

Particulate transport through heterogeneous porous media; numerical studies using finite element method

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ABSTRACT

The complexity of natural systems often prohibits our understanding of governing principles of the systems. The prediction of flow and solute transport through large-scale geological systems is challenging, since accurate predictions involves a detailed characterization of the spatial distribution of hydrologic parameter values. For simplicity reasons, most of the past studies of groundwater flow and solute transport assumed homogeneous aquifers. Numerical methods of estimating hydrologic properties of aquifers used the homogeneity assumption because of mathematical challenges associated with the heterogeneity of aquifers. In the present work we investigate the transport processes in watersheds using a two-dimensional model for flow and particulate transport in the subsurface system. The study reveals that the particle dispersion depends strongly on the heterogeneity of the aquifer. Thus, the particles exhibit a slower speed in the regions of low conductivity. Moreover, the particles exhibit a preferential path, following the path of minimum resistance.

Keywords: Heterogeneous porous medium, Groundwater flow, Particle dispersion, Darcy's law, Finite element method

1. INTRODUCTION

The understanding of subsurface flow and solute transport processes is of critical importance for effective and efficient management of environment and water resources. The hydrosystem within a watershed comprises many hydrological, morphodynamic, and environmental processes, such as rainfall, runoff, groundwater flow, infiltration, evapotranspiration, recharge, upland soil erosion, sediment transport, and contaminant transport. These processes may significantly affect water quality and aquatic ecosystems.

In the past decades the numerical modeling has emerged as efficient and effective tool to investigate these processes and evaluate their effects. Thus, numerous models have been developed for the analysis of aquifer heterogeneity, flow and transport. Most of these models are based on the stochastic field/process concept [6, 7, 9, 10, and 13]. However, the accuracy of this concept is yet to be assessed. The challenges posed by the use of this concept stem from the fact that the aquifer heterogeneity and associated flow and transport processes, at some scales, are not as irregular and complex as those at other scales.

Efficient and accurate evaluation of the flow velocity is mandatory for any numerical model of multidimensional transport through porous media. On the other hand, the

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computational efficiency is of particular importance for the simulation of randomly heterogeneous medium, since hundreds of realizations are necessary for a detailed description of the transport process. For particle tracking techniques, the performance of numerical models depends on the prediction of velocity field. The Finite Difference Method (FDM) and Finite Element Method (FEM) are the most commonly used numerical techniques for groundwater flow and transport. Generally, the numerical methods first solve for the hydraulic head (potential) at the grid points and then obtain the velocity by numerical differentiation. This is usually associated with the loss of one order of accuracy, in the velocity computations, and discontinuities in velocity components at the element boundaries. Generally, at the interface of two different materials, the velocity component normal to the interface should be continuous while the tangential component exhibits a discontinuity.

Extensive research has been conducted in the past two decades to analyze the effect of geological heterogeneity on contaminant transport [1–15]. Experimental and numerical studies have shown that the transport of solutes in porous media can be significantly influenced by the spatial variability in physical and geochemical parameters, such as hydraulic conductivity, porosity, and sorption coefficient [1–3].

Previous studies showed that the physical heterogeneity of the porous medium plays a key role in the contaminant transport [14]. These studies showed that the flow and transport in groundwater are strongly affected by the hydraulic properties of the medium, and thus accurate prediction of these groundwater processes requires advanced modeling. Generally the transport processes in the subsurface exhibit temporal and spatial variability, and thus it is assumed that the heterogeneous nature of aquifers determines a random behavior of flow and transport. The present work concerns the effects of hydrodynamic heterogeneities on the contaminant transport in aquifers using numerical modeling.

