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Surface and Ground Water
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Numerical generation of porous structure with fractal properties

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Abstract

Many natural porous geological rock formations, as well as engineered porous structures, have fractal properties. In the present paper a new numerical method for generating a three-dimensional porous medium with any desired probability density function (PDF) and autocorrelation function (ACF) is presented. The well-known Turning Bands Method (TBM) is modified to generate three-dimensional synthetic isotropic and anisotropic porous media with a Gaussian PDF and exponential-decay ACF. Porous media with other PDFs and ACFs are generated with a nonlinear, iterative PDF and ACF transformation, whereby the arbitrary PDF is converted to an equivalent Gaussian PDF which is then simulated with the classical TBM. Different 3D synthetic porous media are simulated by varying the porosity and the correlation structure of the random field. The performance of the simulations is evaluated by checking the ensemble statistics, the mean, variance and ACF of the simulated random field. For a Gaussian PDF an average fractal dimension of approximately 2.76 is obtained which is in the range of values of actually measured fractal dimensions of molecular surfaces. For a porous medium with a non-Gaussian quadratic PDF the calculated fractal dimension appears to be consistently higher and averages 2.82. The results show also that the fractal dimension is neither strongly dependent of the porosity nor of the degree of anisotropy assumed.

1 Introduction

Numerous experimental studies of the last decade have shown that many natural porous geological rock formations, as well as engineered porous structures, have fractal properties; i.e., they are self-similar or, more specifically, self-affine over several length scales (cf. Avnir *et al.*, 1984; Katz and Thompson, 1985; Krohn and Thompson, 1986; Krohn, 1988; Bunde and Havlin, 1991; Thompson, 1991; Adler, 1992; Dullien, 1992; Cox and Wang, 1993). These studies show that the fractal range of a porous rock or structure, as measured by its pore surface or its pore volume, usually starts somewhere beneath the long-length, non-fractal Euclidean regime of the order of the grain size and extends over several orders of magnitude to the very short-range regime. Other experiments with wave-scattering- or surface adsorption techniques have indicated fractal regimes down even to the molecular level of the crystals that form the porous aggregate (Avnir *et al.*, 1984; Martin and Hurd, 1987). A fractal structure has also been observed, on a large scale, for many natural geological and geophysical fractures, particularly seismic fault planes (cf. Okuba and Aki, 1987), and on the small-scale, for ruptured metal- or rock surfaces (cf. Mandelbrot *et al.*, 1984). Numerous flow processes in a porous medium have also been found to be fractal as well (Feder, 1988; Adler, 1992; Koch, 1993; Dullien, 1992).

These studies demonstrate that the quantitative determination of the fractality; i.e., the fractal dimension of the porous medium, is by no means of pure theoretical interest in the fundamental physics of nature alone, but has far-reaching practical applications in general soil science and subsurface hydrology. As computer simulations of the various aspects of flow and transport in porous medium become of ever-increasing importance, so is the desire for an efficient numerical generation of test medium of certain stochastic nature, with possibly, fractal character.

In spite of the many experimental and theoretical studies above on how to quantify a fractal porous medium and on how to determine its fractal dimension, the numerical generation of a fractal pore structure with predefined statistical and scaling properties is somewhat scarcer. Here a new technique for generating a three-dimensional synthetic isotropic and anisotropic porous medium with any desired probability density function (PDF) and autocorrelation function (ACF) is proposed. The method can easily be implemented in large-scale stochastic simulations of flow and transport in a porous medium to numerically test the previously established experimental relationships between various soil properties and the fractal dimension of the porous medium.

2 Theory

2.1 The turning bands generation of Gaussian and non-Gaussian random fields.

The numerical method used employed is based on a modification of the Turning Bands Method (TBM) (Tompson et al., 1989). The TBM, starting from a second-order stationary isotropic or anisotropic normal random distribution $Y(x)$ with $N(0, \sigma^2)$, and a covariance function $R_{yy}(\tau) = E[Y(x)Y(x + \tau)]$, with τ the separation distance, produces a realization of a stationary, correlated, multi-dimensional random field by reducing a two- or three-dimensional random field simulation to a series of one-dimensional simulations carried out along a finite set of lines radiating from an origin and subsequent superposition of this series.

