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A Stochastic Model for Solute Transport in Porous Media: Mathematical Basis and Computational Solution

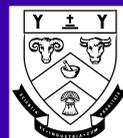
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A Stochastic Model for Solute Transport in Porous Media: Mathematical Basis and Computational Solution

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In this paper, we develop a computational model of solute dispersion in saturated porous media by considering fluid velocity as a fundamental stochastic quantity. The velocity can be considered as having a random part correlated in space and δ -correlated in time superimposed on the Darcian velocity. The spatial correlation depends on the geometric and other properties of porous media. The stochastic partial differential equation that describes the mass conservation of a solute in an infinitesimal volume is derived by assuming the variables are irregular, continuous random variables which require higher order terms in the Taylor series to model the spatial variation. This partial differential equation can be written in the form of a stochastic differential equation with a drift term and a diffusion term. The diffusion term can be expressed in terms of a Hilbert space valued Wiener process which is a function of the spatial correlation of the random part of velocity. This spatial correlation is modelled in terms of a covariance function with an exponential kernel having a fixed correlation length, and Karhunen-Loeve expansion based on the orthonormal basis functions for the exponential kernel is used in the solution. A numerical scheme was developed to solve the model based on the definition of Ito integral.

1. INTRODUCTION

Computational models can often be used to investigate the phenomena they describe through experimentation with the model. In this paper, we develop a model that describes the solute dispersion in a porous medium saturated with water considering velocity of the solute as a stochastic variable. When we consider the hydrodynamic dispersion of a solute in flowing water in a porous medium, there are two ways the solute gets distributed over the medium. The solute can mechanically disperse due to fingering effects of the granular medium and it can diffuse due to solute concentration differences. In deriving the advection-dispersion equation for solute transport, the dispersive transport is modelled by using a Fickian assumption which gives rise to the hydrodynamic diffusion coefficient (Fetter, 1999). The hydrodynamic diffusion coefficient has been found to be dependent on the scale of the experiment. The

hydrodynamic dispersion contributes to making the velocity of solute particles a random variable by changing direction and magnitude in an unpredictable manner. In this paper, we propose a model which addresses this fundamental nature of the dispersion phenomena in porous media

2. DEVELOPMENT OF A STOCHASTIC MODEL

Let us consider a 1-dimensional problem of a solute dispersion in a saturated porous medium. Consider concentration $C(x,t)$ as a stochastic variable with, for example, g/m^3 as units, $V(x,t)$ is the velocity (m/h) and $J(x,t)$ is the contaminant flux at x in $g/m^2.h$. As C , V , and J are stochastic functions of space and time having irregular (sometimes highly irregular) and continuous realisations, it is important to consider higher order terms to the Taylor series expansion when formulating the mass conservation model for the

solute. Consider an infinitesimal cylindrical object having a cross sectional area, A (Figure 1).

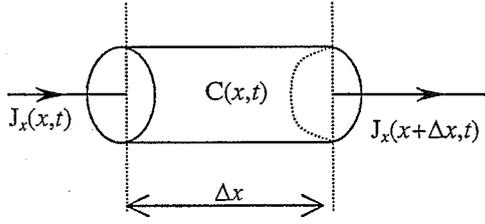


Figure 1 An infinitesimal cylindrical object within the porous medium having the solute concentration of $C(x,t)$

Writing the mass balance for the change in solute during a small time increment, Δt ,

$$\begin{aligned} \Delta C(x,t) A \Delta x &= (J_x(x,t) - J_x(x+\Delta x,t)) A \Delta t \\ \therefore \left(\frac{\Delta C}{\Delta t} \right)_{x,t} &= \frac{(J_x(x,t) - J_x(x+\Delta x,t))}{\Delta x} \end{aligned} \quad (1)$$

For convenience, let us indicate $J_x(x,t)$ as J_x and $J_x(x+\Delta x,t)$ as $J_{x+\Delta x}$.

From the Taylor series expansion,

$$\begin{aligned} J_{x+\Delta x} - J_x &= \frac{1}{1!} \frac{\partial J_x}{\partial x} \Delta x + \\ &\frac{1}{2!} \frac{\partial^2 J_x}{\partial x^2} (\Delta x)^2 + \\ &\frac{1}{3!} \frac{\partial^3 J_x}{\partial x^3} (\Delta x)^3 + R(\varepsilon) \end{aligned}$$

where $R(\varepsilon)$ is the remainder of the series.

