A new model for predicting saturated hydraulic conductivity and diffusion coefficient of granular soils using fractals

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Abstract

There is a general interest in quantifying soil structure to obtain physically based parameters relevant to transport processes. Fractals offer new opportunities to address the relation between structure and a range of physical processes occurring in the soil. In this paper, a random model matrix satisfying the particle size distribution and porosity of a heterogeneous soil structure is constructed. This model is used to predict the saturated hydraulic conductivity and the diffusion coefficient of granular soil. A comprehensive study is conducted to evaluate the usefulness of the proposed model using fractals by comparing the results with the available experimental data.

Keywords: fractal, hydraulic conductivity, diffusion.

Introduction

Modern hydrological models require information on the macroscopic transport properties such as hydraulic conductivity and diffusion coefficient. The fractal geometry theory has been proven to be powerful means for analysis of porous media with complex and random microstructures and its developments have led to a better understanding of material properties and apparently chaotic processes in nature. In many aspects, soil structure is a fractal. A connection between geometry and transport is facilitated when geometry can be described by a small set of parameters such as with a fractal model and assuming fractal scaling of various physical properties of a porous medium [1]. Fractal models also applied to the prediction of two important soil hydraulic properties, i.e. hydraulic conductivity and the soil-water retention characteristic based on a theoretical relationship between the geometry of a porous medium and the flow through it [2]. Crawford et al. (1993) discussed the use of fractal dimensions in diffusion theory applied to pedal soil [3]. Anderson et al. (1996) applied this theory to images of different soil types [4]. Subsequently, the possibility of using image analysis of soil thin sections to compare the relative diffusivities of soil samples was explored and the key structural parameters that determine the magnitude of the diffusivity coefficient were identified by determining their relative importance [5]. A fractal permeability model for bi-dispersed porous media was developed [6] and the analytical expression for the permeability and the Kozeny–Carman constant based on the fractal geometry theory was derived [7]. The inner surface of a porous medium is commonly determined from digital images of soil thin sections or soil blocks [8, 9, 4, 5, 10, 11, 12, 13, 14, 15].

In this paper, a new random model matrix satisfying the particle size distribution and porosity of a heterogeneous soil structure is proposed with the working assumption that there exists a theoretical relationship between the geometry of a porous medium and the flow through it. Each generated model is considered as soil thin section and used to predict the saturated hydraulic conductivity and the diffusion coefficient of granular soil based on structural characteristics within the tortuous porous media by measuring related fractal dimensions. At last, the available experimental data are used to compare with the predicted transport coefficients to evaluate the applicability of this model.

The fractal characteristics of soil

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Fractals provide a unique quantitative framework for integrating soil biological, chemical and physical phenomena over a range of spatial and temporal scales. There are several fractal dimensions of interest and for complete characterization of soil structure and scaling of different properties of soil physical processes, more than one fractal dimension need to be measured [4, 11, 16].

Calculating Fractal dimensions

The box counting method can be used to measure fractal dimensions, or more specifically, fractal capacity dimensions of the pore and the matrix phase. These dimensions can be described by the ratio between the logarithm of an iteration rule and the logarithm of the scale increment. The measurement method takes advantage of the assumed self-similar scaling behavior, which allows applying the equation:

$$N(\lambda) \propto \lambda^{-D} \tag{2}$$

The power law describes the number of boxes N of a specific feature as a function of their side length r with an exponent D. Thus, whenever measured box counts can be described by Eq. (2) using a non-integer value for D, the feature is considered to be a fractal with D as the fractal dimension.

The binary image is covered with square grids of progressively larger sizes, i.e., each time the size is increased; a square encloses a larger number of pixels. For each size square, λ_i, the total number of squares enclosing pixels representing the property of interest is counted, and later plotted as a function of λ_i. Special care was taken so that none of the pixels in the object were obscured by grid lines. Thus, for fractal objects a double-logarithmic plot yields a straight line:

$$\log N(\lambda) = -D \log \lambda + c \tag{3}$$

and D can be determined as the absolute value of its slope. The constant c describes the ordinate intercept. Fig. 1 shows an example of the technique applied to the scaling of pore area.