Once an arbitrary Gaussian random field $Y_s(x)$ has been simulated (see Sun and Koch, 1998, for details), by setting a threshold level Y_0 in the PDF, similar to the experimental setting of the light intensity in a porous thin section of scanning microscope (Quiblier, 1984; Krohn and Thompson, 1986; Krohn, 1988),

$$j, k) = \begin{cases} 0 & Y_s(x) \leq Y_0 & \text{pore} \\ 1 & Y_s(x) > Y_0 & \text{solid} \end{cases} \quad (1)$$

a random porous medium of given porosity $U(i, j, k)$ can be generated. Y_0 is chosen from the inverse F^{-1} of the normalized cumulative distribution function

$$F(Y_0) = \int_{-\infty}^{Y_0} p(\tau) d\tau \quad (2)$$

with $p(\tau)$ the normalized Gaussian PDF. For example, for a medium with a porosity of 0.4 (=40%), using the standard tables of the normal distribution, the corresponding threshold value will be $Y_0 = -0.255$.

Sun and Koch (1998) have extended the approach above to non-Gaussian random fields. However, in such cases both the PDF and the ACF need to be transformed before the TBM can be used. Following an idea of Joshi (1974), a linear transformation

$$R_{zz}(\tau) = \sum_{m=0}^{\infty} C_m^2 R_{yy}(\tau) \quad (3)$$

between the desired non-Gaussian ACF $R_{zz}(\tau)$ and the input Gaussian ACF $R_{yy}(\tau)$ can be set up. The C_m 's are calculated from the measured PDF $p(y)$ of a set of thin sections through

$$C_m = (m!)^{-0.5} \int_{-\infty}^{\infty} f(y) p(y) H_m(y) dy \quad (4)$$

where $H_m(y)$ are the Hermite polynomials and $f(y)$ is a nonlinear inverse probability transformation between the Gaussian and the non-Gaussian PDF $p(y)$. Eq. (3) can then be solved by an iterative Newton method (see *Sun and Koch, 1998*, for details).

2.2 Calculation of the fractal dimension of surface area of porous media.

The surface area A_a of a synthetic porous medium can be integrated by:

$$= \sum_{i=1}^{nx} \sum_{j=1}^{ny} \sum_{k=1}^{nz} (\delta |_{U(i,j,k) * U(i+a', j+b', k+c)} \quad (5)$$

where δ is the surface area measuring scale, and $U(i,j,k)$ is the porous indicator value (0,1) of Eq. (1). a', b', c' are the increments of a space point coordinate i, j, k corresponding to δ , and nx, ny, nz is the total number of grid points in each direction.

Eq. (5) can be implemented using a chosen δ as the basic surface area measuring scale and allowing δ to "walk" through the synthetic three-dimensional sample domain. Because the surface area of the pore space in the synthetic sample is a rough surface, as the measuring scale δ is decreased, the measured surface area A_a should increase in form of a certain functional relationship. More precisely, using the classical "coastline-divider rule" approach (*Mandelbrot, 1982; Feder, 1988*) for a fractal object, the relation between the measuring pixel scale δ (sq. unit) and the surface area $A(\delta)$ of the porous media is given by

$$A_a(\delta) = a_0 \delta^{(2-D)/2} \quad (6)$$

Therefore, the fractal dimension D can be determined from the slope $\alpha = (2-D)/2$ of the logarithmic plot $A_a(\delta)$. One also notices from Eq. (6) that for a fractal dimension $D=2$ a smooth surface will be obtained.