2. COMPUTATIONAL METHOD AND MODELS

2.1. COMPUTATIONAL METHOD

Contaminants are transported, in the porous medium, by the pore water flow. The governing equations for the single phase flow of a fluid (a single component or a homogeneous mixture) in a porous medium are given by the conservation of mass, Darcy's law, and an equation of state. Laboratory and small-scale field experiments have substantiated the validity of Darcy's law for flow through porous media [3–7]. The one-dimensional Darcy law is given by Equation (1)

$$Q = -KA(dh/ds) \quad (1)$$

where Q is the discharge rate in the s direction and the constant of proportionality K is the hydraulic conductivity in the s direction, a property of the porous medium and the fluid filling the pores. In Equation (1), A represents the cross-sectional area of a sand column and dh is the head difference between the manometers. The Darcy law for 3D flow can be written as:

$$\begin{aligned} q_x &= -K_x \partial h / \partial x \\ q_y &= -K_y \partial h / \partial y \\ q_z &= -K_z \partial h / \partial z \end{aligned} \quad (2)$$

For a confined aquifer, the 1D flow equation can be obtained from the mass balance and Darcy's combined with the specific storage (S_s):

$$\frac{\partial}{\partial x} \left(K_x \frac{\partial h}{\partial x} \right) = S_s \frac{\partial h}{\partial t} \quad (3)$$

Equation (3) assumes that the spatial gradient of water density is negligible (mostly fresh water). For a 3D flow the general equation is:

$$\frac{\partial}{\partial x} \left(K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial h}{\partial z} \right) = S_s \frac{\partial h}{\partial t} \quad (4)$$

Thus, the hydraulic head ($h = h(x, y, z)$) must obey this PDE to be consistent with both the Darcy's law and mass balance. It is worth noting that Equation (4) also makes use of the assumption that the spatial gradient of the water density is negligible, and the principal conductivity axes must be aligned with the coordinate axes. Equation (4) is the most universal form of the saturated flow equation for a confined aquifer, allowing flow in three dimensions, transient flow $\left(\frac{\partial h}{\partial t} \neq 0 \right)$, heterogeneous conductivities (e.g., K_x , K_y , K_z are spatially variable), and anisotropic porous medium (K_x , K_y , K_z). From Equation (4)

$$-\nabla \cdot \vec{q} = S_s \frac{\partial h}{\partial t} \quad (5)$$

and making use of $\vec{q} = \bar{\bar{K}} \nabla h$, where $\bar{\bar{K}} = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix}$, we obtain the most general flow equation

$$\nabla \cdot (\bar{\bar{K}} \nabla h) = S_s \frac{\partial h}{\partial t} \quad (6)$$

It is worth noting that Equation (4) is just a reduced form of the most general equation, given the condition that conductivity principal directions are aligned with the coordinate axes. Less general forms of flow equations can be derived from Equation (4) by making various simplifying assumptions. Thus, if the hydraulic conductivities are assumed to be homogenous (K_x , K_y , K_z are independent of x , y , z), the general equation can be written as:

$$K_x \frac{\partial^2 h}{\partial x^2} + K_y \frac{\partial^2 h}{\partial y^2} + K_z \frac{\partial^2 h}{\partial z^2} = S_s \frac{\partial h}{\partial t} \quad (7)$$

An alternative form of the flow equation can be obtained by substituting the Darcy's law, Equation (2), in Equation (4). The new equation is given by

$$-\left[\frac{\partial}{\partial x} (q_x) + \frac{\partial}{\partial y} (q_y) + \frac{\partial}{\partial z} (q_z) \right] = S_s \frac{\partial h}{\partial t} \quad (8)$$

$$\text{or } -\nabla \cdot \vec{q} = S_s \frac{\partial h}{\partial t} \quad (9)$$

In the present work the equations are solved using the finite element method (FEM). The flow domain is represented by a rectangular mesh composed of square cells; each cell is

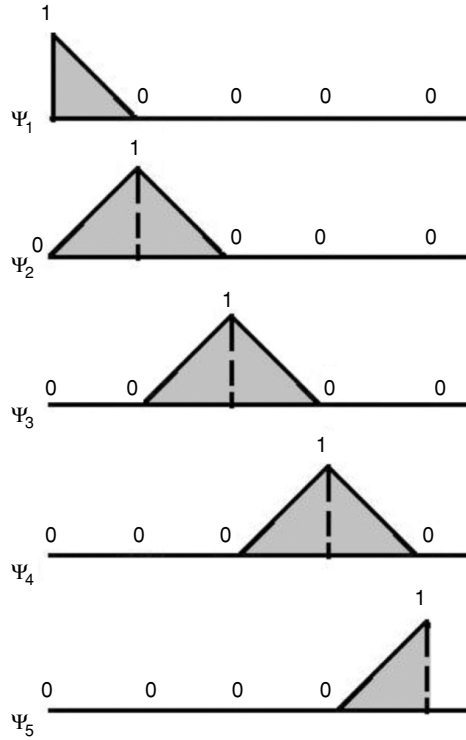


Figure 1 Basis functions in one dimension.