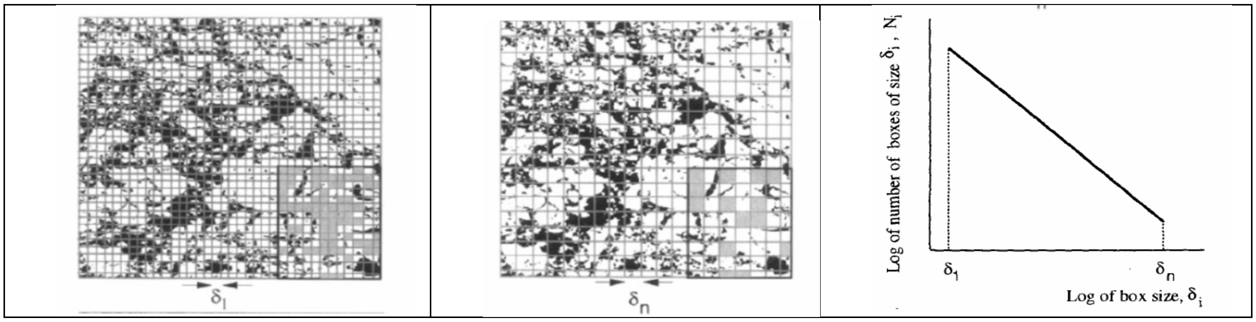

Figure 1: Example of a box-counting technique applied to the scaling of pore area.

Fragmented fractal dimension D

PSDs have been analyzed with power-law functions relating cumulative number of particles to diameter and mass of particles to diameter, and the exponents interpreted as fragmentation fractal dimensions (D) [17, 18, 19, 20, 21]. For different types of objects, a power-law relation between the number and size of objects has been proposed [22, 17]:

$$N(r > R) = CR^{-D} \tag{4}$$

where $N(r > R)$ is the number of objects per unit volume, C is a constant of proportionality. The mass-based is compatible with data obtained from experimentation, where usually mass fractions rather than number fractions are measured. The mass–size form of the Eq. (4) used in this study is expressed as [18]:

$$\frac{M(r < R)}{M_T} = \left(\frac{R}{R_{lu}}\right)^{3-D} \tag{5}$$

where M(r<R) is the mass of soil particles with a radius smaller than R, M_T is the total mass of particles with radius less than R_{Lu}, the upper size limit for fractal behavior, and D is the fragmentation fractal dimension. The radii R of particles satisfying Eq. (5) are confined between $R_{Ll}<R<R_{Lu}$, where R_{Ll} is the lowest limit of validity of the fractal

behavior. Eq. (4) can be rearranged in a log–log scale, thus providing the way of finding the fractal dimension from the slope of the regression log[M $(r<R)$ /M_T] vs. log[R].

Pore area fractal dimension D_f

The pore area fractal dimension D_f can be determined based on the box-counting method [23]. This method is based on the image analysis of a unit cell or a sufficiently large cross-section of a sample along a plane normal to the flow direction. In this method, the cross section under consideration is discretized using square boxes of size, λ, then the number, N (λ), of boxes required to completely cover the pore areas is counted. The pore area fractal dimension, D_f, can be determined by the value of the slope of a linear fit through data on a logarithmic plot of the cumulative number of pores N $(L > \lambda)$ versus the pore size λ.

Tortuosity fractal dimension D_t

There is a similarity of tortuosity of flow pathways between clusters and between particles within clusters; thus, it is need to determine only the tortuosity of pathways between clusters. Because the tortuosity of flow paths between clusters is very similar to the streamtubes in heterogeneous media or coastlines, therefore, the tortuosity dimension D_t can also be determined by the box-counting method. The same software is now applied to find the tortuosity fractal dimension D_t of this flow pathways based on the box-counting method.

Spectral dimension d

The spectral dimension is a measure of connectivity in a percolating fractal network and can also be useful when describing the physical processes such as diffusion confined to a fractal network [24]. A number of eight connected random walks (that is, to any of the eight pixels surrounding the current pixel) are conducted to estimate the spectral dimension. For each walk, a starting pore pixel is randomly picked and then the random walk steps are taken till the stopping criteria of the program satisfied. If after each random walk step a new pixel has been visited, then 1 is added to the number of distinct site visited (Sn) and if a site has been visited previously (a null step) then 1 is added to the number of steps taken and 0 is added to Sn. The program is set to stop after 100 null steps for each individual walk or an edge of the image is hit and the number of walks used in this study is 50. The spectral dimension is calculated from a plot of ln(Sn) vs. ln(number of steps taken, n). The slope of this line is taken to be equal to d/2 [3]. This method is shown diagrammatically in Fig.2.

