FRACTAL THEORY TO SIMULATE UNSATURATED TRANSPORT PROPERTIES

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ABSTRACT

We investigate fractal characteristics of solute transport as viewed from dye experiments. Experiments performed within the EU-sponsored research HYDROMED (a research program on hill reservoirs in the semiarid Mediterranean periphery) are used to test two different fractal model concepts; the diffusion limited aggregation and the random cascade model. Solute transport properties as indicated from dye coverage experiments displayed fractal properties as viewed by power spectrum analyses and probability distribution characteristics. The diffusion limited aggregation model was calibrated and verified for two plots. The verified model agreed very well to observed data. The random cascade model was calibrated for one experimental plot. Some over-estimation appeared to be the case. However, the general spatial pattern appeared to agree well with observed data. It remains to perform a rigid statistical test for the performance of the random cascade model.

INTRODUCTION

Field properties of preferential pathways for water and solutes are still not well understood (e.g., Booltink and Bouma, 1991; Bouma, 1991). Due to this and an increasing awareness of its importance for groundwater and general environmental quality, preferential flow at unsaturated field conditions has become an increasingly important research issue (e.g., Beven and Germann, 1982; Hillel, 1991). A reason for observed discrepancy between field scale transport and results from homogeneous media assumption may be that our tools of observation at field scale are not yet detailed enough to yield information at the relevant scales. Often it is the complicated three-dimensional flow structures at micro-scale that determines the actually observed field scale variation.

A technique to investigate actual field scale transport patterns at micro-scale may be to use dye tracers (e.g., Flury et al., 1994). Images of dyed soil transects provide an excellent resolution at the spatial scale. However, they usually give no information at the temporal scale. Dye data, however, may lead to the development of new model concepts that more accurately can depict complicated spatial patterns of solute transport (e.g., Schwartz et al., 1999).

A possible way to consider scaling in soil transport properties as well as modeling the observed dye formations may be to use fractal theory. Fractal patterns or soil properties are often observed at the field scale for related subsurface transport (e.g., Feder, 1988; Kemblowski and Wen, 1993; Baveye et al., 1998). Similarly, fractal transport models have been developed by several researchers (e.g., Wheatcraft and Tyler, 1988; Flury and Flühler, 1995; Mukhopadhyay and Cushman, 1998; Pachepsky and Timlin, 1998).

In the present paper we investigate fractal properties of observed dyed soil transect images at field conditions. Experimental data from an ongoing European Union cooperation (HYDROMED, a research program on hill reservoirs in the semiarid Mediterranean periphery) were used within this study (see e.g., Öhrström et al., 2000). We use the data to indicate fractal properties and also to test two different fractal models to generate observed properties; diffusion-limited aggregation and random cascade process. We close with a discussion on further development.

MATERIALS AND METHODS

Theory

Diffusion-limited aggregation (DLA)

Witten and Sander (1981) introduced this model concept already two decades ago. An advantage is that the DLA model can generate fractal transport patterns (e.g., Flury and Flühler, 1995; Meakin, 1991). In general, the DLA model generates spatial clusters of the solute by randomly walking particles. Particles are randomly generated from a line source at some distance below the soil surface. By random walk the particles may finally reach up to the line seed (soil surface). When the particles reach the seed they become part of the seed and remain attached at that position (Flury and Flühler, 1995). New particles that reach the seed permanently attach and form a gradually increasing cluster. The process can be halted once some pre-defined maximum depth is reached by the growing cluster z_{max}. The randomly walking particle can consequently move in four directions depending on probabilities, P_u, P_d, P_r, and P_l, corresponding to upward, downward, right and left walk in the two-dimensional grid, respectively.

$$P_u + P_d + P_r + P_l = 1.0 \tag{1}$$

An isotropic random walk model has the following probability distribution:

$$P_u = P_d = P_r = P_l = 0.25 \tag{2}$$

By changing these probabilities, anisotropic conditions may be simulated. Also, layered soils may be simulated by including different walking probabilities for different soil depths (see further e.g., Flury and Flühler, 1995). The DLA model should be seen as a conceptual model within the microscale. Therefore, output from the DLA model has to be averaged over a suitable space in order to be comparable to the scale of observations (see further Persson et al., 2000).

