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APPLICATION OF MONTE-CARLO METHOD TO MODELLING INFLUENCE OF SELECTED SOIL HETEROGENEITY ON MACRODISPERSION OF POLLUTANTS IN UNSATURATED SOIL MEDIUM

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Abstract: The influence of soil heterogeneity on miscible solute transport in soil is analyzed. The transport process is simulated numerically using the Monte-Carlo method. This paper shows how different types of soil heterogeneity influence the process of contaminant spreading. If independent flow paths exist in the soil, the degree of the mixing of pollutants in the outflow from the soil profile is larger. If the preferential flow paths are shorter, the degree of mixing, related to the heterogeneity of the velocity field, is smaller. These effects can be captured using the Monte-Carlo method.

Keywords: macrodispersion, transport in porous media, Monte-Carlo method, preferential flow, unsaturated soil

1. Introduction

The transport of substances dissolved in water flowing through a heterogeneous and unsaturated soil medium is termed hydrodynamic dispersion (depending on the scale, either microdispersion or macrodispersion). The migration of pollutants through a soil medium involves different transport mechanisms (convection, hydrodynamic dispersion). Each mechanism depends on the type and structure of the soil, as well as on a group of physical and physicochemical phenomena, like non-uniform velocity field, molecular diffusion, reactions between dissolved substances; and can lead to spatial and temporal variations of the concentration of a solute substance in groundwater. Hydrodynamic dispersion is mainly of importance in the case of highly permeable porous media, while molecular diffusion occurs at low pore velocity, typical of semi-permeable formations.

2. Basic equation of contaminant transport in soil medium

Hydrodynamic dispersion phenomena are typically described by advection-diffusion models [1, 2]. To describe the process of solute transport in a soil profile, it is assumed that the solute particles are moving at the average speed of the solvent (averaged over an elementary, representative surface or volume). Therefore, to each particle we must apply the mass conservation principle, which can be written in the form of a continuity equation:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial q_i}{\partial x_i} + s \tag{1}$$

where:
q_i – total mass flux of a substance dissolved in groundwater,
$\rho = C\theta$ – solute density in groundwater,
θ – volumetric water content,
C– concentration,
s – sink term,
x_i – spatial coordinate,
t – time.

The total mass flux q_i can be written as a superposition of the dispersive contribution q_i^d and the advective contribution $\overline{q}_i$:

$$q_i = q_i^d + \overline{q}_i \tag{2}$$

The advective flux can be written as:

$$\overline{q}_i = C\theta\overline{v}_i \tag{3}$$

The dispersive flux is proportional to the concentration gradient [3]:

$$q_i^d = -D_{ij}\theta\frac{\partial C}{\partial x_j} \tag{4}$$

where D_{ij} – components of the hydrodynamic dispersion tensor, thus Equation (2) can be written in the form:

$$q_i = -D_{ij}\theta\frac{\partial C}{\partial x_j} + C\theta\overline{v}_i \tag{5}$$

The components of the hydrodynamic dispersion tensor depend on the groundwater flow velocity, as well as on the molecular diffusion coefficient in the soil and can by defined as:

$$D_{11} = D_L\frac{v_1^2}{|v|^2} + D_T\frac{v_2^2}{|v|^2} + D_d \tag{6}$$

$$D_{12} = D_{21} = (D_L - D_T)\frac{v_1 v_2}{|v|^2} \tag{7}$$

$$D_{22} = D_L\frac{v_2^2}{|v|^2} + D_T\frac{v_1^2}{|v|^2} + D_d \tag{8}$$

where:
D_L – longitudinal dispersion coefficient,

D_T – transverse dispersion coefficient,
D_d – molecular diffusion coefficient,
v_i, v_j – components of average linear groundwater velocity in their respective directions.

The advection-dispersion equation, describing the transport of a substance dissolved in groundwater, can be obtained by introducing Equation (5) into Equation (1):

$$\frac{\partial(C\theta)}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\theta\frac{\partial C}{\partial x_j}\right) - \frac{\partial(C\theta\overline{v}_i)}{\partial x_i} + s \tag{9}$$