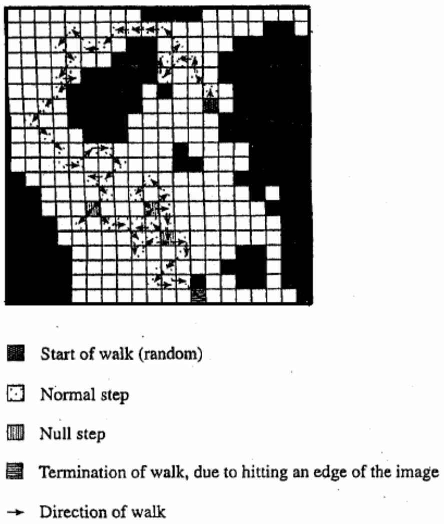

Figure 2: A simplified example of one random walk through the pore space

Mass fractal dimension D_m

The mass fractal dimension is used to describe the fractal properties of space-filling objects. If the object did fill space uniformly, then $D_m = D_E$, the Euclidean dimension, while for fractal objects D_m is less than the embedding dimension. The mass of a fractal object increases with the characteristic radius (r) by a simple power law

$$M \propto r^{D_m} \tag{6}$$

The D_m can be measured for pore or solid space of soil thin sections with progressively larger boxes. Based on the box counting method by constructing a grid which covers the digital image of box size λ and counting the number of boxes that included part of the object as a function of grid spacing λ, the value of D_m is estimated from a plot of ln(number of pore/solid λ pixel) vs. ln(λ). The range of grid spacing that would produce such a relation would be between the pixel size p and the image size L.

Diffusion

The diffusion process is most applicable to the transport of gases, non-reactive solutes and gee-swimming microbes in soils. A particle moving through a fractal network is restrained to that fractal network, so diffusion of solutes in a fractal pore network does not obey Fick's law. Crawford et al. (1993a) described diffusion process by replacing the constant diffusion coefficient in the classical diffusion equation with a term that includes fractal dimensions for both the pore size distribution and the particle trajectory [3]. For fractal networks, the conventional diffusion coefficient, D, is replaced by a length-dependent diffusion coefficient, D(r), where r is the Pythagorean length [24]. Anderson et al. (2000) presented a full expression for the diffusion coefficient as [5]:

$$D(r_c) = D_0 \phi(r_c)^{\zeta} (r_c / r_1)^{-\eta} : \quad \begin{cases} \zeta = \left[2(1 - D_m / d)\right] / (D_m - 2) \\ \eta = 2(D_m - d)/d + D_m - 2 \end{cases} \tag{7}$$

The value of r1 is the value of the length scale below which there is significant departure from linearity and both porosity $\Phi(r_c)$ and sample size r_c influence the value for the diffusion coefficient. The heterogeneity and connectivity, as quantified by the mass fractal dimension (D_m) and spectral dimension (d), respectively, are estimated from sections of random model.

Saturated Hydraulic Conductivity

Saturated hydraulic conductivity, K_{sat}, is an important soil property in various fields such as ground water flow, water/oil reservoirs, chemical engineering, medicine, biochemical and electrochemical engineering. An analytical expression for the permeability in homogeneous porous media based on the fractal characters of porous media and capillary model was derived. The proposed model is expressed as a function of fractal dimensions, porosity and maximum pore size [7]:

$$K = C_f \left(\frac{\phi}{1-\phi} \right)^{(1+D_T)/2} \lambda_{\max}{}^{2} \tag{8a}$$

where the coefficient Cf is also related to porosity

$$C_f = \frac{(\pi D_f)^{(1-D_t)/2} \left[4(2-D_f)\right]^{(1+D_T)/2}}{128(3 + D_T - D_f)} \tag{8b}$$

which indicates that the permeability is a function of the pore area fractal dimension D_f, tortuosity fractal dimension D_T, porosity Φ and maximum pore size λ_{max}. Comparing with other permeability–porosity relations such as Kozeny–Carman equation, this analytical permeability (with no empirical constant) has more fundamental physical significance. This equation with four microstructure parameters (D_f, D_T, Φ and λ_{max}) is a more generalized permeability model and can be used to calculate saturated hydraulic conductivity.