Random cascade process

Dyed soil transects may also be modeled within a multifractal framework. In terms of statistical moments, scaling implies that for the random field $R(\mathbf{x})$ the average qth order moment of the coarse-grained field R_λ relates to the coarse-graining scale λ as

$$\left\langle R_\lambda^q \right\rangle \propto \lambda^{-K(q)} \tag{3}$$

where angle brackets denote (ensemble) averaging. Coarse-graining means decreasing the resolution of the field by taking spatial averages over non-overlapping squares of side λ (see, e.g., Davis et al., 1994). If the function $K(q)$, which essentially represents an infinite hierarchy of fractal dimensions, is nonlinear (convex) the data can be described as multifractal (Frisch and Parisi, 1985). The multifractal behavior as expressed by (3) is related to the exponents obtained from probability density functions and spectral analyses. According to, e.g., Mandelbrot (1974), for $q>q_{cr}$ $K(q)$ becomes linear due to the divergence of moments. It should, however, be mentioned that an asymptotically linear $K(q)$-function has also been deduced as a general property of scaling (or self-similar) fields (Menabde et al., 1997). Further, for (3) to be valid it is required that β is less than the Euclidean dimension of the observed space, i.e., $\beta<2$ for spatial fields (e.g., Menabde et al., 1997).

Assuming an underlying multiplicative cascade process with a Lévy-distributed generator Schertzer and Lovejoy (1987) parameterized $K(q)$. In a multiplicative cascade process, the investigated quantity is transferred to successively smaller scales by means of multiplicative weights, and the generator specifies the statistical distribution of these weights (see e.g., Davis et al., 1994). The approach of Schertzer and Lovejoy (1987) was termed a 'universal multifractal model' in which $K(q)$ is expressed as

$$K(q) = \begin{cases} \dfrac{C_1(q^\alpha - q)}{\alpha - 1} & \alpha \neq 1 \\ C_1 q \log(q) & \alpha = 1 \end{cases} \tag{4}$$

where α and C_1 characterize the Lévy-distribution. The parameters may also be interpreted in fractal terms; α specifies the degree of multifractality and C_1 characterizes the fractal behavior of the mean process. A method known as 'double trace moments' may be employed for parameter estimation (e.g., Lavallée, 1991; Tessier et al., 1993). For a field R transformed into R^η, $K(q)$ becomes $K(q,\eta)$ and these two functions are related as

$$K(q,\eta)=\eta^{\alpha}K(q) \tag{5}$$

which means that α may be estimated by plotting $K(q,\eta)$ as a function of η in a log-log diagram. With a known α, C_1 may be estimated using (4) by $K(q)=K(q,1)$. It is possible to check the validity of the estimated parameters by comparing (4), e.g., with the 95% confidence interval of the empirical $K(q)$-functions.

In the universal multifractal model, the deviation from conservation is specified by the parameter H given by

$$H=\frac{\beta-(1-K(2))}{2}=\frac{\beta-1}{2}+\frac{C_1(2^{\alpha}-2)}{2(\alpha-1)} \tag{6}$$

which is an estimation of the power law filtering exponent required to obtain conservation (e.g., Tessier et al., 1993).

Experimental data

Experimental data from an ongoing European Union cooperation (HYDROMED, a research program on hill reservoirs in the semiarid Mediterranean periphery) were used within this study (see Öhrström et al., 2000). Experiments were conducted in the M'Richet el Anze catchment located 110 km southwest of Tunis in Tunisia. At the time of experiments (October 1996) the soils lay fallow. The average amount of rainfall in the area is 455 mm per year and the yearly average temperature is 16.6 °C. The soil may be described as a Typic Xerochrepts according to the classification of Soil Survey Staff (1996).

