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Modeling plot scale dye penetration by a diffusion limited aggregation (DLA) model

Magnus Persson[a,*], Hiroshi Yasuda[b], Jean Albergel[d], Ronny Berndtsson[a], Patrick Zante[d], Slah Nasri[c], Pernilla Öhrström[a]

[a]Lund University, Box 118, 221 00 Lund, Sweden
[b]Tsukuba University, Japan,
[c]Institut National de Recherche du Génie Rural, des Eaux et Forêts, Tunisia
[d]Institut de Recherche pour le Développement, Tunisia

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Abstract

Solute transport in the unsaturated zone often occurs in preferential flow paths. There are several reasons for this, e.g., water repellency, the occurrence of fissures and cracks, animal burrows, decomposed root threads etc. The resulting flow patterns often display a fractal resemblance which is difficult to predict using conventional transport models. A way to preserve the fractal property of observed data is to use the diffusion limited aggregation (DLA) model concept. In the present paper we use dye infiltration data to further develop the DLA model concept as applied to solute movement in soils. The DLA model is first calibrated against detailed field observations of dye infiltration. The model is shown to give a good description of observed mean and variance of dye penetration. After this, the calibrated model is verified against independent data from a nearby plot. The model is shown to reproduce observed dye patterns in a satisfactory way also at the verification plot. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Solute transport; Diffusion limited aggregation; Dye image; Fractal

1. Introduction

Pathways of water and solutes at field conditions are still poorly understood (Booltink and Bouma, 1991; Bouma, 1991). Due to this, studies of preferential flow, especially for unsaturated field soil conditions, have become an important issue (Beven and Germann, 1982; Hillel, 1991). In general, it may be stated that observed transport phenomena are not in accordance with more or less idealized models based on the commonly used Richards equation and the convection-dispersion equation based on the homogeneous media assumption. A reason for this discrepancy may be that our tools of observation especially at the field scale are not yet detailed enough to yield information at the relevant scales. Often it is the complicated three-dimensional flow structures at the micro-scale that determine the actually observed field scale variation.

Dye tracers are frequently used to study field scale flow patterns in structured soils (Flury et al., 1994). Dye image data can provide an excellent resolution in the spatial scale, but give no information in the temporal scale. Unless the dye is combined with a tracer with known concentration it is difficult to assess

* Corresponding author. Fax: +46-222-4435.
E-mail address: magnus.persson@tvrl.lth.se (M. Persson).

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quantitative characteristics such as dispersion and flow velocity. Dye tracer data, however, are able to give more detailed visual information on three-dimensional flow structures caused by preferential flow, macropores, etc. In this context, dye data may be used to develop and test new model concepts that can more accurately depict spatial physical processes occurring in the soil (Schwartz et al., 1999).

During recent years a new solute transport model concept has been developed based on diffusion-limited aggregation (DLA) (Flury and Flühler, 1995). Witten and Sander (1981) introduced the model concept based on DLA in physics two decades ago. Advantages using the DLA concept to model transport of solutes in soil are that complicated three-dimensional patterns can be simulated in a simple way. Not only structured soils but also seemingly homogeneous soil structures often display preferential flow patterns (Bowman and Rice, 1986; Jaynes et al., 1988; Berndtsson et al., 1996; Persson, 1999). Another advantage is that the DLA model can generate fractal transport patterns. This property is often observed in subsurface flow phenomena (Feder, 1988; Kemblowski and Wen, 1993; Baveye et al., 1998). In Flury and Flühler (1995), a DLA model was used to simulate solute concentration in three field plots that had different accumulated infiltration. One single DLA realization was calibrated for one plot and then compared to the other plots. However, since each DLA realization will give slightly different results, it should be possible not only to simulate average solute transport but also the variability.

In the present paper we make use of the advantages posed by the DLA model concept to simulate complicated fractal flow properties for an unsaturated soil. We start with a brief analysis to show the fractal behavior of unsaturated transport data as indicated by dye stained soil sections. Thereafter, the DLA model used is described and calibrated for an experimental plot. The model parameters are then verified against independent data from a nearby plot.

2. Materials and methods

2.1. Experimental conditions

Experimental data from an ongoing European Union cooperative effort (HYDROMED, a research program on hill reservoirs in the semiarid Mediterranean periphery) were used in this study. 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).

