathbf{r})$ is generated which consists of statistically independent Gaussian random variables $X \in \mathbb{R}$ at each lattice point $\mathbf{r}$. Secondly, the field $X(\mathbf{r})$ is passed through a linear filter which produces a correlated Gaussian field $Y(\mathbf{r})$ with zero mean and unit variance. The reference correlation function $G_{EX}(\mathbf{r})$ and porosity $\phi(\mathbb{S}_{EX})$ enter into the mathematical construction of this linear filter. Finally, the correlated field $Y(\mathbf{r})$ is then passed through a nonlinear discretization filter which produces the reconstructed sample $\mathbb{S}_{GF}$. Our implementation of the method follows [14] and is described in detail in Ref. [27].

The simulated annealing (SA) reconstruction model is a second method to generate a three-dimensional random microstructure with prescribed porosity and correlation function. The method generates a configuration $\mathbb{S}_{SA}$ by minimizing the deviations between $G_{SA}(\mathbf{r})$ and a predefined reference function $G_0(\mathbf{r})$ using a simulated annealing algorithm based on the Monte Carlo method of statistical physics. An advantage is that the method is not limited to correlation functions but can be used to reconstruct other geometric characteristics such as contact distributions [28]. Of course in the sample prepared here we use only the two-point pixel–pixel correlation function and we have again the Fontainebleau sandstone as reference, i.e., $G_0(\mathbf{r}) = G_{EX}(\mathbf{r})$. For further discussions of the method and its problems see Refs. [29,28].

Finally, the reconstruction model SK is new and we describe it here briefly. Its idea is to use the simulated annealing algorithm but to update only a subset of all voxels. In the present implementation an initial configuration is constructed as follows. First, a close packing of hard spheres with diameters uniformly distributed in the range from $13.6a$ to $18.4a$ is produced. The remaining pore space between spheres is then filled randomly with matrix voxels until the desired porosity of $\phi = 0.1355$ is obtained. The added matrix voxels in the initial configuration are declared movable, while the original matrix voxels in the spheres are immobile. The movable matrix voxels are updated sequentially in the same manner as in the SA algorithm until a specified set of geometric observables has been matched exactly. Of course, other initial configurations and another separation into movable and immobile voxels are possible. In the present implementation we match the two-point correlation function in thirteen different directions. We choose many directions to improve the isotropy of the resulting reconstruction. Simpler implementations with fewer directions were found to be potentially anisotropic [29] depending on the nature of the reconstructed correlation function. For more details of the model we refer to Ref. [20].

We collect the basic geometrical properties of the four samples in Table 1. The first row is the porosity ϕ, i.e., the volume fraction of pore space. The second row gives the specific internal surface, i.e., the ratio of internal surface area to sample volume, measured from the slope of the correlation function according to the formula $S_G = -4dS(0)/dr$, where $S(r)$ denotes the voxel–voxel correlation function [9]. The third row is again an estimator for the specific internal surface calculated not from the correlation function but from integral geometric formulae as described in detail in Ref. [30]. The third row gives the integral of the mean curvature κ calculated recursively according to Hadwigers theory [30], and the fourth row is the Euler or connectivity number E giving a measure of the number of connectedness components per unit volume. A positive sign of κ indicates that the matrix space is on average convex shaped, while a negative number indicates concavity of $\mathbb{M}$. A positive Euler number E indicates that on average there are isolated components of $\mathbb{M}$ while a negative value indicates the presence of isolated pores. For a detailed description and the geometric characteristics of the samples EX,DM and SA we refer to Ref. [27].

The porosity ϕ and the specific surface S of all four samples are identical within the statistical uncertainties or imperfections (in the case of GF) of each method. We also find that the average mean curvature is very similar in all models. We attribute the fact that it is negative to the creases and sharp corners. A clear difference between EX on the one hand and GF,SA and SK on the other appears for the Euler number E. A more detailed geometrical analysis [31,27] based on local porosity theory [32–34,9] reveals that the three models GF,SA and SK are more homogeneous in their geometrical properties than the experimental sample EX. Furthermore, we find differences in the connectivity properties. A first indication of this fact can be seen from the value of the specific Euler number E. A clearer view of the phenomenon is obtained using the total fraction of percolating cells introduced in local porosity theory [32]. The total fraction of percolating cells gives the fraction of cubic subblocks of sidelength L that are percolating in all three coordinate directions. A subblock is called percolating in the x-direction if it contains a path inside the pore space connecting the two opposite faces of the sample that are perpendicular to the x-direction. In the last row of Table 1 we give the results for the total fraction $p_3(60a)$ of percolating cells for all four samples for measurement cells of size $60a$ where a is the lattice constant. We find that none of the models matches the values for the original sample EX. Based on the clear differences in connectivity seen in these data, it may be conjectured [27] that the $p_3(L)$ function from local porosity theory is a geometrical indicator for permeability.