3 Numerical Simulations and Results

Numerous different synthetic porous media are simulated by varying the correlation structure of the spatially correlated random field. The performance of the simulations of the random fields was checked by calculating the ensemble statistics, the mean, variance and the ACF of the simulated random field. These statistical parameters provide a clue of how well the simulated field is approaching the theoretical values (*Tompson et al., 1989*). In order to get reasonable statistical representation about 30 Monte Carlo simulations for each predefined statistical distribution were carried out.

Fig. 1 illustrate one typical realization of a 3D isotropic Gaussian porous structure (porosity =50%) with correlation lengths $\beta=(3,3,3)$.

Fig. 2 depicts log-log graphs of the average measured surface area $A_a(\delta)$ for different porosities as a function of the normalized measuring scale δ . The relatively straight lines obtained over the range of δ investigated are evidence for a fractal behavior, in accordance with Eq. (6). In addition, since the slopes of these lines are more or less identical, the fractal dimensions are invariant of the porosity assumed.

The average fractal dimension D_{av} computed from the line-slopes of Fig. 2, using Eq. (6), is approximately $D_{av} = 2.76$. This value is within the lower range ($2.67 < D < 2.92$) of fractal dimensions of porous surfaces obtained experimentally by *Avnir et al. (1984)* through molecular adsorption and even closer to those obtained by *Krohn and Thompson (1986)* and *Krohn (1988)* and for various sandstone, shales and carbonates by means of scanning-electron-microscopic and thin-section images.

For a porous medium with a non-Gaussian PDF, the fractal dimension obtained for the surface area can be different (*Sun and Koch, 1998*). For example, for realizations with an exponential ACF and a non-Gaussian, quadratic PDF $Y=(x-a)^2$, depending on the porosities used, the fractal dimensions calculated range from $D=2.81$ to $D=2.85$, with an average $D_{av}=2.82$. The corresponding log-log graphs of $A_a(\delta)$ are plotted in Fig.3 for six different porosities. Again, the slopes of these lines are more or less

identical for the various porosities assumed; i.e. the fractal dimension is rather independent of the porosity of the structure.

The fractal dimensions D obtained from numerous realizations of four Gaussian and one non-Gaussian pore structure with different correlation lengths are depicted in Fig. 4 as a function of the porosity selected. In accordance with the statement above, the lines of D are relatively flat over the porosity range and D for the non-Gaussian case $\beta = (1.9, 1.9, 1.9)$ is consistently higher than those obtained for the Gaussian structures. However, the overall range of the variations of D is only between 0.1 and 0.2.

The variations of the surface area A_a as a function of the porosity for various measuring scales δ are analyzed in *Sun and Koch (1998)*. There a convex functional course is obtained, whereby A_a increases gradually as the porosity is raised from zero to 50%, and decreases hereafter monotonically again to eventually zero as the porosity is increased further to 100% (a totally void sample). In addition, with the same sample volume and at the same measuring scale δ , it is illustrated that synthetic porous medium with a larger correlation scale β have a smaller surface area A_a . On the other hand, isotropic and anisotropic porous media with the same average correlation scale β have roughly the same surface area A_a .

4 Conclusions

One of major assets of the new method of the numerical generation of a fractal surface is that it can be applied to a three-dimensional porous medium with an arbitrary probability density functions (PDF) and autocorrelation function (ACF). In the case of an isotropic or anisotropic porous media with a Gaussian PDF the Turning Bands Method (TBM) can be used directly. For non-Gaussian PDF with an exponential-decay ACF, the latter has to be transformed first through an inverse polynomial iteration procedure to an equivalent ACF representing an Gaussian PDF, before the TBM can be applied in the same way. Once the surface area is estimated numerically for a given porosity, its fractal dimensions are measured by classical fractal perimeter/area relationships. Different synthetic porous media with varying porosities and correlation structures of the spatially correlated random field are simulated. For a Gaussian PDF an average fractal dimension of approximately 2.76 is obtained which is in the range of values of actually measured fractal dimensions of molecular surfaces. For a porous medium with a non-Gaussian quadratic PDF the calculated fractal dimension averages 2.82. The results show that the average fractal dimension vary strongly neither

with the porosity nor with the correlation length.

