

Stochastic geometry and transport in porous media

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The work is part of the research project “**Fimotum** = First principles-based **m**odels for **t**ransport in **u**nsaturated **m**edia”, joint by ETH Zurich, TU Braunschweig and University of Stuttgart.

A special issue of Advances in Water Resources is planned for results from Fimotum.

Overview

- 1 Introduction
- 2 Characteristics
 - Minkowski functionals
 - Other characteristics
- 3 Simulating pore spaces
 - Simulated annealing
 - Boolean models
 - Thresholded Gaussian models
- 4 Results
 - Comparing other geometric characteristics
 - Permeability
 - Water retention curves
- 5 Discussion

Background

The **goal of soil physics** is to describe and predict the transport of water, air and solutes through the pores between the soil surface and the aquifer.

This is a largely unsolved problem: The pore space is not known for applications and too complex for solving the hydrodynamic equations (Navier-Stokes).

To some extent, continuum theory (Richards equation) is applicable. It requires a parametrization of the relations between saturation and pressure and between hydraulic conductivity and pressure. These are purely empirical.

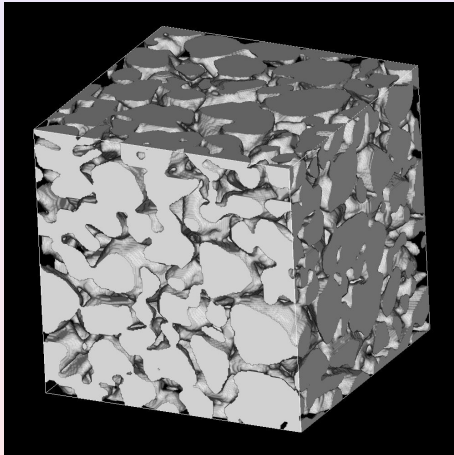
Aim of the Fimotum project

The Fimotum project aims to improve the understanding of the influence of the pore structure at the microscale on transport properties.

It uses recent progress in imaging technology: We have 3d-binary images of two sand samples (coarse and fine). An image consists of 800^3 voxels of size $(11\mu)^3$.

It also uses progress in the numerical solution of the Navier-Stokes equation with complicated boundary conditions (Lattice Boltzmann method).

Coarse sand image



Permeability and water retention curve

For this measured pore space, we can compute the saturated **permeability** by solving the Navier-Stokes equation.

Permeability is viscosity times flow rate divided by applied pressure gradient. Saturated means that the pore space is completely filled with the fluid.

With a pore network model, we can also compute the **water retention curve**, i.e. saturation as a function of applied pressure (starting with the saturated condition).

Our main questions

For a better understanding, we would like to find **simple geometric characteristics** of the microstructure of porous media that determine the transport properties of the medium.

When we have candidates for such characteristics, we want to **generate artificial pore spaces** with prescribed values of these characteristics and compute the permeability and the water retention curves for them.

As prescribed values, take those of the real sand probes and vary them in a systematic manner.

Minkowski functionals

It is clear that transport properties of a porous medium depend on the **volume**, the **surface** (because of friction at the solid walls) and some measures of **connectivity**.

The Euler characteristic is a measure of $3d$ connectivity. Because of the Crofton formula, the mean curvature is a measure of average $2d$ connectivity.

Hence we use the 4 Minkowski functionals as our candidates for the geometric characteristics. The Hadwiger theorem can be seen as an indication that they might be sufficient.

Minkowski functionals for openings

One can argue that when draining a porous medium by increasing the suction, pores of different size are emptied at different suctions. This means the Minkowski functionals not for all pores, but for those with a given diameter are relevant.

Hence consider the Minkowski functionals of the **morphological openings** with balls of radius r as a function of r . We call these the **Minkowski functions**.

Chord length

Another characteristic that might be relevant is the **chord length** distribution because this also describes how frequent pores of different width are.

In the following, we simulate pore spaces with prescribed values for the 4 Minkowski functionals. We then use the Minkowski functions and the chord length distribution as an indication how different the simulated and the real pore spaces are.