Fig. 1: Example of a dye image from plot 1.

At six plots, within a small catchment, dye stained water was applied. The tracer used was food-grade dye pigment Vitasyn-Blau AE 85 (Swedish Hoechst Ltd.), similar to the more commonly used Brilliant Blue. This dye has been used in several field experiments due to its good visibility, low toxicity, and weak adsorption on soils (e.g. Flury et al., 1994; Aeby et al., 1997). A rainfall simulator (Bernard, 1987) was used to simulate a heavy rainstorm during about 1.5 hrs over 1.0 m^2. Placing an iron frame of size 1 by 1 m at each site created the 1.0 m^2 plots. In order to avoid border effects, totally about 9 m^2 were covered by the rainfall simulator. Surface runoff was collected through a discharge weir in the iron frame. A total of about 45 mm were infiltrated at each plot. The surface plots did not contain any visible vegetation and the soil surface was homogenized down to depth of 2 cm. After the simulations, the plot was covered to avoid evaporation. About 24 hrs after the rainfall, a trench was dug and vertical sections of 2.5 cm thickness were excavated, resulting in 41 sections at each plot. Photos were taken of the vertical sections by a 35-mm camera with Kodachrome 64 film. The color photos were converted to black and white images bye use of the Adobe Photoshop™ (version 4.0, Adobe Systems, Inc.) software (Fig. 1). The resolution of the converted black and white images corresponded to a pixel size of 0.14 cm. However, when the images were compared to the DLA model simulation, they were re-scaled to a pixel size of 4 by 4 cm. This leads to a lower resolution, however, the horizontal average of the dye structures did not change significantly with the pixel size.

RESULTS

DLA model simulations

Initial tests for fractal behavior of the data were performed by power spectrum analyses and probability distributions (see Olsson et al., 2000). The power spectrum typically displayed power-law behavior extending over the entire frequency range. The probability distribution analyses displayed a hyperbolic tail for the majority of the plots. Consequently, both analyses indicate a fractal behavior.

Figure 2 shows an example of the general procedure to use the DLA model concept and the comparison to dye images. It should be noted that the DLA is a stochastic model that gives a randomly varying output. Therefore, individual model outputs and observations can not be compared directly. Instead, statistical properties of model output and observations have to be compared. This is seen in Fig. 3, which shows a comparison between average and standard deviation of dye coverage with depth for simulations using the calibrated DLA and observations at plots 1 and 2.