divided into two triangular elements. The computational domain is shown in Figure 1. Linear basis functions are used in the finite element formulation. After solving the hydraulic head h , the x and y components of the average interstitial velocity vector are computed by

$$V_x = -\frac{K}{n} \frac{\partial h}{\partial x} \quad (10)$$

$$V_y = -\frac{K}{n} \frac{\partial h}{\partial y} \quad (11)$$

where n is the porosity. The velocity vectors are used for computing the flow paths and advective movement of fluid particles. It is worth noting that in a flow field with nonuniform velocity, a cloud of fluid particles will tend to spread. This spreading can be described by the spatial variance (in the x and y directions) of particle positions

$$S_{xx} = \frac{1}{N} \sum_{i=0}^N (X_i - x_c)^2 \quad (12)$$

$$S_{yy} = \frac{1}{N} \sum_{i=0}^N (y_i - y_c)^2 \quad (13)$$

In Equations (12) and (13) N is the total number of fluid particles, x_i and y_i are the x and y coordinates of the i -th particle, x_c and y_c denote the x and y positions of the center of mass, defined as

$$x_c = \frac{1}{N} \sum_{i=0}^N x_i \quad (14)$$

$$y_c = \frac{1}{N} \sum_{i=0}^N y_i \quad (15)$$

If each fluid particle is assumed to carry a fixed amount of solute mass, then particle spreading is analogous to macro-scale solute dispersion. In the macro-dispersion approach, the small-scale variation of velocity is not explicitly simulation. Instead, solute spreading is characterized by a dispersion tensor. The components of the dispersion coefficients can be estimated by

$$D_{xx} = \frac{1}{2} \frac{dS_{xx}}{dt} \quad (16)$$

$$D_{yy} = \frac{1}{2} \frac{dS_{yy}}{dt} \quad (17)$$

As already mentioned, the equations of groundwater flow are solved using the finite element method. The finite element method (FEM) and finite difference method (FDM) are equivalent in the view of their accuracy. The only difference between the FEM and FDM is the way of approximating the flow equations. The FEM approximates the equation by integration while the FDM approximates the equation by differentiation. The mathematical approach to solve the unknown heads is briefly described in the following. For 2D flow in a confined aquifer the equation is

$$\frac{\partial}{\partial x} \left(T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial h}{\partial y} \right) + Q - S \frac{\partial h}{\partial t} = 0 \quad (18)$$

where Q in $[L^3/T]$ stands for the external sources and sinks and T in $[L^2/T]$ stands for transmissivity. When the boundary conditions are expressed in terms of the hydraulic head or flux, one must find the head distribution h that satisfies Equation (18) everywhere inside the domain at every instant in time. The exact head distribution cannot be determined in complex systems. Generally FEM approximates the solution of h by piecewise linear functions. To illustrate the FE approximation, let us consider a four elements model, as shown in Figure 1.

The governing flow equation is

$$\frac{\partial}{\partial x} \left(T \frac{\partial h}{\partial x} \right) - S \frac{\partial h}{\partial t} = 0 \quad (19)$$

In 1D for a given time, straight lines as elementwise approximation for the head distribution are found

$$\hat{h} = a + bx \quad (20)$$

where $\hat{h}$ represents the approximate head. Let us consider four elements.

$$\hat{h} = \begin{cases} h_3 + \frac{h_4 - h_3}{x_4 - x_3}(x - x_3) & x_3 \leq x \leq x_4 \\ 0 & \text{elsewhere} \end{cases} \quad (21)$$

An alternative way to express $\hat{h}$ is by using interpolation functions, also referred to as basis functions, ψ defined by Equation (22) and shown in Figure 1, and by formulating $\hat{h}$ as a weighted average of the nodal values h_3 and h_4 .