Simulated annealing I

Assume we have m functionals $F_1, \dots, F_m$ and m real numbers $f_1, \dots, f_m$ and an observation window W . We want to generate one or many pore spaces $P \subset W$ such that

$$\frac{F_j(P)}{\text{vol}(W)} = f_j \quad (j = 1, \dots, m).$$

This can be done by minimizing the cost function

$$J(P) = \sum \alpha_j \left| \frac{F_j(P)}{\text{vol}(W)} - f_j \right|.$$

Simulated annealing is a stochastic minimization algorithm which avoids being trapped in local minima.

Simulated annealing II

Simulated annealing proceeds iteratively

- Choose a simple modification of $P' = T(P)$ randomly (e.g. flipping the values of two voxels).
- If $J(P') \leq J(P)$, always accept the modification. Otherwise, accept with probability

$$\exp(-\beta(J(P') - J(P))).$$

- Increase β and iterate.

Practical issues are the choice of the basic modifications, of the weights α_j and of the speed with which we increase β with the number of iterations.

Simulated annealing III

In theory, with an appropriate choice of $\beta \rightarrow \infty$, we end up sampling from the uniform distribution on the set $\{P; J(P) = 0\}$.

In the literature, successes with simulated annealing are reported. Our own experience is less positive. If we match only the Minkowski functionals, we often obtain strange “non-stationary” P . Using additional functionals, we have problems with convergence even though we worked only in $2d$.

Boolean models I

For Boolean models, we can express the four (specific) Minkowski functionals in terms of the intensity of the germs and the 3 expected Minkowski functionals of the typical convex grain. (Davy 1978, Mecke 2000). Moreover, this relation is invertible.

Hence we need to construct grain distributions with prescribed values of the expected Minkowski functionals.

Boolean models II

We use the Boolean model for the solid phase and choose ellipsoids for the grains. For a fast algorithm there are at least two possibilities:

Choose ellipsoids where two half axes are the same, and take the two different half axes to be independent (Arns et al., 2003). Choose ellipsoids of the form $Z \cdot E_0$ where E_0 is fixed and Z is random (our solution).

Open questions: Can we obtain all possible specific Minkowski functionals with ellipsoid grains ? How do we obtain the “least eccentric” grains?

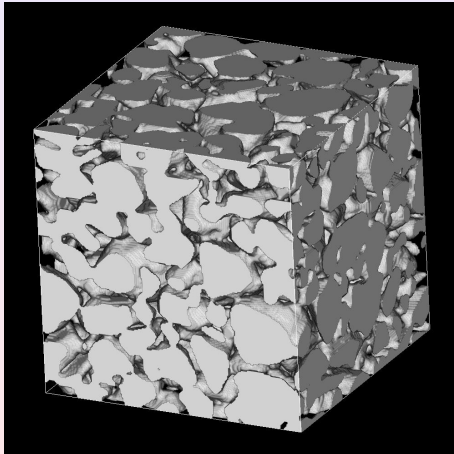
Thresholded Gaussian models

Consider a Gaussian stationary and isotropic random field $(Z(x))$ with correlation function ρ and the thresholded binary field

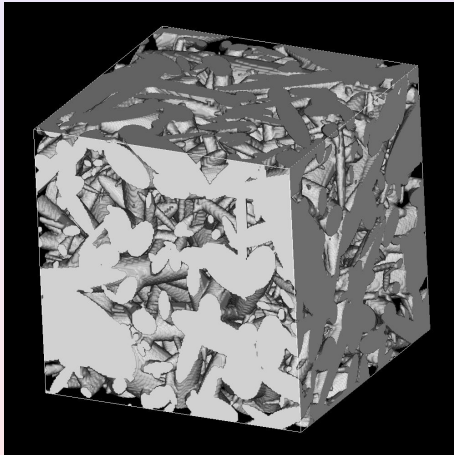
$$\Xi(x) = 1_{[a,b]}(Z(x)).$$

Results of Adler show that the four specific Minkowski functionals depend only on the thresholds a, b and the second derivative of ρ at the origin. Hence we can obtain in this way only a $3d$ subset of the $4d$ space of all specific Minkowski functionals. By chance (?) the values of the real sand images are very close to this $3d$ subset.