We have calculated the exact values of permeability by solving the Stokes boundary value problem (1) numerically for all four samples. On the sample surface the pressure is fixed while von Neumann conditions are applied for the velocity. This computation is a demanding task in terms of computation time and memory. For the above geometries with up to 27×10^6 grid points, such calculations of k are possible only on parallel computers. The iterative algorithm for the solution of Eq. (1) was terminated when the condition $\max_{\mathbf{r} \in \mathbf{P}} |\Delta \mathbf{v}(\mathbf{r}) - \nabla p(\mathbf{r})| < 10^{-6}$ for the dimensionless left-hand side of (1a) was fulfilled for the first time. Typically, the convergence required between 10 000 and 50 000 iterations in the pressure correction equation for samples EX and SK. The

Table 2
Permeability for the four porous samples

Permeability (mD)	EX	GF	SA	SK
k_{zz}	692	20	35	505
k_{yy}	911	20	22	522
k_{xx}	790	20	20	497
$\bar{k}$	798	20	26	508
$\bar{k}^*$	1150	24	38	731

k_{ii} is the permeability in mD in the direction $i = x, y, z$. The experimentally measured permeability was $k^* = 1300$ mD (see text).

program was run on a Cray T3E with usually 128 processors in parallel, and required between 1 and 3 h run time. For samples SA and GF on the other hand, the number of iterations increased by roughly a factor of 10. This was a consequence of the poor connectivity of the sample.

The first three rows in Table 2 give the numerical results for the diagonal elements k_{xx}, k_{yy}, k_{zz} of the fluid permeability tensor. The off-diagonal elements were found to be small. In all cases their numerical value was at least one order of magnitude below the smallest diagonal element, and hence we neglect them here. The permeabilities of the simulated annealing SA and Gaussian field reconstruction GF are found to be an order of magnitude smaller than those of EX. This finding confirms the geometrical predictions from [27]. It seems as if the stochastic reconstruction models of the two-point correlation function cannot reproduce the high degree of geometrical connectivity of the original sandstone. Correct reproduction of the geometrical connectivity however is an indispensable precondition for reproducing the dynamical connectivity that determines transport properties. The hybrid model SK gives somewhat better results than SA and GF. The improved degree of geometrical connectivity is already seen in the value of $p_3(60a)$. Correspondingly, the permeability values of the SK model are found to be higher than those of SA and GF, but do not quite reach those of the experimental sample EX. In the fourth row of Table 2, labelled $\bar{k}$, we give the averages of the diagonal elements k_{xx}, k_{yy}, k_{zz}.

We can now compare the numerically calculated permeabilities to the experimental value. The value of the permeability for the original experimental core from which the later digitized subsample was cut has been measured in the laboratory to be $k^* = 1300$ mD. Of course this value can differ substantially from the permeability of the digitized subsample EX. In fact already the porosity of the original core $\phi^* = 0.1484$ differs from that of the digitized sample. There is a well-known experimental correlation between porosity and permeability of Fontainebleau sandstone [23]. It is usually approximated in the form

$$k = A\phi^b , \tag{4}$$

where A and b are constants (see Ref. [23, p. 46]). In the porosity range of interest around $\phi \approx 0.13$–0.15 this correlation shows an exponent of $b \approx 4$, although it should be kept in mind that this value is very inaccurate because the experimental data scatter strongly. The power-law fit in Eq. (4) amounts to fitting a tangent to a general

correlation of the form $\log k = f(\log \phi)$. Moreover, the data are uncertain and scatter for the same value of ϕ by roughly a factor of 2. Using the rough estimate $b \approx 4$ we can extrapolate the numerically measured permeabilities $k_{\mathsf{EX}}, k_{\mathsf{GF}}, k_{\mathsf{SA}}, k_{\mathsf{SK}}$ into the predictions

$$\bar{k}_i^* = \bar{k}_i \left(\frac{\phi^*}{\phi_i} \right)^b , \tag{5}$$

where $i \in \{\mathsf{EX}, \mathsf{GF}, \mathsf{SA}, \mathsf{SK}\}$ and the constants A_i have dropped out. These predictions are the corrected values that might be compared with the experimental value of $k^* = 1300$ mD. We see that the predicted permeability of the digitized sample EX agrees very well with the experimental value. It has to be kept in mind that the geometry of the digitized sample EX is always inaccurate because of the finite resolution of $a = 7.5$ μm. Hence a deviation of only 13% in k can be viewed as very good agreement. On the other hand, the values for the GF and SA models are more than an order of magnitude too small. The value for SK is again better as expected and falls within a factor of 2 of the experimental result. Because of the initial conditions in the SK model we expect this result to depend strongly on the details of the implementation and statistical fluctuations.

In summary we have analysed geometrical and physical properties of Fontainebleau sandstone and three reconstruction models. We find that the straightforward Gaussian field and simulated annealing reconstructions of the correlation function differ in many respects from the original sample. The new model SK gives a somewhat better agreement for the permeability, and connectivity indicators. However, further studies are necessary to study statistical fluctuations in this result. Our results also show that numerical solutions of the flow problems are becoming feasible to investigate the quantitative accuracy of geometrical models as well as approximate physical theories. The correlations between geometry and transport in porous media are in this way becoming accessible to numerical experiment.

Acknowledgements

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