At two plots (plots 1 and 2), separated by about 8 m, 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 (Flury et al., 1994; Aeby et al., 1997). A rainfall simulator (Bernard, 1987) was used to simulate a heavy rainstorm during about 1.5 h. Placing an iron frame of size 1 by 1 m at each site created two 1.0 m^2 plots. In order to avoid border effects, the rainfall simulator covered totally about 9 m^2 at each plot. Surface runoff was collected through a discharge weir in the iron frame. A total of 47.1 and 41.9 mm infiltrated at plots 1 and 2, respectively, during the experiment. 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 prevent evaporation. About 24 h after the simulated 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 with a 35-mm camera with Kodachrome 64 film. The slides were scanned with a diapositive scanner. More information about the field experiments can be found in Palmquist and Tullberg (1997). The color photos were converted to black and white images bye use of Adobe Photoshop™ (version 4.0, Adobe Systems, Inc.) software. An example of one black and white image from plot 1 is given in 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 distribution did not change significantly with the pixel size.

2.2. DLA modeling concept

Witten and Sander (1981) introduced the DLA concept based on a study of aggregation of solid particles. The DLA model is a conceptual model describing the process where solid particles irreversibly attach to each other and form aggregates and the process is limited by diffusion. An interesting characteristic of the DLA model is that the generated clusters are fractal (Meakin, 1983a,b). It has been shown that there is an analogy between DLA and various physical processes obeying the Laplace equation. Consequently, the DLA model has been used to model several physical phenomena (Niemeyer et al., 1984; Flury and Flühler, 1995).

Meakin (1983b) introduced a DLA model of a so-called line seed type, which is used in the present study since it mimics the boundary condition of the solute transport experiments. Basically, the DLA model generates clusters by randomly walking particles. Particles are randomly generated from a line source at some distance below the soil surface. The distance between the DLA cluster and the line source is set only a few grid units larger than the distance from the line source and the maximum depth of the growing clusters. This considerably shortens the computational time but does not affect the shape of the resulting cluster (Flury and Flühler, 1995). As the cluster grows, the line source is shifted downwards. By random walk the particles may finally reach up to the line seed (soil surface). When the particles reach the seed they remain attached at that position (Flury and Flühler, 1995). New particles that reach the seed or previously attached particles 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 $z_{\max}$. If the DLA cluster is to be compared with experimental results, observed $z_{\max}$ has to be used. 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.

$$P_u + P_d + P_r + P_l = 1.0$$

An isotropic random walk model has the following probability distribution:

$$P_u = P_d = P_r = P_l = 0.25$$

By changing the probabilities, anisotropic conditions may be simulated. Also, layered soils may be simulated by including different walking probabilities for different soil depths (Flury and Flühler, 1995). The DLA model used in this study was written in FORTRAN code and follows the model structure described in Flury and Flühler (1995).

2.2.1. Calibration of the DLA model

It should be noted that the implicit assumption of the DLA model, i.e., diffusion type movement of particles, is not strictly applicable to the infiltration case. However, as a pattern descriptor, the DLA model can be used as a conceptual model of solute transport within the microscale. Output from the DLA model therefore has to be averaged over a suitable space in order to be comparable to the scale of observations. Flury and Flühler (1995) compared the average solute concentration determined from ten cylindrical soil cores with the average cluster coverage of ten synthetic measurements at each depth. The synthetic measurements were used to convert the DLA cluster from the microscale to macroscopic concentration. The synthetic measurements were calculated by counting all particles within a circle and by dividing this value by the area of the circle. A calibration coefficient was then needed to convert the cluster coverage to solute concentration. This coefficient had to be calculated for every comparison between measured and simulated data. Thus, the model could not be used for prediction of the actual concentration for an independent site.

In our study, the DLA model was used to simulate the properties of dye images. A black and white transformed dye image contains information according to the number of pixels per unit area. Each pixel has the value 1 if it is stained with dye and the value 0 if it is unstained. However, the actual concentration of dye can be different for different pixels since the lowest detectable dye concentration may be rather low (Aeby et al., 1997). In order to convert the DLA model to macroscopic dye distribution the number of particles in a 4 by 4 grid area was counted. If the number of particles was higher than a threshold number C_{d0} the entire grid area was assumed to be stained with dye

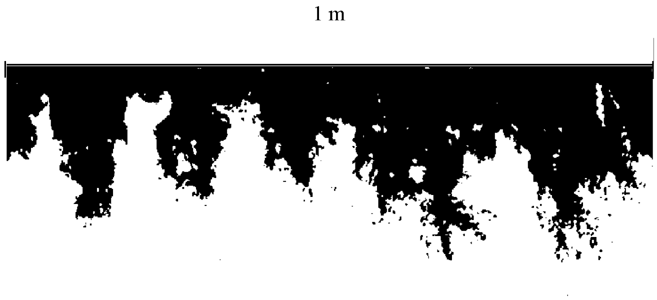

Fig. 1. Example of one dye image from plot 1.