3. Numerical solution

The advection-dispersion equation can be solved using a variety of methods, such as the finite difference method, the finite element method or the finite volume method. In this work, the transport equation is solved with the Monte-Carlo method [4–6]. In contrast to the finite element and finite difference methods, the Monte-Carlo method does not generate numerical dispersion. This method involves a numerical solution for virtual particles of the dissolved substance. It is based on stochastic process theory [7–9]. An algorithm for the computer simulation of random variables was described in detail by Maciejewski and Gorczewska-Langner [10]. The Monte-Carlo method consists in developing an equivalent formulation of the advection-dispersion equation in terms of the Kolmogorov equation and the Ito stochastic equation. The Kolmogorov equation is written as [11, 12]:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_i}(m_i f) = \frac{1}{2}\frac{\partial^2}{\partial x_i \partial x_j}(b_{ij} f) \tag{10}$$

and the corresponding Ito stochastic equation is:

$$dx_i = m_i dt + \sigma_{ik} dB_k \tag{11}$$

where:
dx_i – displacement,
f – probability density,
m_i, b_{ij} – coefficients,
B_k – Wiener process, which is the theoretical model of Brownian motion,
x_i, x_j – spatial coordinates,
t – time.

The relationship between matrices $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ is given by:

$$b_{ij} = \sigma_{ik}\sigma_{jk} \tag{12}$$

The advection-dispersion equation for a solute dissolved in groundwater (9) with the omission of the sink term, can be transformed into the Kolmogorov equation in the following way:

$$\frac{\partial(C\theta)}{\partial t} + \frac{\partial}{\partial x_i}\left[\left(\overline{v}_i + \frac{\partial D_{ij}}{\partial x_j} + \frac{D_{ij}}{\theta}\frac{\partial\theta}{\partial x_j}\right)C\theta\right] = \frac{1}{2}\frac{\partial^2}{\partial x_i \partial x_j}(2D_{ij}C\theta) \tag{13}$$

By comparing the above relations, we obtain:

$$2D_{ij} = \sigma_{ik}\sigma_{jk} \tag{14}$$

From the Ito stochastic equation (11) and the Kolmogorov equation (13) it follows that the coordinates of the vector $\boldsymbol{m}$ can be written as:

$$m_i = \overline{v}_i + \frac{\partial D_{ij}}{\partial x_j} + \frac{D_{ij}}{\theta}\frac{\partial \theta}{\partial x_j} \tag{15}$$

The difference approximation of Equation (11) can be written as follows:

$$\Delta x_i = m_i \Delta t + \sigma_{ik} V_k \sqrt{\Delta t} \tag{16}$$

where:
V_k – normal random variable,
Δt – time step.

4. Simulation examples

In this work we focus on the numerical simulation of stochastic processes described by the Ito stochastic equation, which enables us to solve the flow and transport problems in a soil profile, as shown in Figure1.

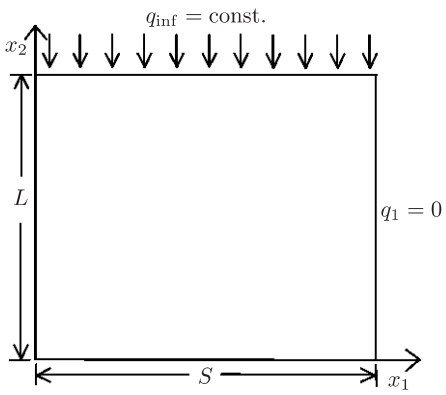

Figure 1. Flow zone of a solute dissolved in groundwater

The concentration profile of the solute injection on the profile surface can be simulated assuming that the total mass M is divided into n particles. Based on the position of particles at time t, we can calculate their position for $t+\Delta t$. Zero concentration was assumed as the initial condition for the transport equation. The upper boundary is permeable for the tracer particles entering the domain, but impermeable for those particles which are inside the domain. The horizontal boundaries are impermeable.

$$\left.\begin{aligned} C(x_1,x_2,0) &= 0 \\ C(x_1,L,0) &= C_0 \\ q_1(x_1,0,t) &= 0 \\ q_1(x_1,L,t) &= 0 \end{aligned}\right\} \tag{17}$$

Based on the distribution of particle positions, we can estimate the concentration field of substances dissolved in groundwater:

$$C(x_2,t) = \frac{M \cdot \sum n(x_2)}{x_1 \cdot \Delta x_2 \cdot \overline{\theta}} \tag{18}$$

where:
M – total mass of tracer,
$\Sigma n(x_2)$ – number of particles corresponding to the mass of tracer dissolved in soil water,
$\overline{\theta}$ – average volumetric water content in the domain.

The number of particles in the domain is proportional to the density of dissolved substances. For a given density and water content in the soil medium, the distribution of the concentration of the pollutant in the soil profile can be calculated for each time step using a numerical simulation program. Moreover, the total amount of the pollutant which flowed out from the soil medium in a given time can be found. The total amount of the pollutant is used to define the distribution of the solute concentration C_F at the outflow:

$$C_F(t) = \frac{1}{S\rho^0 q^w} \frac{dM(t)}{dt} \tag{19}$$

where:
$M(t)$ – total mass of the solute flowing out from the soil medium between $t = 0$ and t,
q^w – outflow flux,
S – outflow surface,
ϱ^0 – water density ($\varrho^0 = 1\,\mathrm{g/cm^3}$).

