Simulation of Solute Transport in Heterogeneous Aquifers using Stochastic Partial Differential Equations

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Abstract   Flow in porous media has been a subject of active research for the last four to five decades. In this paper, a simulation model developed using stochastic partial differential equations to describe hydrodynamic dispersion of a tracer in a confined aquifer is presented with appropriate visualisations. Since the velocity of a tracer particle depends very much on the pore structure of the medium, it can be described by the average Darcian velocity and a Wiener process in space and in time accounting for uncertainty in the pore structure. We can simulate random paths of tracer particles using this stochastic process for the velocity and correlation functions can be used to control the behaviour. In this way, we can model the hydrodynamic dispersion of a tracer without resorting to perturbation solutions in a porous medium. In addition, pore-scale diffusion is modelled as a stochastic differential equation relating the instantaneous concentration gradient of the solute at a specific location to the stochastic diffusive flux through a coefficient containing noise. This noise term is also characterised in terms of a Wiener process in space and in time with its correlation functions. The total stochastic flux is the sum of the flux due to the velocity and the flux due to pore-scale diffusion. Based on these concepts, a stochastic solute transport model is developed incorporating the properties such as porosity and hydraulic conductivity either as deterministic functions or as random quantities from appropriate distributions if sufficient amount of data is available from the porous formation. The stochastic transport model is solved numerically for 1-dimensional, 2-dimensional and 3-dimensional cases.

1.   INTRODUCTION

Flow in porous media has been a subject of active research for the last four to five decades. Field experiments show that spatial heterogeneity is the most significant factor affecting dispersion of solutes in natural formations such as aquifers (Anderson, 1979; Gelhar et al., 1985; Freyberg, 1986). Dagan (1988) concluded that the concentration of a solute can be considered as a random variable, which can be described by its statistical moments, and the expected value of concentration does not necessarily satisfy an advective-dispersive type equation based on the continuum approach; and even if the latter is satisfied, the dispersion coefficient increases with the travel time reaching an asymptotic value. Cushman (1987) stated that the transport process in natural formations can not be modelled by the advective-dispersive equation because of stochastic (random) fluctuations in flow velocity due to natural heterogeneity in the pore structure and failure of Fick's type diffusion equation to describe the pore scale dispersion. Scale dependence of the dispersion process has been examined in the light of the spatial distribution of hydraulic conductivity in many studies (Dagan, 1988, 1990). Serrano (1988) argued that small random variations in the perturbation expansion solutions (Gelhar and Axness, 1983) should have small variance for the

differential equations to be valid. One could argue that if the variances of the processes involved are indeed small as required by the perturbation solutions, then a completely deterministic model could be used as a sufficient tool for prediction purposes. Cushman (1987) made similar conclusions after an in-depth analysis of the perturbation solutions provided by Gelhar and Axness (1983).

The objective of this paper is to develop a computational model for solute transport in a saturated heterogeneous porous medium by treating velocity as a stochastic variable and by providing ways to incorporate stochasticity in pore scale diffusion. The model is developed in a manner so that hydraulic conductivity and porosity can be either deterministic functions or stochastic variables. The advantage of such a computational model is that we can use the model to see whether we could characterise the variability in the concentration field using the stochasticity in velocity and pore-scale diffusion. We discuss the development of the model and associated numerical solutions briefly and present a selected number of visualisations of the concentration field.

2. STOCHASTIC VELOCITY

Since the velocity of a solute particle is central to formulating a model of transport processes, it is important to develop the concept of stochastic velocity to describe the motion of a particle in a porous medium. Velocity of a tracer can be described in Cartesian coordinates by the average Darcian velocity and a random component accounting for uncertainty due to pore structure:

$$\underline{V}(x,t) = -\frac{K(x)}{\varphi(x)}\nabla\phi(x,t) + \underline{W}(x,t) \tag{1}$$

Here K is hydraulic conductivity, φ is porosity, ϕ is piezometric head, W is a random component in the velocity due to pore structure, x denotes spatial coordinates and t is time. The random part is assumed to be noise correlated in space and δ-correlated in time. This assumption allows us to obtain stochastic differential equations having separable time and space, and at the same time provides a mechanism to model irregular variations in the system in a realistic manner (Unny, 1989). W(x,t) is assumed to be a Wiener process (in some literature it is called a Brownian process) in time and in space and it is the only stochastic process having continuous paths as well as stationary independent increments with zero mean (Knight, 1981).