and the area was given the value 1. The parameter C_{d0} was set to one particle per 4 by 4 grid area. Now the horizontal average of the 4 by 4 grid DLA model can be compared with the horizontal average of the dye image. For this comparison, the dye image was rescaled to a pixel size of 4 by 4 cm in order to have both the dye image and the DLA simulation in the same scale. The procedure is described in Fig. 2. Schwartz et al. (1999) simulated dye penetration using a random walk model using a similar procedure for comparison between model results and dye images. It should be noted that this procedure omits the need for the calibration coefficient used by Flury and Flühler (1995).

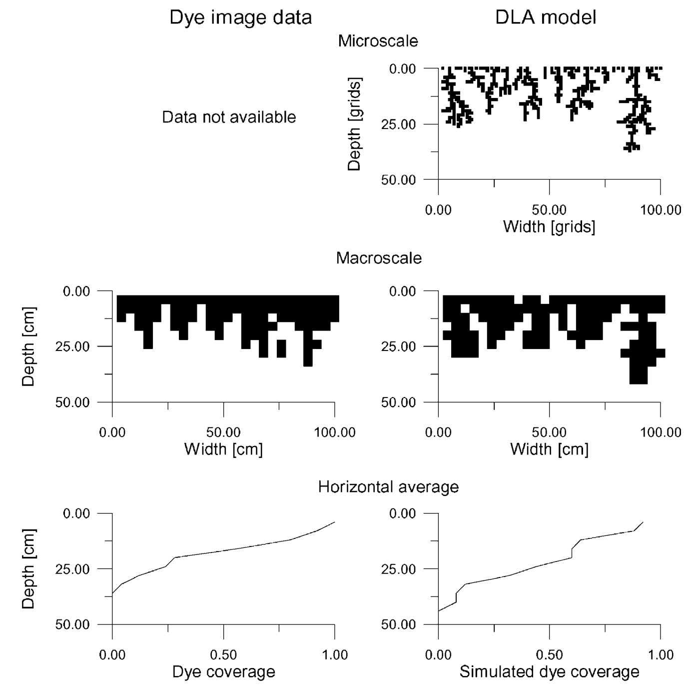

Fig. 2. Example of the DLA model concept and a comparison between model results and observations. The top row shows the microscale data from the dye image and the DLA model. No data is available for the dye image at this scale. The DLA model shows one realization of a DLA cluster with $z_{\max} = 0.30$ m and P_u, P_d, P_r, and P_l equal to 0.305, 0.295, 0.2, and 0.2 respectively. The second row shows the macroscale data. The dye image data is converted to a pixel size of 4 by 4 cm. Note that the dye image data was calculated from the dye image shown in Fig. 1. The DLA cluster is averaged over each 4 by 4 grid area. If the area contains at least one particle the area is given the value 1 (black). The third row shows the horizontal average of the macroscale data.

Table 1
Distribution of the maximum dye penetration z_{maxdye} for the 41 dye images from plots 1 and 2

z_{maxdye} (cm)	Plot 1 (no. of images)	z_{maxdye} (cm)	Plot 2 (no of images)
19–23	2	10–15	4
24–28	12	16–20	6
29–33	21	21–25	12
34–38	4	26–30	16
39–43	2	31–35	3

According to the above, choosing the grid size of the DLA model is an important issue. A small grid size results in a fast simulation time but the variation between the different realizations is larger compared to a larger grid size. For calibration purposes a low variation is desired since this makes comparisons between each parameter set easier. However, the dye images showed large individual variation and in order to simulate this variation a rather small grid was necessary. In the present paper a two-dimensional modeling domain corresponding to a 100 by 100 grid net was used since it proved to be a good compromise. The grid area over which the DLA cluster is averaged in order to convert the microscale DLA cluster to macroscopic concentration or, as in the present study, dye coverage, is also critical to the outcome of the model. If the DLA cluster is averaged over a larger area, the variability will be smaller. Furthermore, in order to maintain the same resolution of the result, a larger grid size is necessary. Consequently, both the grid size and the grid area over which the DLA cluster is averaged should be treated as calibration parameters when the DLA model is used for prediction of the variability.