$$\psi_i = \begin{cases} 0 & |x| > x_{i-1} \\ 0 & |x| < x_{i-1} \\ \frac{x - x_{i-1}}{x_i - x_{i-1}} & x_{i-1} \leq x \leq x_i \\ \frac{x_{i+1} - x}{x_{i+1} - x_i} & x_i < x \leq x_{i+1} \end{cases} \quad (22)$$

The approximation for the head distribution in element 3 is

$$\hat{h} = \begin{cases} h_3 + \frac{h_4 - h_3}{x_4 - x_3}(x - x_3) & x_3 \leq x \leq x_4 \\ 0 & \text{elsewhere} \end{cases} \quad (23)$$

The approximation for the entire head distribution results from the summation of the contribution of each element and it is found that

$$\hat{h} = h_1\psi_1 + h_2\psi_2 + h_3\psi_3 + h_4\psi_4 + h_5\psi_5 \quad (24)$$

Equation (24) represents an approximate solution to the flow problem, but the nodal head values h_i are still unknown. The solution becomes exact for an infinitesimal discretization:

$$h = \lim_{n \rightarrow \infty} \sum_{i=1}^n h_i \psi_i \quad (25)$$

where n represents the number of nodes. For a finite n , the solution remains an estimate:

$$h \approx \hat{h} = \sum_{i=1}^n h_i \psi_i \quad (26)$$

Consequently we find for the 1D case

$$\frac{\partial}{\partial x} \left(T \frac{\partial \hat{h}}{\partial x} \right) - S \frac{\partial \hat{h}}{\partial t} = \varepsilon \neq 0 \quad (27)$$

where ε is the residual. The nodal heads h_i are still undetermined. It is worth noting that from a numerical point of view the residual ε must be kept small since $\varepsilon = 0$ corresponds to the exact solution. Although the governing flow equation cannot be satisfied everywhere, we determine h_i such that the residual on average is forced to converge to zero over the solution domain as expressed in $\int_x \varepsilon dx = 0$. Locally ε will not generally be zero. To force the residual

on average to zero, the FEM applies the weighted residuals. Using this method the residual weighted by an arbitrary function $f(x)$ demanding that the area integral still be zero:

$$\int_x \varepsilon f(x) dx = 0 \quad (28)$$

Since there are only n unknowns, only n conditions or functions can be applied to Equation (28). The popular Galerkin method is a special form of weighting method in which the n interpolation functions ψ_i are chosen as the n weighting functions μ_i

$$f(x) = \mu_i = \psi_i \quad (29)$$

Thus, Equation (28) becomes

$$\int_x \varepsilon \mu_i dx = 0 \text{ for } i = 1 \div n \quad (30)$$

Combining Equations (26), (27) and (30) we obtain

$$\int_x \left[\frac{\partial}{\partial x} \left(T \frac{\partial}{\partial x} \sum_{i=1}^n h_i, \mu_i \right) - S \frac{\partial}{\partial t} \sum_{i=1}^n h_i, \mu_i \right] \mu_j dx = 0 \quad (31)$$

for $j = 1 \div n$.

Developing Equation (31) step by step, a set of algebraic equations is formed for the unknown groundwater heads h_i . The discretized equations are given by:

$$\begin{aligned} & \frac{1}{6} \left[\frac{h_{i+1,k+1} - h_{i+1,k}}{\Delta t} + 4 \frac{h_{i,k+1} - h_{i,k}}{\Delta t} + \frac{h_{i-1,k+1} - h_{i-1,k}}{\Delta t} \right] + \varepsilon \frac{q_{i+1,k+1} - q_{i-1,k+1}}{2\Delta x} \\ & + (1 - \varepsilon) \frac{q_{i+1,k} - q_{i-1,k}}{2\Delta x} = 0 \end{aligned} \quad (32)$$

In the present problem the boundary conditions are of Dirichlet type. For more details on the FEM, the reader is referred to [5].

2.2. COMPUTATIONAL MODEL

Generally, groundwater flow in aquifers is modeled as two-dimensional in the horizontal plane. This holds accurate results since most aquifers have large aspect ratio, with horizontal dimensions hundreds times greater than the vertical thickness [5]. Thus, it can be assumed that the groundwater flows along the horizontal plane, meaning that the spanwise velocity component is small. The computational domain is illustrated in Figure 2.