In spite of the versatility of the present numerical approach of the generation of a fractal porous structure for the use in Monte-Carlo type computer simulations of various aspects of flow and transport in a porous medium, several reservations are in order. The TBM program only generates stationary, homogenous porous structures with a single, uniform porosity. However, a real heterogenous porous media may have widely different properties. The fractal properties of such a heterogenous porous media can only be inferred from comparisons of numerous realizations of homogenous anisotropic synthetic media with varied correlation structures. An accurate statistics can then be established by following the general method presented above; i.e., by simulating a large number of desired porous media structures and calculating the specific surface areas and the corresponding fractal dimensions.

References

- Adler, P.M., *Porous Media: Geometry and Transports*, Butterworth-Heinemann Press, London, 1992.
- Avnir, D., Farin, D. and Pfeifer, P., Molecular fractal surfaces, *Nature*, 308, 261-263, 1984.
- Bunde, A. and S. Havlin, *Fractals and Disordered Systems*, Springer, New York, NY, 1991.
- Cox, B.L. and J.S.Y. Wang, Fractal surfaces: Measurement and application in the earth science, *Fractals*, 1, 87-115, 1993.
- Dullien, F. A. L., *Porous Media, Fluid Transport and Pore Structure*. Academic Press, Orlando, FL, 1992.
- Feder, J., *Fractals*. Plenum Press, New York, NY, 1988.
- Joshi, M. Y., *A class of stochastic models for porous media*, Ph.D Dissertation, University of Kansas, Lawrence, KS, 1974.
- Katz, A.J. and A.H. Thompson, Fractal sandstone pores: Implications for conductivity and pore formation, *Phys. Rev. Lett.*, 54, 1325--1328, 1985.
- Koch, M., Modeling the dynamics of finger instabilities in porous media: Evidence for fractal and nonlinear system behavior, In: *Advances in Hydroscience and -Engineering, Volume I*, Wang, Sam S.Y. (ed.), pp. 1763--1774, Center for Computational Hydroscience and

- Engineering, The University of Mississippi, Oxford, MS, 1993.
- Krohn, C.E., Fractal measurements of sandstone, shales and carbonates, *J. Geophys. Res.*, 93, 3297-3305, 1988.
- Krohn, C.E., and A.H. Thompson, Fractal sandstone pores: Automatic measurement using scanning-electron-microscopic images, *Phys. Rev., Sect. B*, 33, 6366-6374, 1986.
- Mandelbrot, B.B., *The Fractal Geometry of Nature*, W.H. Freeman and Company, San Francisco, CA, 1982.
- Mandelbrot, B.B., D.E. Passoja, and A.J. Pauley, Fractal character of fracture surfaces of metals, *Nature*, 308, 721-722, 1984.
- Martin, J.E. and Hurd, A.J., Scattering from Fractals, *J. Appl. Crystallogr.*, 20, 61-78, 1987.
- Okuba, P.G. and K. Aki, Fractal geometry in the San Andreas fault system, *J. Geophys. Res.*, 92, 345-355, 1987.
- Quiblier, J.A., A New Three-Dimensional Modeling Technique for Studying Porous Media. *J. Colloid and Interface Sci.*, 98, 84-102, 1984.
- Sun, H and M. Koch, Fractal generation of surface area of porous media, *J. Stochast. Hydrology*, 1998 (In Press).
- Tompson, A.F.B., Ababou, R. and Gelhar, L.W., Implementation of the three-dimensional turning bands random field generator. *Water Resources Research*, 25, 2227-2243, 1989.
- Thompson, A.H., Fractals in rock physics, *Annu. Rev. Earth Planet. Sci.*, 19, 237-262, 1991.