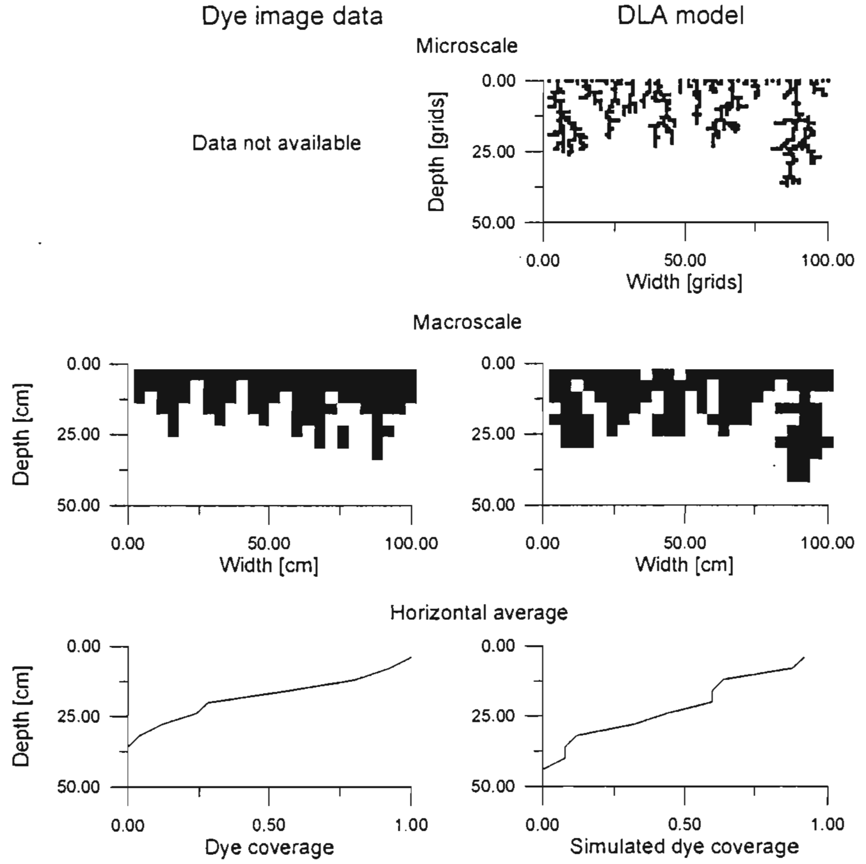

Fig. 2: Example of DLA model concept and a comparison between model results and observations. Note that the macroscale dye image data was calculated from the dye image shown in Fig. 1.

As seen from the figure model results and observations agree well between the average dye penetration and the average of 369 DLA model realizations. To test the DLA model against independent data the calibrated model was verified using data from plot 2. This is seen in Fig. 3 showing a comparison between simulated and observed dye coverage with depth. Here, it should be stressed that model parameters were kept constant and no information from plot 2 other than the distribution of maximum dye penetration was used when running the model. Even so, as seen from the figure, the match between model and observations is quite satisfactory with a r^2 value of 0.997 between the average dye penetration and the average of 369 DLA model realizations. This confirms the applicability of the model concept and that the DLA can be used to simulate both average and variation in the soil at the field site with limited observations.

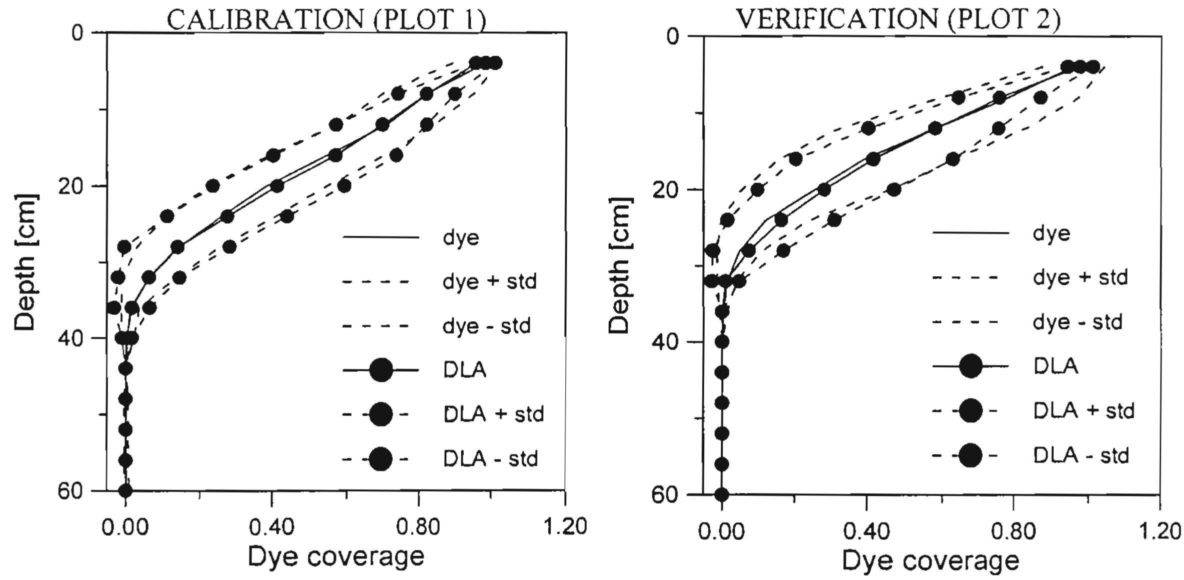

Fig. 3 : Average and standard deviation of dye coverage for the calibrated (plot 1) and verified (plot 2) DLA model.