The concentration C_F represents an average value measured at the outflow, which is in general different from the point values measured at various locations in the porous domain.

Numerical simulations were performed for five different cases (Figure 2). These cases reflect the heterogeneity of the soil. The simulation results are shown below as the distribution of the solute concentration in the soil profile and in the outflow from the soil profile. In each case, the flow problem can be represented as a one-dimensional problem. It was solved for a soil profile of length $L = 120\,\mathrm{cm}$ and width $W = 50\,\mathrm{cm}$.

Each of the subdomains was assigned a random value of the hydraulic conductivity. The values were generated as random Gaussian variables, assuming the same average value of 1 cm/d and the standard deviation of 10% in every test problem. In each case, the solutions were obtained for a constant longitudinal

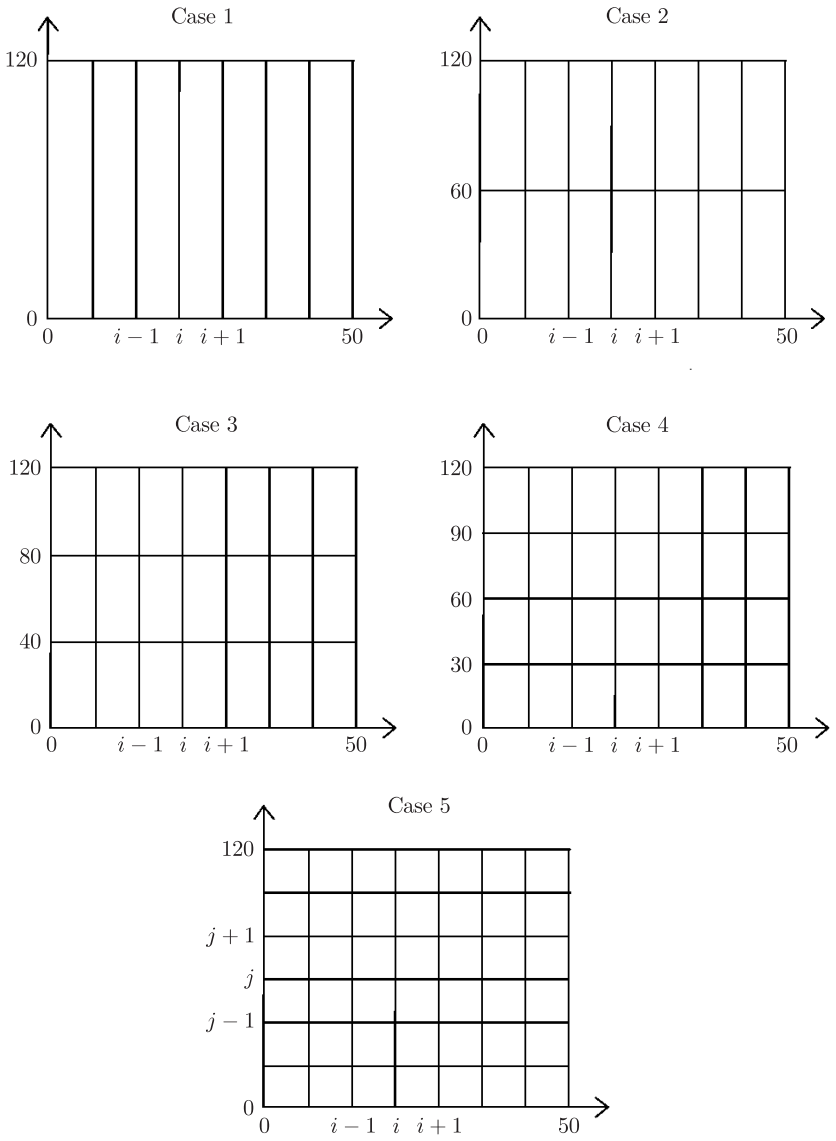

Figure 2. Division of a random field for the 5 cases considered

dispersion coefficient D_L of either $0\,\mathrm{cm}^2/\mathrm{d}$ or $0.1\,\mathrm{cm}^2/\mathrm{d}$. The transverse dispersion coefficient D_T, as well as the molecular diffusion coefficient D_d, were assumed to be zero. Assuming $D_L = 0\,\mathrm{cm}^2/\mathrm{d}$ allowed us to observe the effect of soil heterogeneity on the flow and transport processes. Eliminating dispersion in this way prevents exchange between individual flow paths, making it possible to study only flow processes depending on the types of soil heterogeneity. In each problem, the average value of the groundwater flow velocity was equal to $1\,\mathrm{cm/d}$.