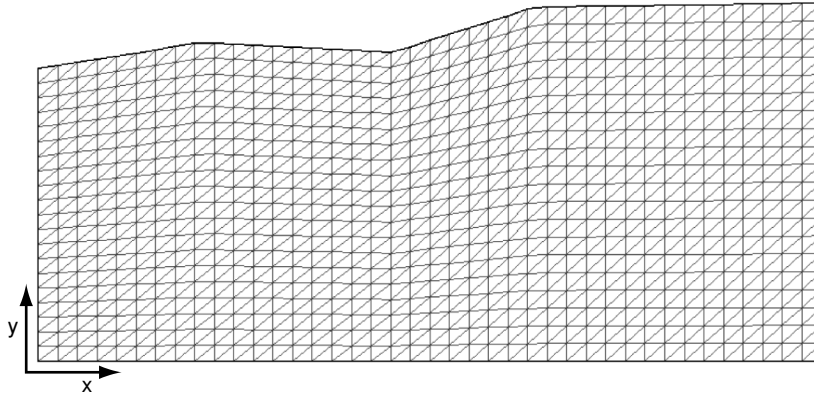


Figure 2 Computational domain.

3. RESULTS AND DISCUSSION

As already motioned the objective of the present study is to investigate the effect of heterogeneous porous medium on the particle dispersion. Figure 3 presents the heterogeneous computational domain. Figure 4 presents the particle dispersion at different instants in time. The study reveals that the particulate phase exhibits a preferential dispersion, which depends on the conductivity of the medium. Thus, the low values of conductivity cause the particles to travel at lower speeds as well forcing the particles to find the path of minimum resistance. This is well illustrated at instant $t = 70$ [days]; when the cluster of particles reaches the low conductivity porous region, the particles try to find a different path of lower resistivity. A good insight into the particles preferential path can be obtained from the observations of particle trajectories at instants $t = 10$ [days] and $t = 70$ [days]. The comparison of particle dispersion at these two instants in time shows that the cluster of particles entering the region of low conductivity (red-color in the middle of the domain) travels at much slower speed. The analysis of particle dispersion at instant $t = 150$ [days] reveals the preferential path of particle trajectories. Thus, most of the particles prefer to travel on the paths of minimum resistance (high conductivity).

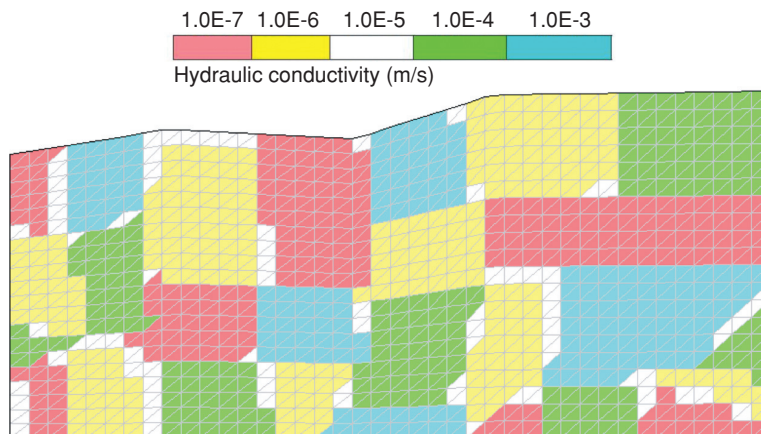


Figure 3 Heterogeneous porous medium.