<u>Random cascade process</u>

A universal multifractal model according to (4) was tested by comparing estimated parameters with the 95% confidence interval of the empirical $K(q)$-functions (Fig. 4). As seen from the figure three out of four plots´ universal function is contained within the 95% confidence limits thus confirming the model.

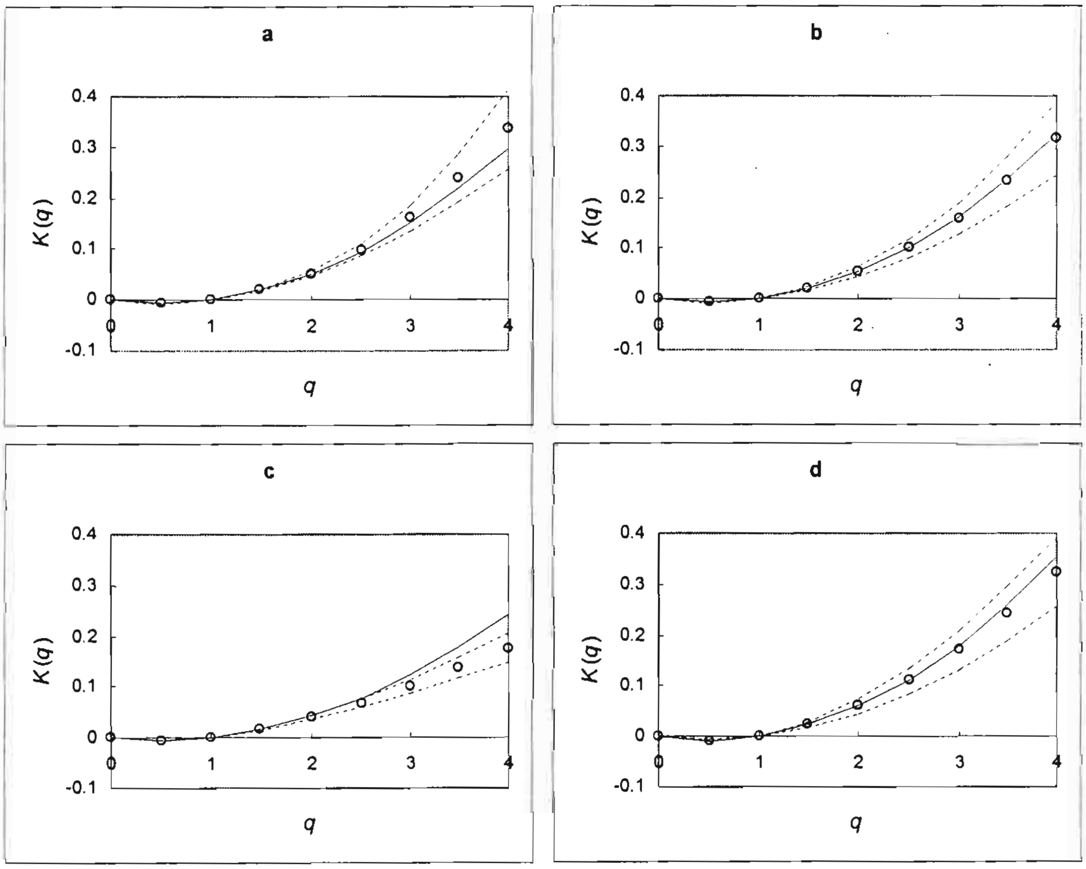

Fig. 4 : Empirical K(q)-function (point values) with 95% confidence intervals (dashed lines) and fitted universal multifractal K(q)-function (solid line) for four typical experimental plots.