The solute concentration in the soil profile for an arbitrary instant of time for case 5 is presented in Figure 3. The simulation was performed for 3

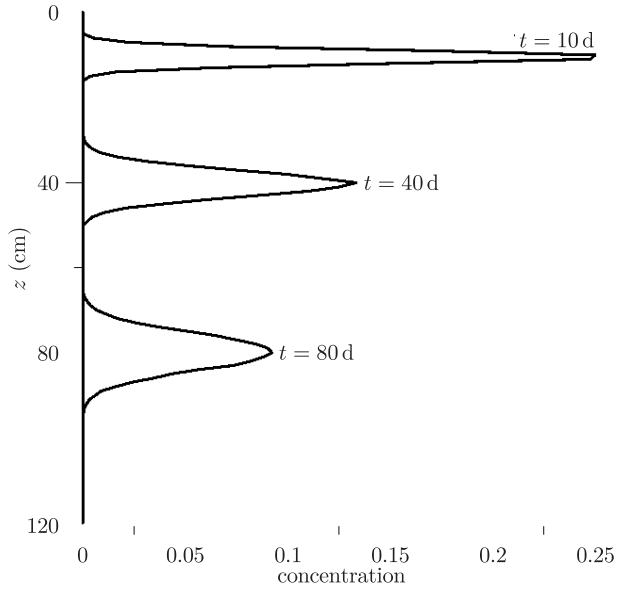

Figure 3. Solute concentration in the soil profile for case 5, $D_L = 0.1\,\mathrm{cm}^2/\mathrm{d}$

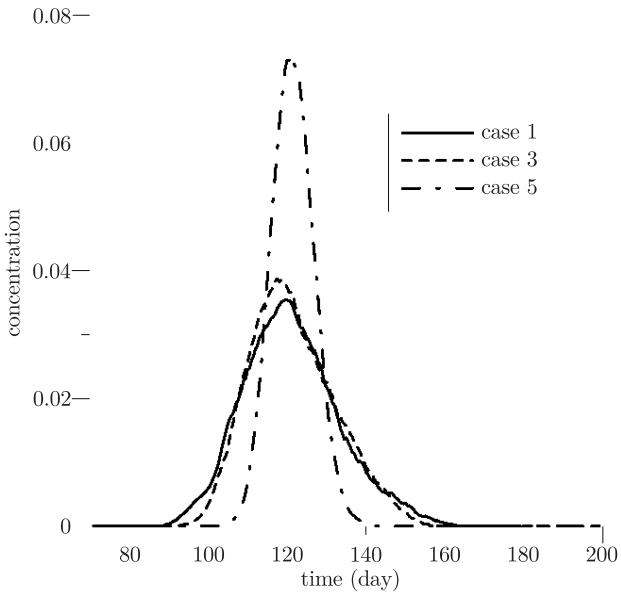

Figure 4. Concentration in the outflow from the soil profile, $D_L = 0.1\,\mathrm{cm}^2/\mathrm{d}$

intermediate times of the solute flow: $t = 10\,\mathrm{d}$, $t = 40\,\mathrm{d}$ and $t = 80\,\mathrm{d}$. The maximum concentration of the tracer decreased with the increase in depth.

Figure 4 presents the concentration distribution of the tracer in the outflow as a function of time for 24000 virtual particles. An increase in the number of flow paths triggers an increase in the maximum value of the concentration, while the curves become increasingly steeper.

Figure 5 presents the total mass of pollutants flowing out from the soil as a function of time for all five cases. As can be easily seen, for the first case the tracer outflow begins at the earliest, and takes the longest time. For case 5, it was observed that the mass outflow is the most delayed and the total mass of the pollutant flows out very quickly in a short period of time. In comparison, for case 1, the total mass of pollutants flowed out after 66.5 d; for case 5, the total amount of pollutants flowed out after 8.5 d. Thus, we believe that the random field compaction reduces the time the pollutants reside in the soil medium.