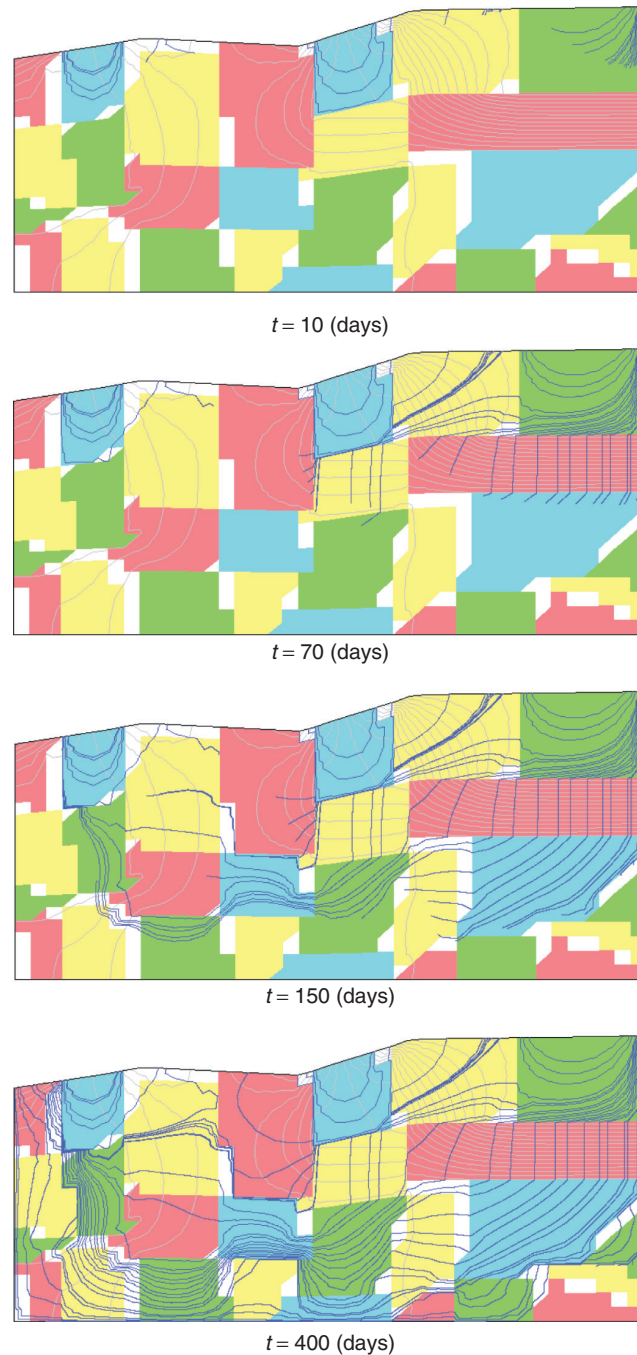


Figure 4 Particle trajectories.

Figure 5 presents the effect of heterogeneous medium on the particle dispersion. To conduct this study a cluster of particles is released at the upper region of the computational domain as shown in Figure 5 at instant $t = 1$ [day]. The analysis of particle dispersion shows that at the initial stage, 10[days], the particles distribute at the upper boundary of low