A stochastic process W(t) is a standard Wiener process if

1. W(0)=0, $\tag{2}$

2. the random variables $W(t_1)$, $W(t_2)$, ..., $W(t_n)$ are n-dimensional Gaussian processes whose parameters are

$$E[W(t)]=0, \quad E[W(t_i) W(t_j)] = \min (t_i, t_j). \tag{3}$$

A general Wiener process in time can be defined by using a correlation function q(t) related in time such that

$$E[W(t)] = 0 \tag{4}$$

and $E[W(t_i) W(t_j)] = \int_0^{\min(t_i,t_j)} q(\tau)d\tau$, q>0. $\tag{5}$

A Wiener process in time and in space, W(x,t) is similarly defined by using a correlation function q(t,x) related in time and in space such that

$$E[W(x,t)] = 0 \tag{6}$$

and

$$E[W(x_i, t_i) W(x_j, t_j)] =$$

$$\int_0^{\min(x_i,x_j)} \int_0^{\min(t_i,t_j)} q(\tau,\zeta)d\tau d\zeta . \tag{7}$$

The general Wiener process, $W(x,t)\in E^0=L^2(R) \times [0, T]$, where E^0 is a separable Hilbert space. Unny(1989) illustrated a procedure to replace the Wiener process increment in E^0, $d\beta = W(x,t) dt$, using stochastic calculus in Hilbert space.

The Wiener process increment in a Hilbert space can be approximated by the series

$$d\beta_m(t) = \sum_{i=1}^m e_i(d\beta(t),e_i) \tag{8}$$

where e_i 's are an orthonormal basis in the Hilbert space E^0, which can be taken as the eigen functions of the correlation operator Q:

$$Qe = \omega\, e \tag{9}$$

Then the Wiener process increments can be written as,

$$d\beta_m(t) = \sum_{j=1}^m e_j \sqrt{\omega_j}\, db_j(t) \tag{10}$$

where db 's are all increments of independent standard Wiener processes. Kumar et al. (1991) used a 4 x 4 positive definite matrix for the space correlation operator Q to model the 2- dimensional space correlation of the random term of a stochastic rainfall input. They have used component values (q_{ij}'s) of the order of 10^{-3} for their numerical simulations with a time step of 0.1 days. In the 1-dimensional case, for example, the correlation operator is a 2 x 2 matrix, and the components, q_{ij}'s , indicate the degree to which the random component at x_i is related to that at x_j for a given time. The standard Wiener process does not have a space correlation coefficient and is entirely time correlated through min (t_i, t_j) which can be thought of as having a unit space correlation component q_{ii} at a given point in space.

Natural formations are anisotropic in general, and it can be assumed that the space correlation of the random component in one direction is independent of the space correlation in another direction. If this assumption is valid, the correlation operator in a given direction is a 2 x 2 matrix. To illustrate the significance of the correlation operator (Q), let us consider paths of tracer particles modelled by (1) in two dimensions.

When (1) is modified by replacing the velocity vector with the time derivative of the displacement vector and multiplying by dt, the following equation can be obtained.

$$d\underline{x} = -\frac{K(x)}{\varphi(x)}\nabla\phi(x,t)dt + \underline{W}(x,t)dt \tag{11}$$

The last term on the right hand side can be replaced by (8), $d\beta(t)$, for each direction; then we have ordinary stochastic differential equations for the x and y directions. These

equations can be solved numerically by using, for example, an Euler scheme or a Milstein scheme which are strong Taylor approximations (Kloeden and Platen, 1994). Figure 1 shows three different realisations of y displacement of a particle in a porous medium having a constant porosity (0.3), a constant hydraulic conductivity (46.0 m/day) and a constant piezometric head gradient (-0.020 m/m). The values of q_{ij} for all i and j were assumed to be 0.001 and this corresponds to equal e_j values (0.707) and equal ω_j values (0.002) in (10). The time increment for simulations was 0.001 days and the simulations were run until the distance traced by a realisation in the x direction was 10.0 m. As shown by Figure 1, realisations of y displacement given by (11) can be quite different from each other.
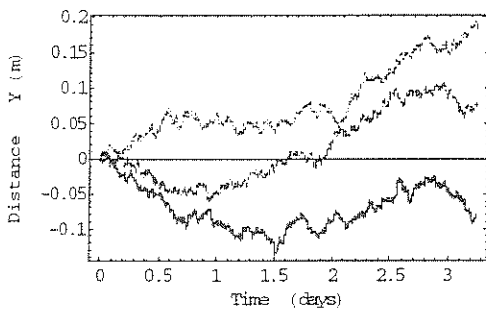

Figure 2: Three realisations of y displacement of a tracer particle given by (11) when q_{ij}s are 0.1.