Figure 6 presents the standard deviation of the concentration for each case. The numerical simulations show that the standard deviation is smaller for

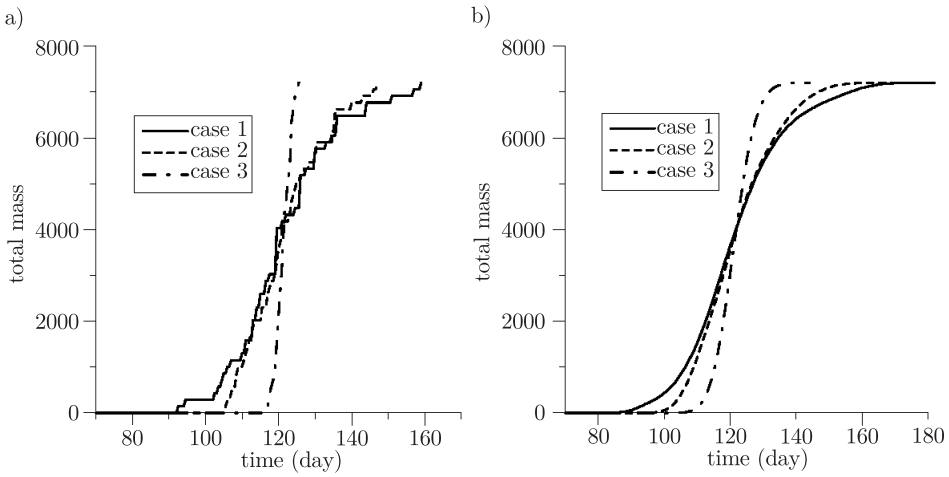

Figure 5. Mass of the solute flowing out from the soil medium, (a) $D_L = 0\,\mathrm{cm}^2/\mathrm{d}$, (b) $D_L = 0.1\,\mathrm{cm}^2/\mathrm{d}$

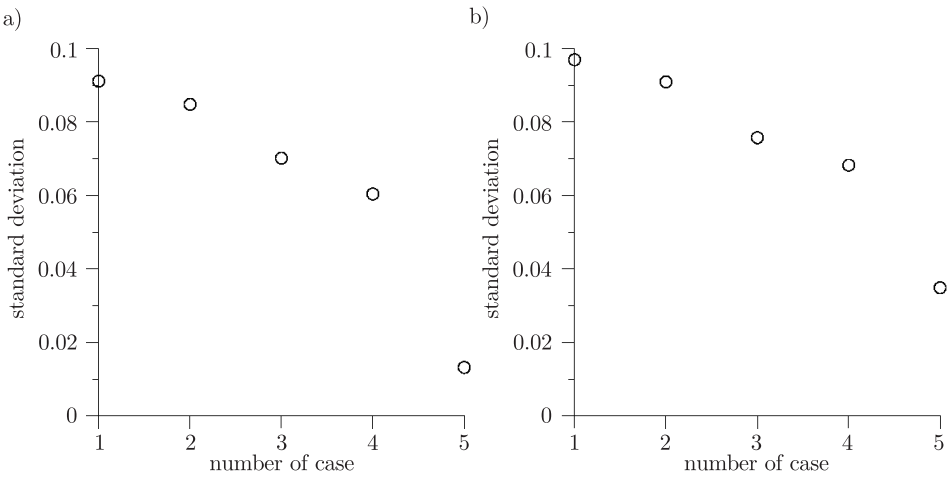

Figure 6. Standard deviation of the concentration for each case, (a) $D_L = 0\,\mathrm{cm}^2/\mathrm{d}$, (b) $D_L = 0.1\,\mathrm{cm}^2/\mathrm{d}$

a condensed random field. For case 1, a standard deviation of 0.091 is obtained, whereas for case 5, the deviation was almost 7.5 times smaller (equal to 0.013).

5. Conclusions

A classical advection-dispersion model was applied to the simulation of solute transport in heterogeneous and porous soil medium. The heterogeneity of the medium can have different characteristics. The properties of the soil, such as hydraulic conductivity, are described by an isotropic random field. In the soil medium, there can also exist numerous flow paths with random hydrodynamic conductivities. The influence of heterogeneity on the mixing of the liquid during transport in soil was analyzed. We showed how different types of soil heterogeneity influence the mixing of contaminants flowing through a porous soil medium. Where independent flow paths exist in the soil, the degree of mixing in the outflow from the soil profile is larger. For shorter preferential flow paths, the degree of mixing, related to the heterogeneity of the velocity field, is smaller. In the simulations, the dispersivity values approaching zero were assumed, so that the degree of mixing depended on the characteristic velocity fluctuations of groundwater flow determined by the soil heterogeneity on the macro scale. The presented calculations demonstrate that the disappearance of flow paths (*cf.* case 5), leads to a decrease in the influence of local velocity fluctuations on the process of mixing. Further simulations are necessary to evaluate the performance of the approach used in this paper for more complex soil heterogeneity patterns. Also, further laboratory experiments are needed to validate the model.

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