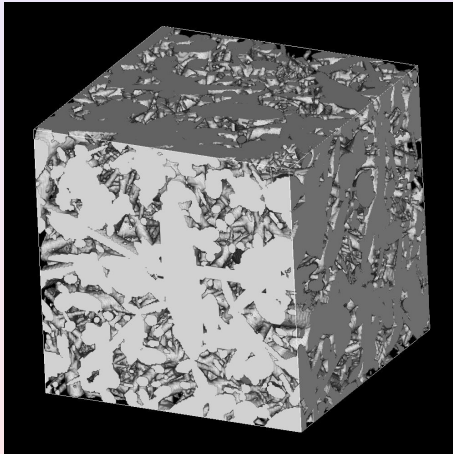
Real sand



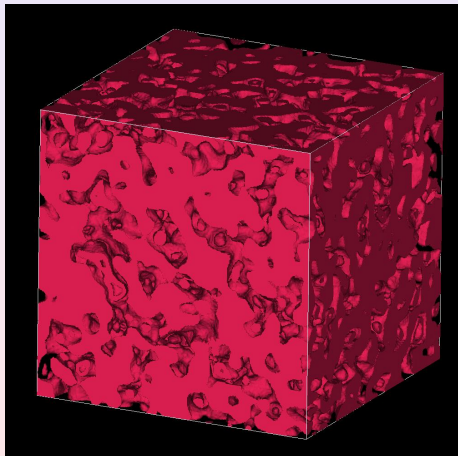
Boolean model, 4 functionals matched



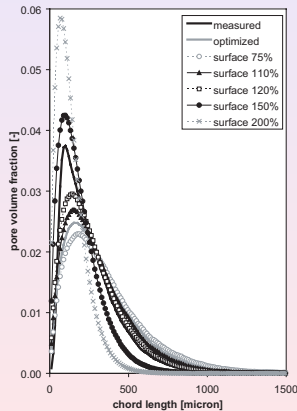
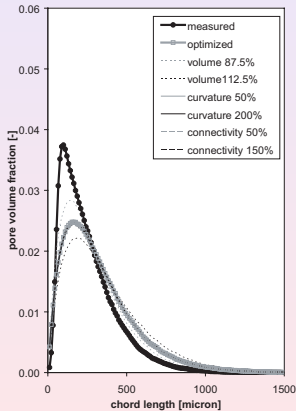
Boolean model, increased surface



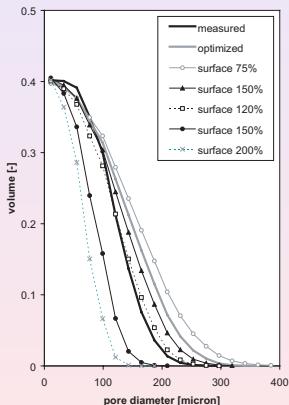
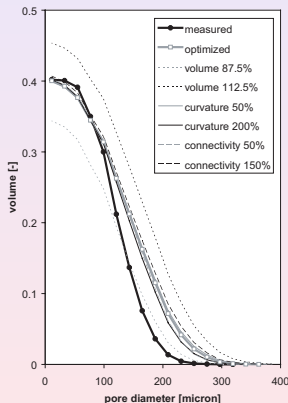
Gaussian model, 4 functionals matched