The encouraging results were used to simulate the dye coverage bye use of a random cascade process. In Fig. 5 this is shown by comparing original and simulated maximum infiltration depth for a typical plot (plot 3).

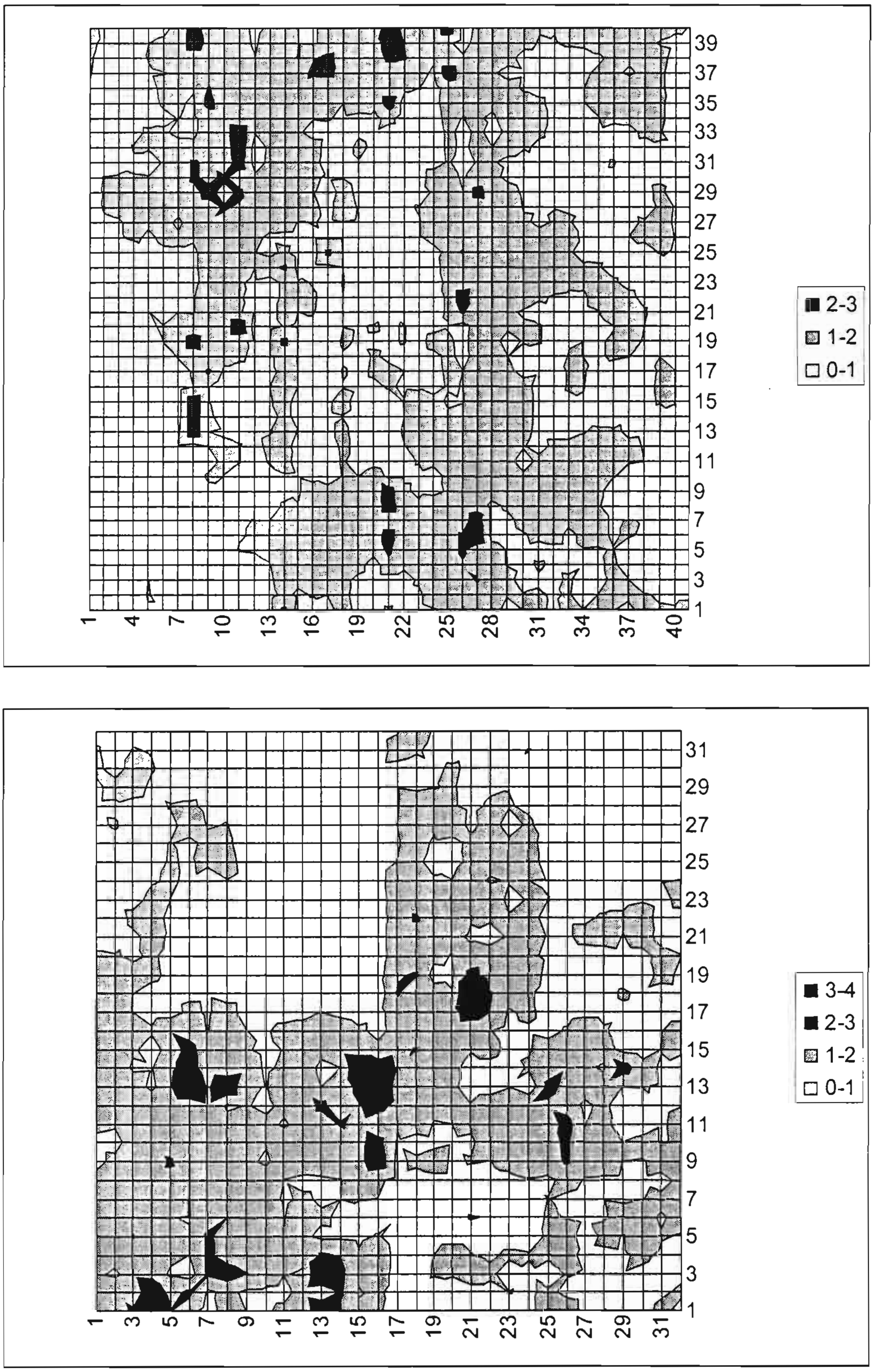

Fig. 5: Observed (upper) and modeled (lower) spatial variation of maximum infiltration depth for experimental plot 3. Simulation was done by discrete cascade simulation of a 32×32 field.

As seen from the figure overall variation is well simulated. Areas of similar infiltration characteristics are generally spatially connected. Some over-estimation appears, however, in the simulated case. Even so it is seen that overall properties seem to be well preserved.

CONCLUSIONS

The conclusions of this study can be summarized as:

1) Solute transport properties as indicated from dye coverage experiments displayed fractal properties as viewed by power spectrum analyses and probability distribution characteristics.
2) Two fractal models were tested and encouraging results were obtained. The tested fractal models were the diffusion limited aggregation and the random cascade model.
3) The diffusion limited aggregation model was calibrated and verified for two plots. The verified model agreed very well to observed data. The random cascade model was calibrated for one experimental plot. Some over-estimation appeared to be the case. However, the general spatial pattern appeared to agree well with observed data. It remains to perform a rigid statistical test for the performance of the random cascade model.

This study showed that fractal models are viable to apply for subsurface flow phenomena. Several previous studies have shown that many soil properties can be viewed as fractal pathways (e.g., Katz and Thompson, 1985; Tyler and Wheatcraft, 1990; Young and Crawford, 1991; Kemblowski and Wen, 1993; Baveye