Figure 1: Three realisations of y displacement of a tracer particle given by (11) when q_{ij}s are 0.001.

At any given time t, the expected value of y displacement is zero and the expected value of x displacement is given by the integration of the Darcian velocity from 0 to t. The second moments of displacements depend on Q and t. In these particular examples, porosity and hydraulic conductivity are taken as constants, but they can either be deterministic functions reflecting their distributions across the spatial domain or be random functions if their changes are highly irregular or be a combination of both. If random functions for porosity and hydraulic conductivity are used, means and variances have to be evaluated using computer generated samples and the central limit theorem. When values of q_{ij} s are increased to 0.1, three of the resulting realisations are given in Figure 2 to illustrate the effect of the random component in 1. Note the differences in the y displacement in Figures 1 and 2: change in Q produces significant changes in the realisations and this means that particle velocity given by (1) could be used to model the dispersion in a porous medium.
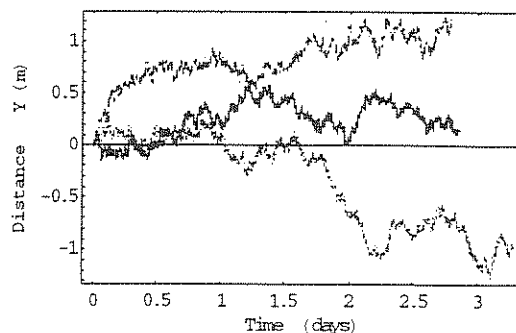
3. A STOCHASTIC SOLUTE TRANSPORT MODEL

The formulation of a stochastic solute transport model based on stochastic variables is briefly described here. This formulation assumes that the solute has similar density and viscosity to those of water; representative values of effective porosity and hydraulic conductivity can be assigned to specific points in a specified domain using either random or deterministic spatially distributed functions; piezometric head is given or can be calculated for a specific point; and velocity at a given point is given by (1).

For the sake of simplicity, consider a small 1-dimensional cylindrical section having a cross sectional area of A and length δx in the X direction. Solute flux at X=x is J_x (kg/m^2 day) and that at X= x+δx is $J_{x+\delta x}$. During a small time duration δt,

the solute mass entering the element = J_x (Aφ(x)) δt, and

the solute mass leaving the element = $J_{x+\delta x}$ (A φ(x+δx)) δt

where $J_{x+\delta x} = J_x + \dfrac{\partial J_x}{\partial x}\delta x$.

the change of solute mass within the element

$$= J_x A\varphi(x)\delta t - \left(J_x + \frac{\partial J_x}{\partial x}\delta x \right) A\varphi(x+\delta x)\delta t.$$

Substituting $\varphi(x+\delta x) = \varphi(x) + \delta\varphi$, and simplifying , the change of solute mass within the element

$$= - J_x A\,\delta\varphi\delta t - \frac{\partial J_x}{\partial x} A\varphi\delta x\delta t - \frac{\partial J_x}{\partial x} A\delta\varphi\delta x\delta t.$$

We define the solute concentration within the element (C (x)) as the mass of solute per unit void volume and assign that value to X=x for small δx. Then the change in solute mass within the element during δt can be written in terms

of concentration. Change in solute mass within the element $= \delta C \varphi A \delta x$.

Therefore,

$$\delta C \varphi A \delta x =$$

$$- J_x A \delta \varphi \delta t - \frac{\partial J_x}{\partial x} A \varphi \delta x \delta t - \frac{\partial J_x}{\partial x} A \delta \varphi \delta x \delta t$$

Simplifying we obtain

$$\varphi \frac{\delta C}{\delta t} = - J_x \frac{\delta \varphi}{\delta x} - \frac{\partial J_x}{\partial x} \varphi - \frac{\partial J_x}{\partial x} \delta \varphi$$

and taking limits as $\delta x \to 0$, $\delta t \to 0$ and $\delta \varphi \to 0$,

$$\varphi \frac{\partial C}{\partial t} = - J_x \frac{\partial \varphi}{\partial x} - \varphi \frac{\partial J_x}{\partial x} \qquad (12)$$

(12) can be simplified further if we can neglect the gradient of the effective porosity within certain regions.