Random Model Matrix (RMM)

Knowing the particle size distribution and porosity of a given soil (cohesive soil) sample, it will be possible to convert the retained mass on each sieve to the number of particles of that specific size. The relative number of the ith size fraction can be obtained from Mi using the equation [25]:

$$M_i = N_i \left(G_i x_i^{\,3} \right) \tag{9}$$

where G_i is a factor that combines the effect of bulk density and aggregate shape, and is considered constant, M_i is the relative mass fraction of size i and N_i is the number of aggregate with size i. Consequently, knowing the porosity, the total volume of the soil sample, V_t, can be measured and a matrix is filled randomly with N_i number of maximum particles of size i. In next step, the matrix is divided into smaller fraction such that the unfilled cells can be filled randomly with smaller particles (N_{i-1}) of size i-1 and this procedure is continued till the minimum particles fill empty cells and a random model matrix will be generated. This matrix is considered as a representative random model of granular porous media. The results of pore-size distribution of soils using fractals on the number-size distribution of voids which is collected in 2-D by image can be extrapolated to 3-D by the relation $D_3 = D_2 + 1$ [13]. This model can be used as soil thin sections to calculate the fractal dimensions of a soil knowing the particle size distribution and porosity of given soil sample.

Results and discussion

Gimenez et al. (1997) determined saturated hydraulic conductivity of six aggregate fractions, with mean aggregate diameters, x_m, of 8.4, 4.7, 2.9, 1.5 and 0.4 mm [12]. A fragmented fractal dimension of 2.12 + 0.15 was determined for this soil where the soil packed as a duplicate coloumn with porosity of Φ=0.45. In this study, a particle size distribution with the same fragmentation fractal dimension was considered and the random model matrix of this soil sample was generated to determine the magnitude of saturated hydraulic conductivity and the diffusion coefficient by calculating fractal dimensions of pore space as shown in Fig. 3. Assuming specific gravity, Gs=2.65, and using Eq. (9) the number of ith aggregate size fraction were obtained from PSD of the soil sample. As discussed previously, a representative random model of soil thin section can be easily constructed.

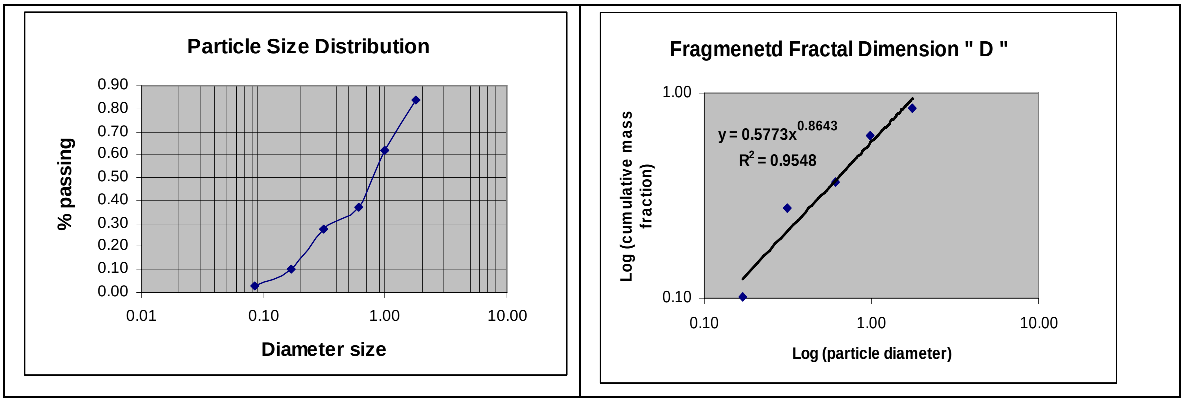

Figure 3: Particle size distribution and method of calculating fragmented fractal dimension.

The number of each aggregate size needed to generate the RMM is presented in Table 1 and two samples of RMM are shown in Fig. 4.