et al., 1998). In this paper we confirmed these results by applying two fractal models to observed dye penetration in unsaturated field soil. Further studies are needed to explore the effects of varying fractal parameters on the investigated models. Also, studies are needed to relate different types of soils to different fractal properties such as fractal and multifractal parameters. We hope to be part of these future studies.

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REFERENCES

AEBY, P., FORRER, J., STEINMEIER, C., and FLÜHLER, H., 1997. Image analysis for determination of dye tracer concentrations in sand columns, Soil Sci. Soc. Am. J., 61, 33-35.

BAVEYE, P., BOast, C.W., OGAWA, S., PARLANGE, J.-Y. and STEENHUIS, T., 1998. Influence of image resolution and thresholding on the apparent mass fractal characteristics of preferential flow patterns in field soils, Water Resour. Res., 34, 2783-2796.

BERNARD, A., 1987. Le simulateur de pluie 2éme génération, Technical report, ORSTOM, Tunis, Tunisia.

BEVEN, K. and GERMANN, P., 1982. Macropores and water flow in soils, Water Resour. Res., 18, 1311-1325.

BOOLTINK, H.W.G. and BOUMA, J., 1991. Physical and morphological characterization of bypass flow in a well-structured clay soil, Soil Sci. Soc. Am. J., 55, 1249-1254.

BOUMA, J., 1991. Influence of soil macroporosity on environmental quality, Adv. Agron., 46, 1-37.

DAVIS, A., MARSHAK, A., WISCOMBE, W., and Cahalan, R., 1994. Multifractal characterizations of nonstationarity and intermittency in geophysical fields: Observed, retrieved, or simulated, J. Geophys. Res., 99, 8055-8072.

FEDER, J., 1988. Fractals, Plenum Press, New York.

FLURY, M. and FLÜHLER, H., 1995. Modeling solute transport leaching in soils by diffusion-limited-aggregation. Basic concept and application to conservative solutes, Water Resour. Res., 31, 2443-2452.