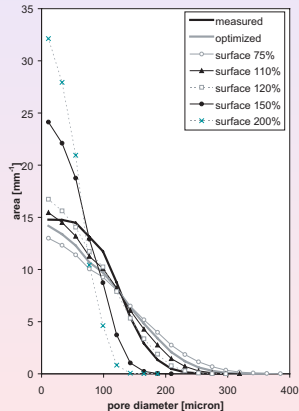
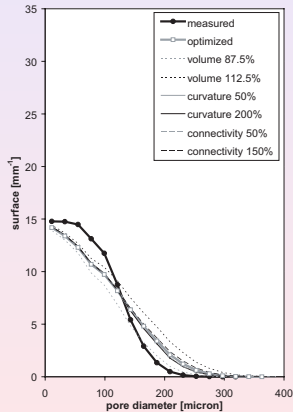
Chord length distributions



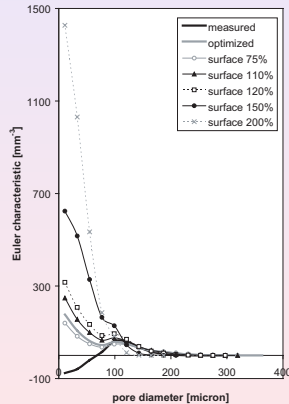
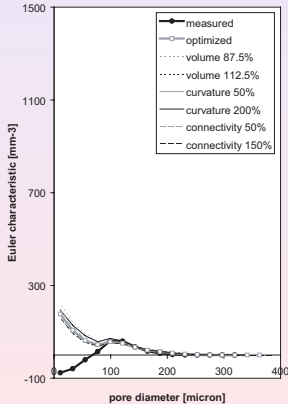
Porosity as a function of pore size



Surface as a function of pore size



Euler char. as a function of pore size

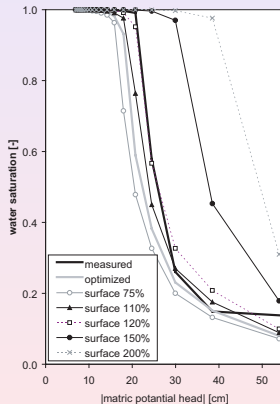
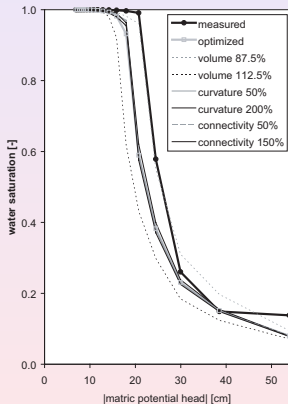


Permeability for real and simulated pore spaces

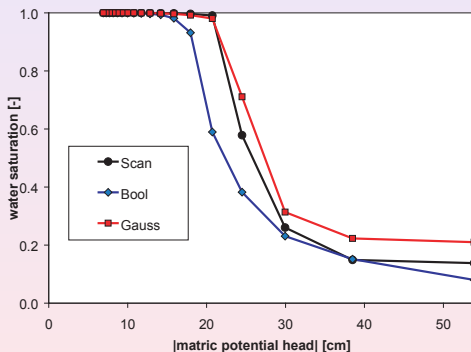
Values for solid phase, relative to real sand probe

origin	volume	surface	curvature	Euler	permeability 10^{-12} m^2
model	0.92	1.0	1.0	1.0	194.6
model	1.0	1.0	1.0	1.5	162.0
model	1.0	1.0	1.0	0.5	161.3
model	1.0	1.0	1.0	1.0	149.0
real	1.0	1.0	1.0	1.0	149.0
model	1.0	1.0	2.0	1.0	148.5
model	1.0	0.75	1.0	1.0	144.9
model	1.0	1.0	0.5	1.0	143.8
model	1.0	1.2	1.0	1.0	105.8
model	1.08	1.0	1.0	1.0	79.5

Water retention curves I



Water retention curves II



Discussion

Boolean models are not suitable for these images, even when we are satisfied with a rough approximation. Thresholded Gaussian models are better, but less flexible.

Minkowski functionals alone are not sufficient for transport properties.

Can we match Minkowski functions ? Are they sufficient for transport properties ?

How would packing of hard or soft grains with random shape and size work ? Could we relate the properties of the grain distribution to transport properties ?