For two dimensional space, for example, (12) becomes

$$\varphi \frac{\partial C}{\partial t} = - J_x \frac{\partial \varphi}{\partial x} - J_y \frac{\partial \varphi}{\partial y} - \varphi \frac{\partial J_x}{\partial x} - \varphi \frac{\partial J_y}{\partial y} . \qquad (13)$$

It should be noted that the fluxes, concentration and porosity are stochastic variables. The main feature of the model given by (13) is that it is expressed in terms of fluxes and no assumption is made relating them to the concentration. Further we avoided using the chain rule for differentiation as the deterministic chain rule is invalid when stochastic variables are involved. Next we introduce the concept of stochastic flux.

3.1 Stochastic Flux

It has been suggested previously that the dominant mode of solute transfer is advection, and if the velocities are low which is the case in aquifers, dispersion may play a significant role giving highly "irregular" concentration contours, even after considerable smoothing (Dagan, 1990). The following model for the stochastic flux is proposed to model the hydrodynamic dispersion:

$$\underline{J} = \underline{V} C - \left(\underline{D} + \underline{W_d} \right) \nabla C \qquad (14)$$

Here $\underline{V}$ is the stochastic velocity given by (1), C is the concentration, $\underline{D}$ is a diffusivity vector which gives *typical values* of the diffusivity for pore scale diffusion and $\underline{W_d}$ models the random components of diffusion using a Wiener process in Hilbert spaces. It should be noted that two

different Wiener processes, W and W_d , have two different correlation coefficients. (14) gives the flexibility to investigate the effects of advection and diffusion separately. It is assumed that the stochastic flux has a high level of randomness where concentration gradients are high. By substituting (1) in (14), we can express the stochastic flux in terms of velocity and concentration, and the Wiener processes can be evaluated by using (10) at any given instance according to the definition of the Ito integral (Kloeden and Platen, 1994). The resulting expression for the stochastic flux and the conservation equation ((14) for 2 -dimensions) constitute a stochastic model for solute transport in porous media. This model has to be solved using numerical schemes with appropriate boundary conditions and initial conditions. The numerical schemes used in this research were developed and tested by the author.

4. COMPUTATIONAL MODELS

Computational models based on the stochastic and 3-dimensional cases with a constant tracer concentration is imposed on the upstream boundary for a given period of time. As an example, the stochastic model can be written for the 1-dimensional porous medium with uniform effective porosity. A numerical routine was developed to solve the above stochastic partial differential equation using (10) and the definition of Ito integral for the Wiener processes, W and W_d. Since the Wiener processes involved are irregular, continuous, non-differentiable processes, special routines were developed for the 1-dimensional model which has a concentration pulse of 1.0 introduced at the upstream boundary over ½ day. The hydraulic conductivity is 46.0 m/day and the piezometric head gradient is 0.020 m/m and the simulations were run with q_{ij}'s = 0.01 for the W Wiener processes. The diffusivity is taken as 0.00008 m^2/day and the q_{ij} s associated with the W_d Wiener process is 0.0001. Realisations of the concentration at 0.4 day and at 1.4 day generated from the model are shown in Figures 3 and 4, respectively.
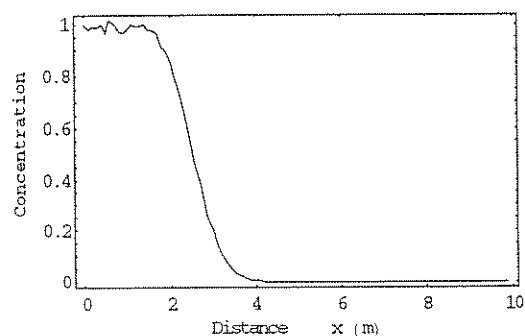

Figure 3: A realisation of the concentration at 0.4 days.
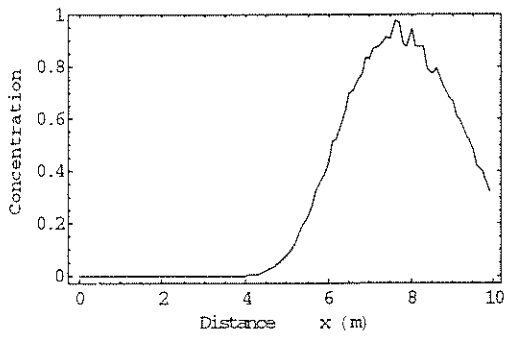
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Figure 4: A realisation of the concentration at 1.4 days.