Table 1: Number of aggregate size obtained from PSD

Particle Size (mm)	Passing (gr)	N for model
28		0
15.6	100.0	0
8.4	84.1	10
4.7	62.0	9
2.9	36.9	14
1.5	27.4	37
0.8	10.2	74
0.4	2.8	174

Fig. 5a shows a logarithmic plot of ln(Sn) vs. ln(number of steps taken, n).The spectral fractal dimension is determined from the slope of the straight line which gives a typical value of d=1.60 for an individual random walk that is terminated after 100 null steps. The capability of the proposed model to simulate the physical processes such as diffusion through a fractal network is shown in Fig. 5b for a random walk which is set to stop after 1000 null steps.

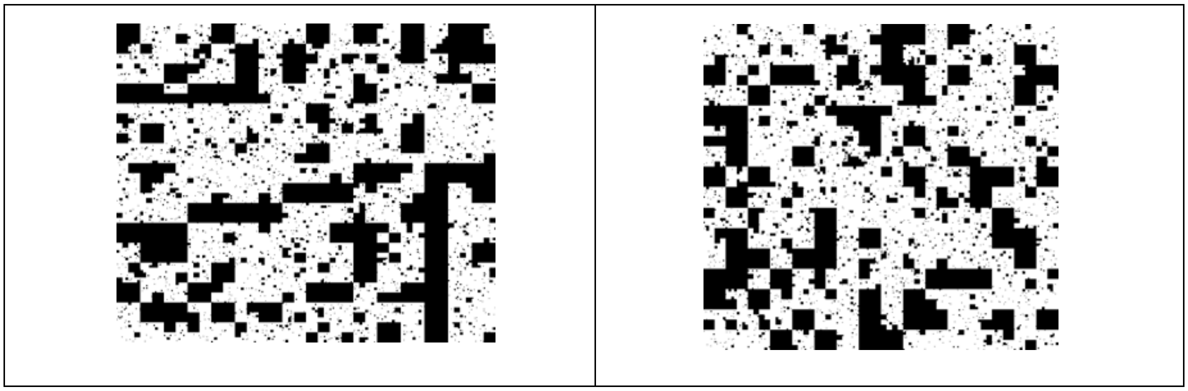

Figure 4: Two samples of random model matrix (RMM)

The procedure to calculate the magnitude of toruosity fractal dimension of random flow pathway using box counting method is demonstrated in Fig. 6a and Fig. 6b presents a random flow pathway between clusters in the porous sample of RMM where the flow is assumed under a pressure gradient from left to right.

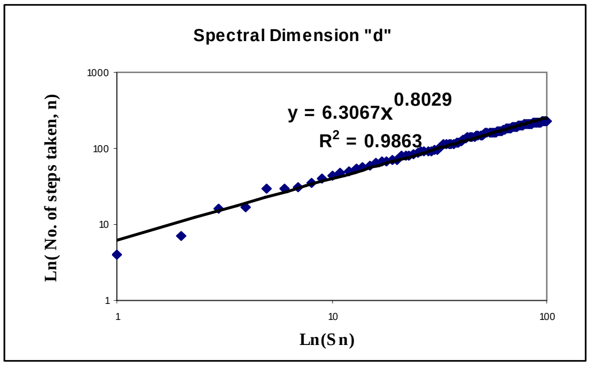

Figure 5a: Determination of spectral fractal dimension for an individual random walk

Figure 5b: A random walk through the pore space with 1000 null steps

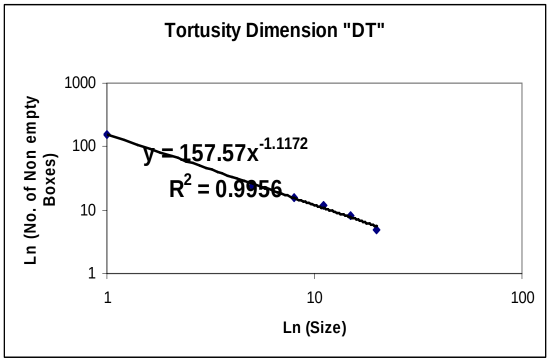

Figure 6a: Determination of tortuosity fractal dimension of a pathway

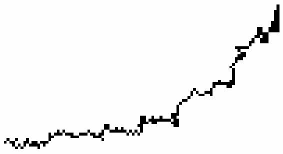

Figure 6b: A tortuous pathway for flow through the porous sample

All fractal dimensions required to predict the saturated hydraulic conductivity and the coefficient of diffusion were calculated by the methods discussed in the foregoing sections.