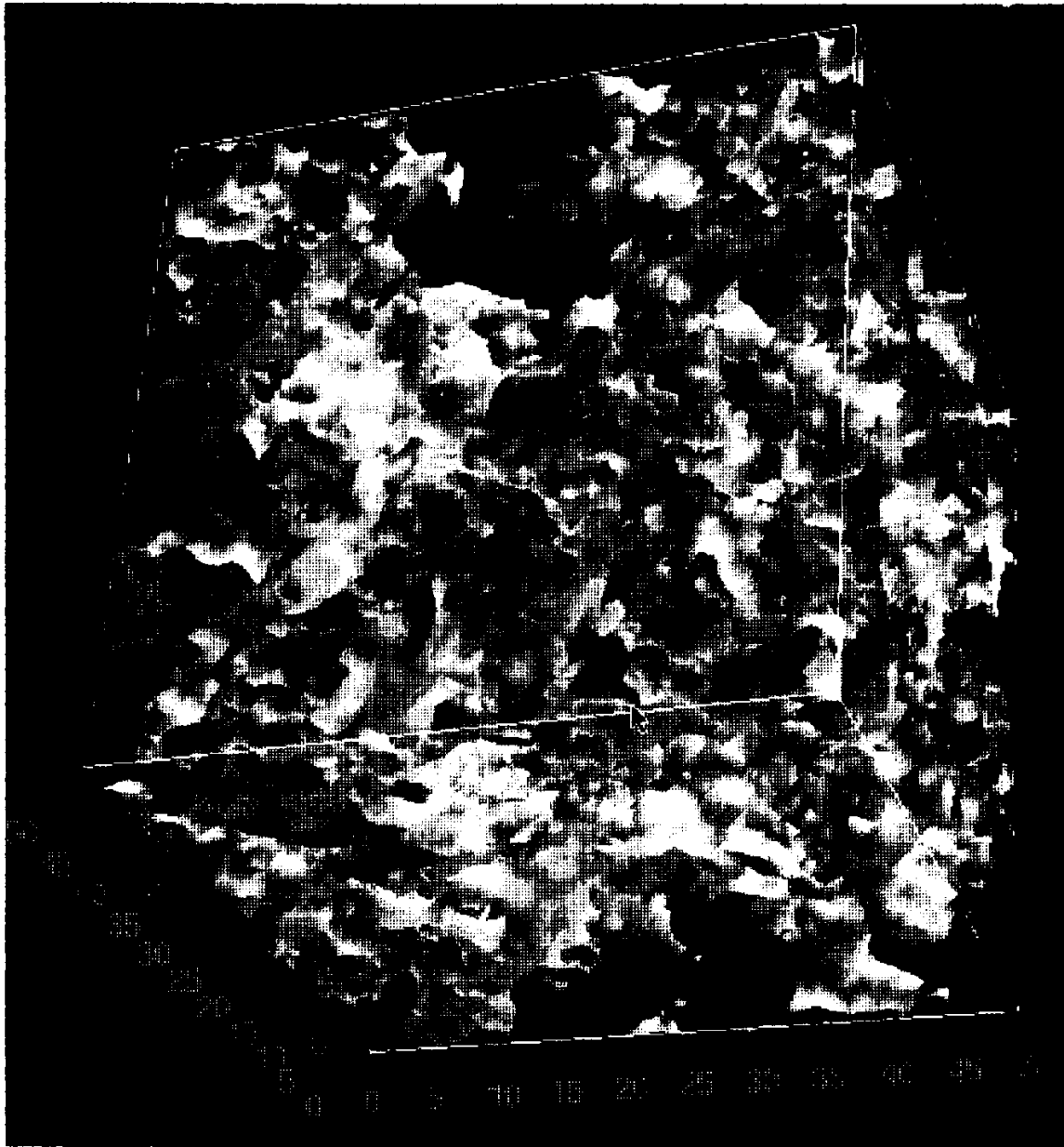


Figure 1. A typical realization of an isotropic Gaussian porous structures with different correlation lengths β ; $\beta=(3,3,3)$;