With q_{ij} 's = 0.1 for the W Wiener process and the same parameters as above, two realisations at 0.4 day and at 1.4 day from the model are shown in Figure 5 and Figure 6, respectively.
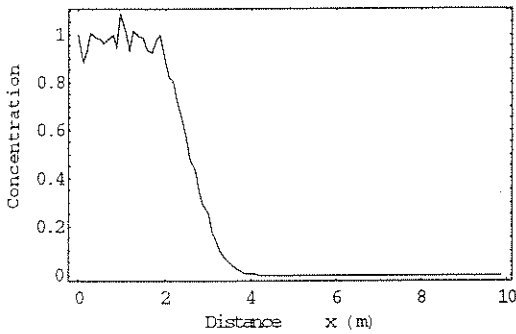

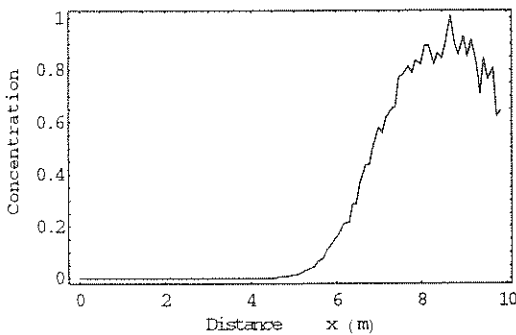**Figure 5:** A realisation of the concentration at 0.4 days.

Figure 6: A realisation of the concentration at 1.4 days.

The effect of the correlation operator, Q, in W can be seen from the above figures, and in general, an increase in Q increases the shape of the concentration spread and the noise level associated with the pulse. Increasing the q_{ij}s associated with the diffusivity (W_d) keeping all other parameters unchanged will also increase the spread of the pulse. This indicates that the model allows us to experiment with the relative significance of the pore-scale

diffusion, advection, related noise terms and variations in parameters such as hydraulic conductivity and head gradient.

A numerical routine was developed to solve the model for the 2-dimensional case. A realisation for a rectangular region of 10 m x 5 m having uniform porosity of 0.3, hydraulic conductivity of 46.0 m^2/day and a uniform pressure gradient of -0.02 m / m along the x axis is shown in Figure 6. The axes are divided into 0.1 m divisions and q_{ij} values for each directions were taken as 0.01. A uniform concentration of 1.0 was applied for x=0 plane for ½ day, and the realisation shown in Figure 7 is sampled at 0.93 day.
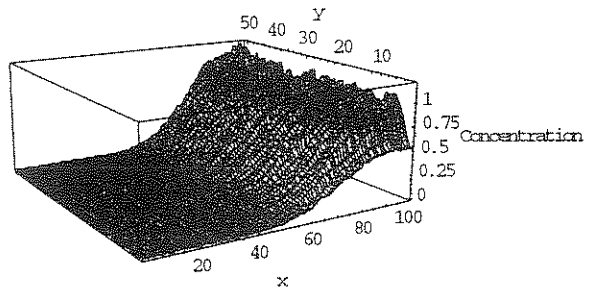

Figure 7a: A realisation of the concentration at 0.93 days.

A contour plot of the same realisation is shown in Figure 7b. Even with a small noise introduced to the stochastic velocity, a significant irregularity is shown in the concentration contours of the advancing concentration front. This situation can be further complicated by the stochasticity introduced by hydraulic conductivity and boundary conditions.
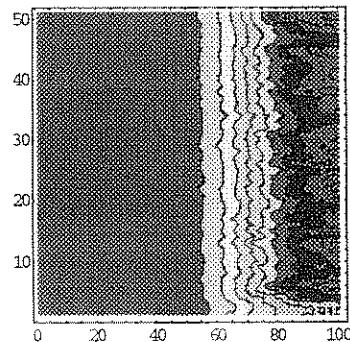

Figure 7b: Contour plot of concentration shown in

Figure 7a.

5. SUMMARY AND DISCUSSION

A stochastic model based on concepts of stochastic velocity and flux was developed; the numerical solutions were developed to solve them for 1, 2 and 3 dimensional cases. In this paper, we showed the influence of the correlation operator in the Wiener process in a few situations and it can be used to characterise hydrodynamic dispersion within porous media. Future research will be aimed towards conceptual validation of the model using simulations and experimental data from artificial aquifers which are being constructed by the Lincoln Environmental at Lincoln University, Canterbury, New Zealand. The numerical solutions for stochastic partial differential equations are still at early stages of development and this work will provide valuable contributions in that area as well. As can be seen from this paper, even with a uniform hydraulic conductivity, it is possible to have irregularity in concentration fields due to randomness in the pore structure. Stochastic differential equations provide a method of modelling this variability; however, their solutions are computationally expensive. With the advancement of distributed computing, this will not be a serious problem in solving stochastic partial differential equations.

6. ACKNOWLEDGEMENT

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