FLURY, M., FLÜHLER, H., JURY, W.A. and LEUENBERGER, J., 1994. Susceptibility of soils to preferential flow of water: A field study, Water Resour. Res., 30, 1945-1954.

FRISCH, U., and PARISI, G., 1985. On the singularity structure of fully developed turbulence, in Turbulence and Predictability in Geophysical Fluid Dynamics and Climate Dynamics – Proceedings of the International School of Physics "Enrico Fermi", edited by M. Ghil, R. Benzi, and G. Parisi, pp. 84-88, North-Holland, Amsterdam.

HILLEL, D., 1991. Research in soil physics: A re-view, Soil Sci. 151, 30-34.

KEMBLOWSKI, M.W. and WEN, J.-C., 1993. Contaminant spreading in stratified soils with fractal permeability distribution, Water Resour. Res., 29, 419-425.

LAVALLEE, D., 1991. Multifractal Analysis and Simulation Technique and Turbulent Fields, Ph.D. Thesis, McGill Univ., Montreal, Canada.

MANDELBROT, B. B., 1974. Intermittent turbulence in self-similar cascades: Divergence of high moments and dimension of the carrier, J. Fluid. Mech., 62, 331-358.

MEakin, P., 1991. Fractal aggregates in geophysics, Rev. Geophys., 29, 317-354.

MENABDE, M., SEED, A., HARRIS, D., and AUSTIN, G., 1997. Self-similar random fields and rainfall simulation, J. Geophys. Res., *102*, 13509-13515.

MENABDE, M., SEED, A., HARRIS, D., and AUSTIN, G., 1999. Multiaffine random field model of rainfall, Water Resour. Res., 35, 509-514.

MUKHOPADHYAY, S., and CUSHMAN, J. H., 1998. Diffusive transport of volatile pollutants in nonaqueous-phase liquid contaminated soil: A fractal model, Transport in Porous Media, *30*, 125-154.

OLSSON, J., PERSSON, M., ALBERGEL, J., ZANTE, P., NasRi, S., and BERNDTSSON, R., 2000. Spatial variability of soil water infiltration: scaling properties and random cascade modeling, manuscript.

PACHEPSKY, Y., and TIMLIN, D., 1998. Water transport in soils as in fractal media, J. Hydrol., 204, 98-107.

PERSSON, M., YASUDA, H., ALBERGEL, J., ZANTE, P., BERNDTSSON, R., NASRI, S., and ÖHRSTRÖM, P. 2000. Modeling plot scale dye penetration by a diffusion limited aggregation (DLA) model, manuscript.

SCHERTZER, D., and LOVEJOY, S., 1987. Physical modeling and analysis of rain and clouds by anisotropic scaling multiplicative processes, J. Geophys. Res., 92, 9693-9714.

SCHWARTZ, R.C., MCINNES, K. J., JUO, A.S.R. and CERVANTES, C.E., 1999. The vertical distribution of a dye tracer in a layered soil, Soil Sci., 164, 561-573.

Soil Survey Staff, 1996. Keys to soil taxonomy, United States Department of Agriculture, Washington, D.C.

TESSIER, Y., LOVEJOY, S., and SCHERTZER, D., 1993. Universal multifractals: Theory and observations for rain and clouds, J. Appl. Meteorol., *32*, 223-250.

WHEATCRAFT, S. W. and TYLER, S. W., 1988. An explanation of scale dependent dispersivity in heterogeneous aquifers using concepts of fractal geometry, Water Resour. Res., *24*, 566-578.

WITTEN, T. A. and SANDER, L.M., 1981. Diffusion-limited aggregation: A kinetic critical phenomenon, Phys. Rev. Lett., 47, 1400-1403.

ÖHRSTRÖM, P., PERSSON, M., ALBERGEL, J., ZANTE, P., NASRI, S., BERNDTSSON, R., and NASRI, S., 2000. Field scale variation of preferential flow indicated from dye coverage, manuscript.