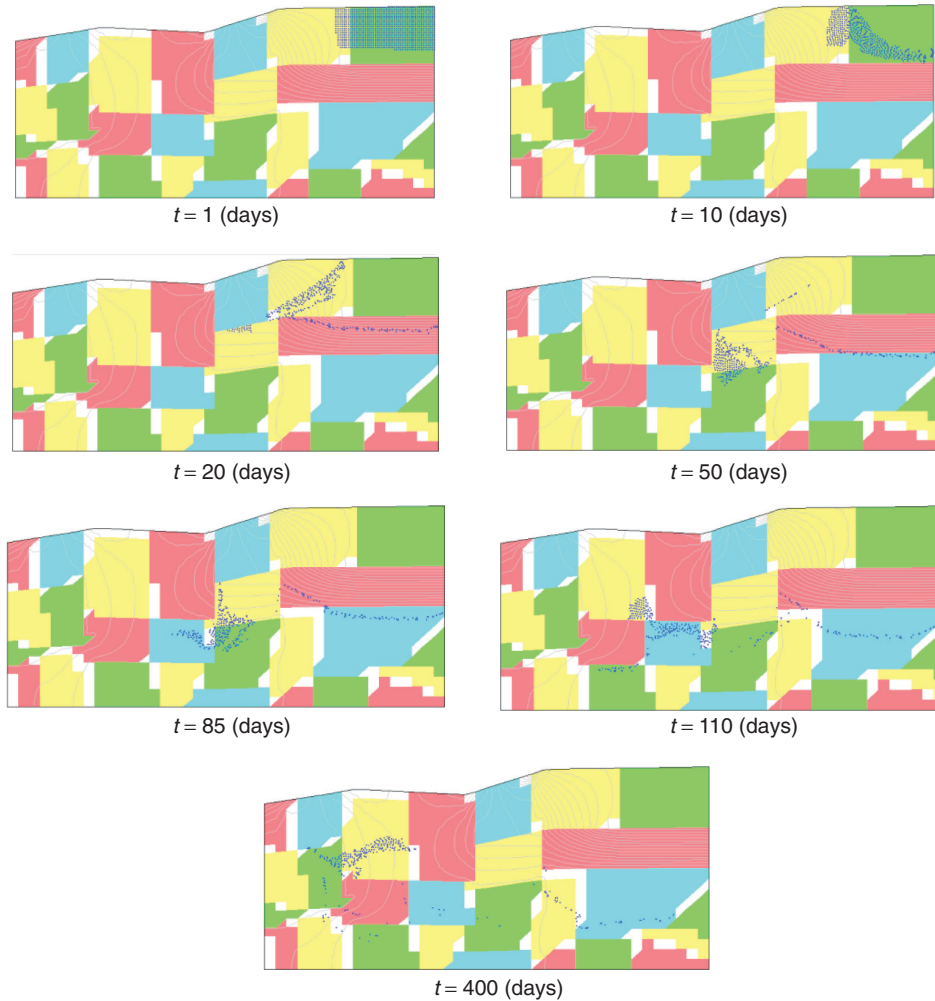


Figure 5 Particle dispersion.

conductivity region (red color). A percentage of the particles, about 35%, transits this low conductivity region, while the rest of particles enter a region of high conductivity, and thus are being transported further. The analysis reveals that the particles transiting the low conductivity region exhibit slow speed when compared with the particles transiting high conductivity regions. The anisotropic nature of the porous medium is reflected on the particle dispersion. Thus, the cluster of particles travels on the paths of minimum resistance. From Figure 5 it can be seen that the cluster of particles make a turn, when encounters the region of low conductivity (red color), searching for paths of minimum resistance. Once the particles reach the regions of high conductivity they travel much faster towards the terminus destination.

As part of this work, a second study is conducted to investigate the effect of a highly randomized heterogeneous porous medium on the particle dispersion. Figure 6 shows a highly random heterogeneous porous medium. In this case we assume that the variation of the heads, in the normal direction, is almost negligible (i.e. $\frac{\partial h}{\partial y} \approx 0$). Figure 7 presents the time-varying particle trajectory at three different instants in time. The analysis of numerical

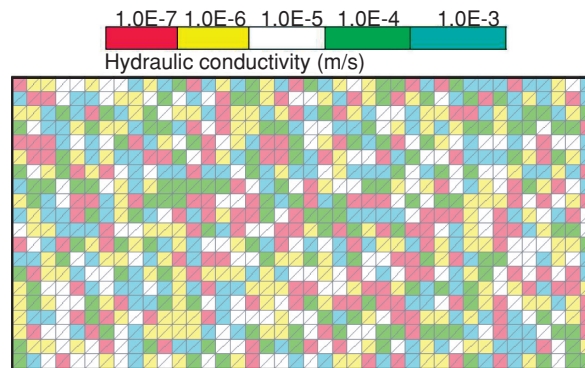
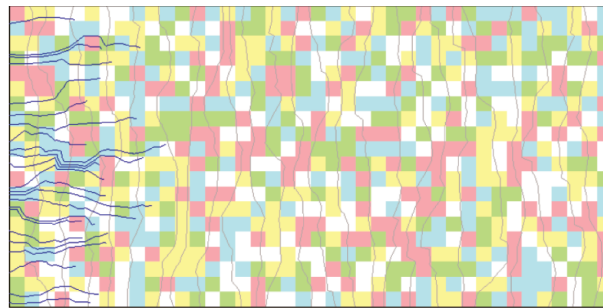
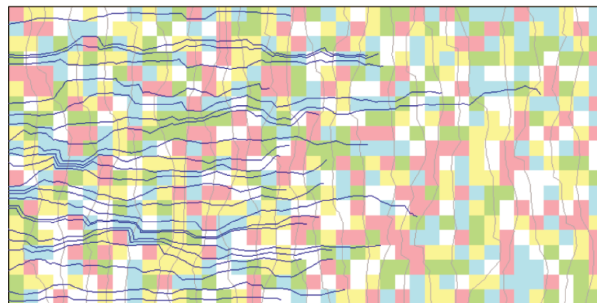