Only two walking probabilities need to be calibrated in the DLA model, P_u and P_d. The remaining probabilities can be calculated by $P_l = P_r = 1 - P_u - Pd$ since the model domain is assumed isotropic in the horizontal direction. The model was calibrated to predict the horizontally averaged dye coverage for all 41 dye images from plot 1. The parameter z_{max} was set to 0.30 m which corresponds to the average dye penetration for plot 1. Each probability was changed with an increment of 0.005 and the r^2 value of the horizontally averaged dye coverage and the DLA model was used to determine the best parameters. This procedure was done manually.

Each DLA realization will be different even if the probabilities are kept constant. In order to determine how many DLA realizations are needed to arrive at robust model results, 400 different DLA realizations were made using the same probabilities and z_{max}. A value of 50 model realizations was found sufficient and was thus used in the DLA model calibration.

Flury and Flühler (1995) used a two-layer model domain with different walking probabilities in their DLA model. Adding more layers will usually give better fit between simulated and measured data. Layers with different walking probabilities should only be included when the modeled soil profile contains clearly defined horizons. For the present soil, no horizons with different soil properties could be distinguished and therefore, a homogeneous model soil domain was kept.

2.3. DLA model simulations

Since the dye images showed a great variation for the maximum dye penetration, z_{maxdye}, it was necessary to run the DLA model with different z_{max} in order to investigate if the DLA model can estimate the variation in the dye images. The distribution of z_{maxdye} for the plots is presented in Table 1. For each z_{maxdye}, nine DLA model realizations were run, resulting in a total of 369 realizations.

The next step was to use the calibrated values of the probabilities for plot 1 and to verify the model for dye penetration of plot 2. The distribution of z_{maxdye} was determined for plot 2 (Table 1) and was then used as input to the DLA model and 369 realizations were run as described above.

3. Results and discussion

The power spectral density of the dye penetration for each pixel column by fast Fourier transform was

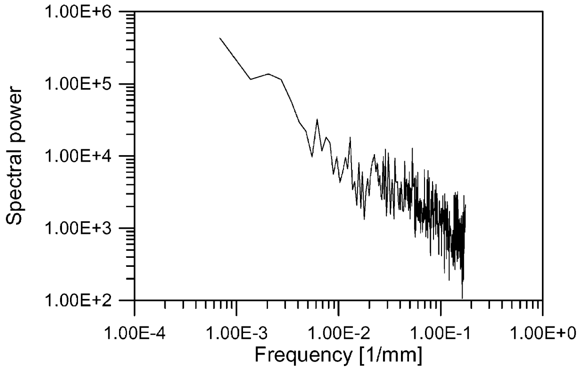

Fig. 3. Mean power spectrum for the dye penetration of plot 1 (six dyed soil transects).

calculated using a pixel size corresponding to 0.14 cm (725 pixel columns per image). Fig. 3 shows the average power spectral density of six observed soil transect images (the images at distances 0, 0.2, 0.4, 0.6, 0.8, and 1.0 m from the border of the plot were chosen for this). The spectral power is plotted in a log–log axis diagram and displays a typical power law relationship over the entire range of frequencies. This is an indication of scaling behavior and possible existence of fractal relationships (Ladoy et al., 1991). In turn, this is a strong motivation to apply a model such as the DLA, which results in fractal clusters.

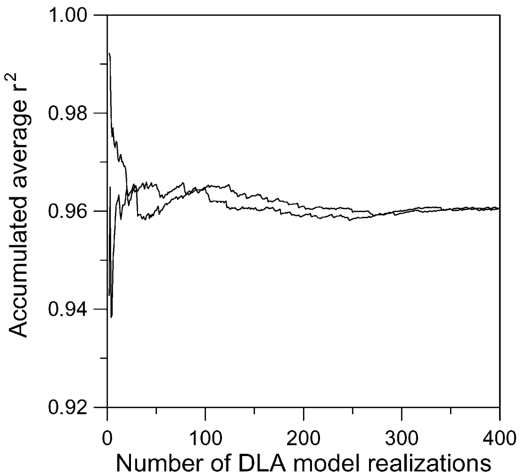

Fig. 4. Accumulated average r^2 value between modeled and observed dye coverage depending on number of realizations using the same z_{max}, P_u, P_d, P_r, and P_l. The two curves were calculated from the same data set, however, the second curve is using the data set in reverse order.