Table 2 contains a summary of results after conducting these procedures for five RMM generations. Although, in each generation a new random model matrix is constructed, however, as shown in Fig.7 it is obvious that the magnitude of averaged saturated hydraulic conductivity and diffusion coefficient converge to a specific value. As indicated in Table 2, the average value of Ksat is equal to 119.4 which is very close to the experimental value for K_{sat} of 115.2 as determined by Gimenez et al. (1997) [12].

Table 2: The results of 5 generation of RMM

Model	λmax, (mm)	Dm	d	Dt	Df	Ksat , (μm s-1)	D/D0, m2/s $*10^{-2}$
1	8.0	1.88	1.53	1.07	1.83	126.1	1.47
2	7.2	1.88	1.57	1.10	1.83	120.1	2.77
3	7.2	1.88	1.66	1.12	1.83	116.3	10.34
4	7.6	1.88	1.58	1.01	1.83	125.4	3.23
5	7.2	1.88	1.68	1.03	1.83	109.0	13.59
Average	7.4	1.88	1.60	1.07	1.83	119.4	6.28

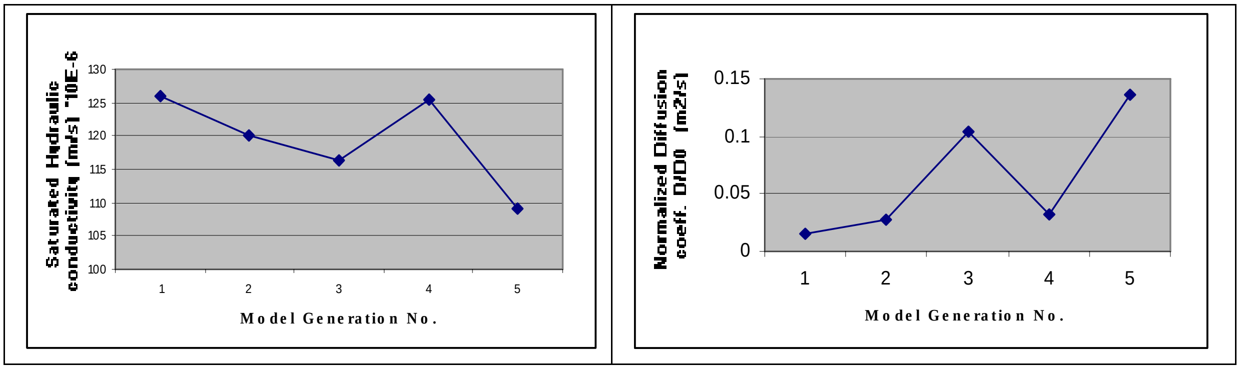

Figure 7: Variation of Saturated hydraulic conductivity and diffusion coefficient for 5 model generation

Conclusion

In this paper, a model was proposed to predict the saturated hydraulic conductivity and diffusion coefficient of granular media. The proposed random model matrix is simply generated from particle size distribution and porosity of the soil media which may be considered as a representative of soil thin section. The model incorporates the pore area and tortuosity fractal dimensions for predicting saturated hydraulic conductivity of the porous media. The model also assumes mass and spectral fractal dimensions for predicting diffusion coefficient of the medium. The generated model was then used to determine the required fractal dimensions. The accuracy of the proposed approach was verified by comparing the model prediction with the available experimental results in literature. The comparison indicated the suitability of the model for prediction of soil parameters such as hydraulic conductivity and diffusion coefficient. However, further works are needed to enhance the model in order to be capable of predicting these parameters for other soil types, such as soils with considerable plasticity.

References

1. Muller, J. and McCauley, J.L. (1992) Implication of fractal geometry for fluid flow properties of sedimentary rocks. *Transp. Porous Media*, **8**, 133-147.

2. Gimenez, D., Perfect, E. Rawls, W.J. and Pachepsky, Ya. (1997a) Fractal models for predicting soil hydraulic properties: a review, *Engineering Geology*, **48**, 161-183.

3. Crawford, J.W., Ritz, K. and Young, I.M. (1993a) Quantification of fungal morphology, gaseous transport and microbial dynamics in soil: an integrated framework utilizing fractal geometry. *Geoclerma*, **56**, 157-172.