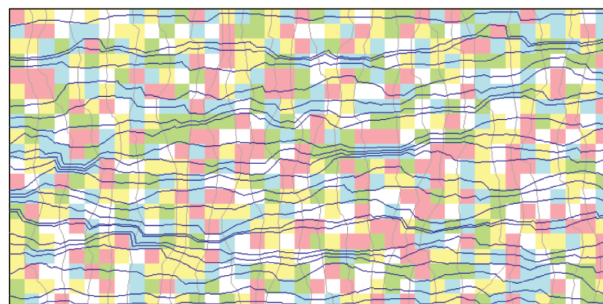
Figure 6 Heterogeneous, randomly sampled computational domain.



$t = 80$ (days)



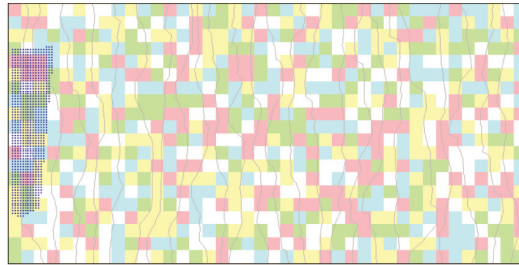
$t = 200$ (days)



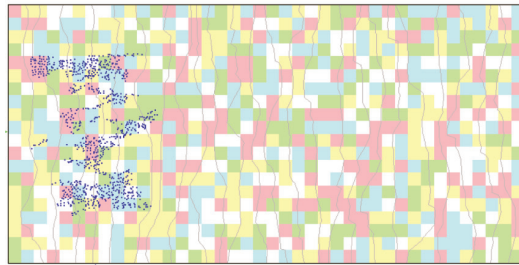
$t = 400$ (days)

Figure 7 Time-dependent particle trajectories.

results emphasizes the preferential dispersion of particles in the heterogeneous medium. Thus, the particles avoid the region of low conductivity and follow the paths of minimum resistance defined by high conductivity. The preferential particle's trend is also well illustrated in Figure 8. At the instant 1[day], the parcel of particles is released into the



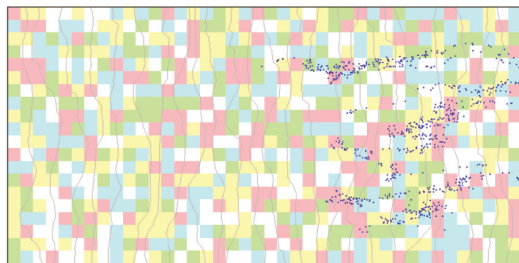
$t = 1$ (days)



$t = 60$ (days)



$t = 150$ (days)



$t = 300$ (days)

Figure 8 Particle dispersion in a randomly heterogeneous medium.

computational domain. The analysis of the numerical results reveals that the particle dispersion is mainly in the horizontal direction. It is also observed that the particles exhibit a preferential dispersion following the paths of minimum resistance.

The present study shows that the heterogeneous nature of the porous medium causes the particles to exhibit different speeds, and thus particles which travel regions of high conductivity would travel faster than the ones traveling through regions of low conductivity. Moreover, the particles always search for the path of minimum resistance. Particles transiting the regions of low conductivity are forced to reside in these regions for long periods of time. This would raise serious concerns for particles posing health hazards. Thus, a detailed knowledge of the subsurface composition would help diminish these health hazards.

4. CONCLUSIONS

A particle tracking algorithm is developed for the study of particle dispersion into porous media. The effect of heterogeneous medium on the particle dispersion is subject of investigation. The study reveals that the particles exhibit a preferential dispersion which depends on the conductivity of the medium. It is observed that the particles travel on the path of minimum resistance. Also the particles traveling through regions of low conductivity exhibit lower speeds than the one traveling through regions of high conductivity. Particles transiting the regions of low conductivity reside in these regions for long periods of time. The FEM is a computationally efficient approach for the prediction of particle dispersion into porous media.

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