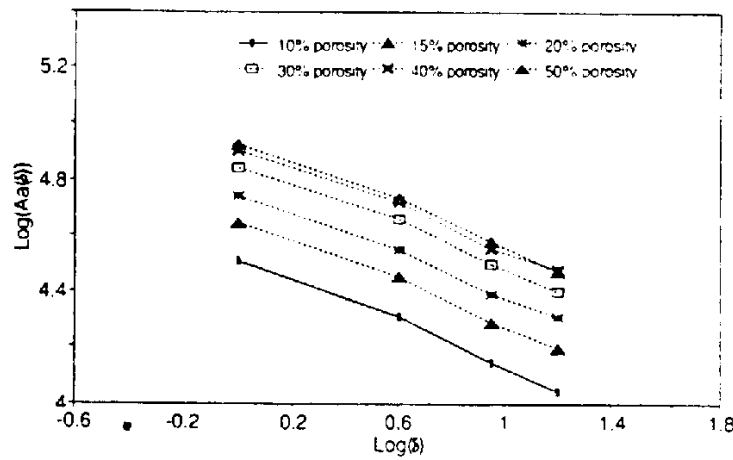


Figure 2. Log-log plot of $A_a(\delta)$ as a function of δ for different porosities of the Gaussian PDF field with an anisotropic structure, $\beta=(1,2,3)$. $D_{av}=2.76\pm.05$.

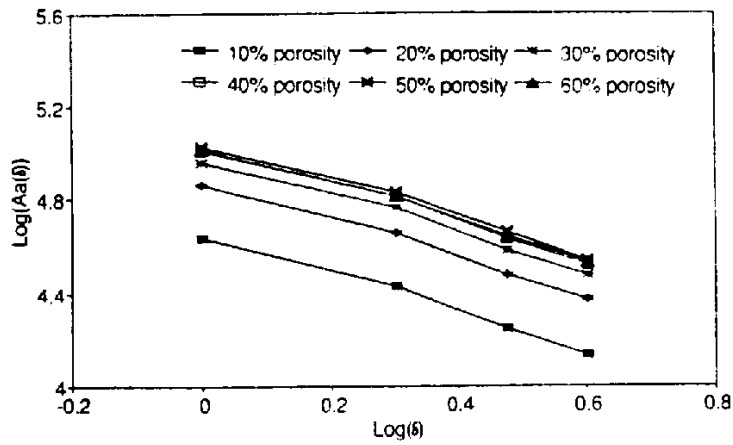


Figure 3. Similar to Fig. 2, but for a non-Gaussian, quadratic PDF, $Y=(x-a)^2$, and an isotropic, structure, $\beta=(1.9,1.9,1.9)$. $D_{av}=2.82\pm.03$.

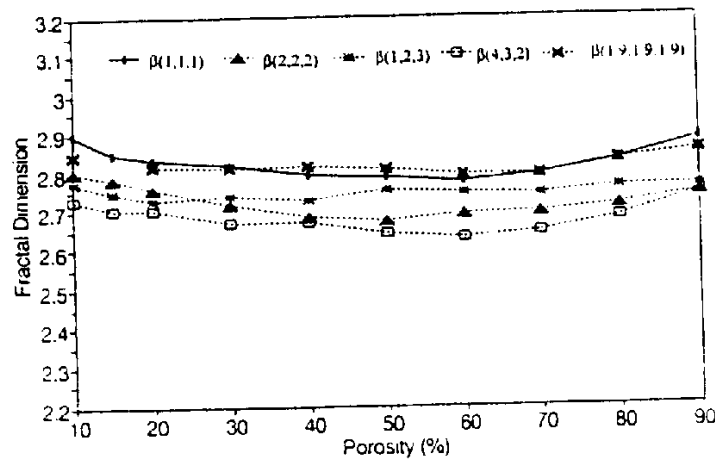


Figure 4. Fractal dimensions D versus porosity for four Gaussian ($D_{av}=2.76\pm.05$) and one non-Gaussian ($D_{av}=2.82\pm.03$) porous structures (case $\beta=(1.9,1.9,1.9)$).