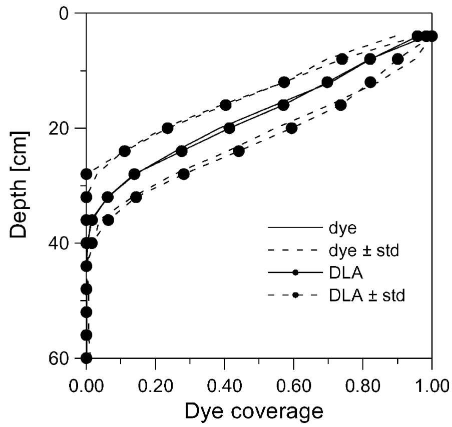

Fig. 5. Depth distribution of dye coverage and its variability of modeled and observed data for plot 1 (calibration plot). The modeled dye coverage is the average of 369 realizations using P_u, P_d, P_r, and P_l equal to 0.305, 0.295, 0.2, and 0.2 respectively and the distribution of z_{max} according to Table 1.

3.1. Calibration of the DLA model

Tests were performed to evaluate the number of simulations necessary to arrive at robust model results. Fig. 4 shows the correlation between modeled and observed dye coverage depending on number of simulations. As seen, after about 20 simulations the variation using different sub-samples as input to the model stabilizes and converges to a more or less constant value. However, to be on the safe side 50 realizations were used. The number of realizations needed will be affected both by the grid size and the averaging method (synthetic measurements).

When the DLA model was calibrated against the horizontally averaged dye coverage, the best fit probabilities were determined to be 0.305, 0.295, 0.2, and 0.2 for P_u, P_d, P_r, and P_l respectively. This parameter set gave a r^2 value of 0.959 between the horizontally averaged dye coverage and the average of 50 DLA model realizations using $z_{max} = 30$ cm. In our case the P_u and P_d were rather similar, but in the study by Flury and Flühler (1995) significantly different P_u and P_d were used.

3.2. DLA model simulations

It should be noted that the DLA is a stochastic model that gives a randomly varying output.

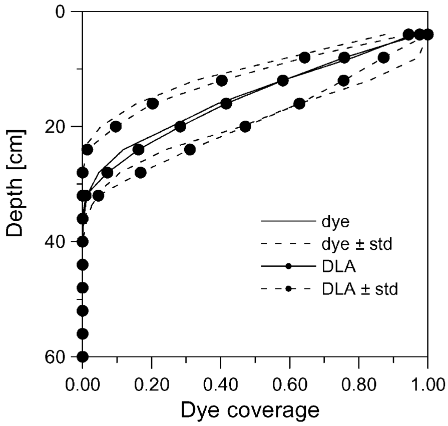

Fig. 6. Depth distribution of dye coverage and its variability of modeled and observed data for plot 2 (validation plot). The modeled dye coverage is the average of 369 realizations using P_u, P_d, P_r, and P_l equal to 0.305, 0.295, 0.2, and 0.2 respectively and the distribution of z_{max} according to Table 1.

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. 5, which shows a comparison between average and standard deviation of dye coverage with depth for simulations using the calibrated DLA and observations at plot 1. As seen from the figure, model results and observations agree well, with a r^2 value of 0.999 between the horizontally averaged dye coverage and the average of 369 DLA model realizations. Consequently, the DLA model can reproduce both the mean and the variation of observations in a satisfactory way.

To test the DLA model against independent data the calibrated model was verified using data from plot 2. This is seen in Fig. 6 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 z_{maxdye} 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 horizontally averaged dye coverage and the average of 369 DLA model realizations. This confirms the applicability of the model concept and that the DLA model can be used to simulate both the average and the variability of dye penetration in the soil at the field site. Another option could be to estimate z_{max} from the amount of infiltrated water and not use the observed distribution of z_{maxdye}. However, this approach would only give the average dye coverage and not the variation.

4. Conclusions

The DLA model was modified to simulate dye penetration observed from infiltration experiments. The model contains only two calibration parameters, i.e., P_u and P_d. However, the variability of the model result for different realizations is also highly dependent on the grid size and the grid area over which the DLA cluster is averaged. Thus, these parameters can also be viewed as calibration parameters although these were kept constant in the present study.

We showed that the dye penetration in a field plot indicated fractal behavior. This is a motivation to use a model capable of reproducing the fractal nature of the solute transport, such as the DLA model. The model was calibrated against horizontally averaged dye coverage of 41 dye images. During the calibration, the z_{max} was set to the average dye penetration of plot 1. When the actual distribution of z_{maxdye} was given as input to the model, the model was able to accurately simulate both the depth distribution of dye coverage and its variability of the 41 dye images. The calibrated model was then used to verify dye penetration at a second plot close to the first. Using the calibrated parameters from plot 1 the model was able to accurately simulate both the depth distribution of dye coverage and its variability of the 41 dye images from this plot as well.

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