4. Anderson A.N., McBratney A.B. and FitzPatrick E.A., (1996) Soil mass, surface, and spectral dimensions estimated from thin section photographs. *Soil Sci. Soc. Am. J.*, **60**, 962-969.

5. Anderson A.N., Crawford, J.W. and McBratney, A.B. (2000) On Diffusion in Fractal Soil Structures. *Soil Sci. Soc. Am. J.*, **64**, 19-24

6. Yu, B.M. and Cheng, P. (2002) A fractal permeability model for bi-dispersed porous media. *Int. J. Heat Mass Transfer,* **45**, 2983–2993.

7. Xu, P. and Yu, B.M. (2007) Developing a new form of permeability and Kozeny–Carman constant for homogeneous porous media by means of fractal geometry. *Advances in Water Res.*, **31** (1), 74-81.

8. Hatano, R., Kawamura, N., Ikeda, J. and Sakuma, T. (1992) Evaluation of the effect of morphological features of the flow paths on solute transport by using fractal dimensions of methylene blue staining patterns. *Geoderma*, **53**, 31-55.

9. Crawford, J.W., Sleeman, B.D. and Young, I.M., (1993b) On the relation between number-size distributions and the fractal dimension of aggregates*. J. Soil Sci.*, **44**, 555-565.

10. Bird, N., Dıaz, M.C., Saab, A. and Tarquisc, A.N. (2005) Fractal and multifractal analysis of pore-scale images of soil. *Journal of Hydrology*, **212** (322), 211–219.

11. Pachepsky, Y. and Timlin, D. (1998) Water transport in soils as in fractal media. *Journal of Hydrology*, **204**, 98-107.

12. Gimenez, D., Allmaras, R.R., Huggins, D.R. and Nater, E.A. (1997b) Prediction of the Saturated Hydraulic Conductivity-Porosity Dependence Using Fractals. *Soc. Am. J.,* **61**, 1285-1292.

13. Dathe, A., Eins, S., Niemeyer, J. and Gerold, G. (2001) The surface fractal dimension of the soil–pore interface as measured by image analysis. *Geoderma*, **103**, 203– 229.

14. Dathe, A. and Thullner, M. (2005) The relationship between fractal properties of solid matrix and pore space in porous media. *Geoderma*, **280** (129), 279–290.

15. Bird, N.R.A. and Dexter, A.R. (1997) Simulation of soil water retention using random fractal networks, *Eur. J. Soil Sci.*, **48**, 633–641.

16. Gimenez, D., Allmaras, R.R., Nater, E.A. and Huggins, D.R. (1997c) Fractal dimensions for volume and surface of interaggregat. *Geoderma*, **77**, 19-38.

17. Turcotte, D.L. (1986) Fractals and fragmentation. J. *Geophys. Res*., **91**, 1921–1926.

18. Tyler, S.W. and Wheatcraft, S.W. (1992) Fractal scaling of soil particle size distributions: analysis and limitations. *Soil Sci. Soc. Am. J.,* **56**, 362–369.

19. Wu, Q., Borkovec, M. and Sticher, S. (1993) On particle size distributions in soils. *Soil Sci. Soc. Am. J.,* **57**, 883–890.

20. Bittelli, M., Campbell, G.S. and Flury, M. (1999) Characterization of Particle-Size Distribution in Soils with a Fragmentation Model. *Soil Sci. Soc. Am. J.*, **63**, 782–788.

21. Filgueira, R.R., Fournier, L.L., Cerisola, C.I., Gelati, P. and García, M.G. (2006) Particle-size distribution in soils: A critical study of the fractal model validation. *Geoderma*, **134**, 327–334.

22. Mandelbrot, B.B. (1982*) The Fractal Geometry of Nature*. W.H. Freeman, New York, 23–57(see also pp. 117–119).

23. Feder, J. and Aharony, A. (1989) *Fractals in Physics*. North-Holland, Amsterdam.

24. Orbach, R. (1986) *dynamics of fractal network. Science*. Washington, DC 231, 814-819.

25. Logsdon, S.D., Gimenez, D. and Allmaras, R.R. (1996) Fractal characterization of aggregate size distribution: The question of scale invariant. *Soil Sci. Soc. Am. J.*, **60**, 1327-1330.