Assuming that the higher order derivatives greater than 3 of the flux are negligible, (1) can be written as

$$\frac{\partial C}{\partial t} = -\frac{\partial J_x}{\partial x} - \frac{1}{2} \frac{\partial^2 J_x}{\partial x^2} dx + R_c(x,t) \quad (2)$$

where,

$$\begin{aligned} R_c(x,t) &= -\frac{1}{6} \frac{\partial^3 J_x}{\partial x^3} (dx)^2 - \\ &\frac{1}{24} \frac{\partial^4 J_x}{\partial x^4} (dx)^3 - \Lambda \end{aligned}$$

Substituting $dx = h_x$

$$\frac{\partial C}{\partial t} = -\frac{\partial J_x}{\partial x} + \frac{h_x}{2} \frac{\partial^2 J_x}{\partial x^2} + R_c(x,t) \quad (3)$$

(3) describes the mass conservation of the contaminant within the cylindrical volume ($A\Delta x$).

$$\begin{aligned} dC &= -\left(\frac{\partial J_x}{\partial x} + \frac{h_x}{2} \frac{\partial^2 J_x}{\partial x^2} \right) dt + \\ &R_c(x,t) dt \end{aligned}$$

Compared to the first term on the right hand side, let us assume that $R_c(x,t)dt \approx 0$. This assumption has to be tested in any given situation.

$$\therefore dC = -\left(\frac{\partial J_x}{\partial x} + \frac{h_x}{2} \frac{\partial^2 J_x}{\partial x^2} \right) dt \quad (4)$$

Let us express the $J(x,t)$ term in terms of the velocity in the x direction and the concentration of the contaminant.

$$J(x,t) = V(x,t) C(x,t) \quad (5)$$

Now the velocity can be expressed as a stochastic quantity which is affected by the nature of the porous medium. The effects of the porous medium can be included within the noise term of the stochastic variable. We model the velocity in terms of the mean velocity and the Gaussian white noise.

$$V(x,t) = \bar{V}(x,t) + \xi(x,t) \quad (6)$$

where

$$\bar{V}(x,t) = -\frac{K(x)}{\varphi(x)} \frac{\partial p}{\partial x} \quad (\text{Darcy's Law})$$

$K(x)$ = a typical value of the hydraulic conductivity in the region

$\varphi(x)$ = the porosity of the material

p = pressure head

and $\xi(x,t)$ is white noise correlated in space and δ -correlated in time such that

$$E[\xi(x,t)] = 0 \quad (7)$$

$$E[\xi(x_1, t_2) \xi(x_2, t_2)] = q(x_1, x_2) \delta(t_1 - t_2) \quad (8)$$

$q(x_1, x_2)$ is the velocity covariance function in space and $\delta(t_1 - t_2)$ is the Dirac delta function.

Substituting (6) into (5)

$$J(x,t) = (\bar{V}(x,t) + \xi(x,t)) C(x,t) \quad (9)$$

$$J(x,t) = \bar{V}(x,t) C(x,t) + C(x,t) \xi(x,t) \quad (10)$$

Substituting (10) into (5)

$$\begin{aligned} dC &= -\frac{\partial}{\partial x} [\bar{V}(x,t) C(x,t) + C(x,t) \xi(x,t)] \\ &\quad - \frac{h_x}{2} \frac{\partial^2}{\partial x^2} [\bar{V}(x,t) C(x,t) + C(x,t) \xi(x,t)] \\ &= -\left(\frac{\partial}{\partial x} + \frac{h_x}{2} \frac{\partial^2}{\partial x^2} \right)^* \\ &\quad [\bar{V}(x,t) C(x,t) + C(x,t) \xi(x,t)] \end{aligned} \quad (11)$$

Let us define the operator in space,

$$A = -\left(\frac{h_x}{2} \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} \right) \text{ for a given } h_x.$$

Then

$$dC = A(\bar{V}(x,t) C(x,t) + C(x,t) \xi(x,t)) dt$$

$$dC = A(\bar{V}(x,t) C(x,t)) dt + A(C(x,t) (\xi(x,t) dt)) \quad (12)$$

(12) is a stochastic differential equation and both terms on the right hand side need to be integrated as Ito integrals to obtain concentration. We introduce $d\beta(t) = \xi(x,t) dt$ where $\beta(t)$ is a Wiener process in Hilbert space for a given x .

Therefore (12) can be written as

$$dC = A(\bar{V}(x,t) C(x,t)) dt + A(C(x,t) d\beta(t)) \quad (13)$$

$$\therefore C(x,t) = \int_0^t A(\bar{V}(x,t) C(x,t)) dt + \int_0^t A(C(x,t) d\beta(t)) \quad (14)$$

where A is the differential operator given above

Unny (1989) showed that $d\beta(t)$ can be approximated by

$$d\beta_m(t) = \sum_{j=1}^m e_j \sqrt{\lambda_j} db_j(t) \quad (15)$$

where m is the number of terms used, $db_j(t)$ is the increments of standard Wiener processes, e_j and λ_j are eigen functions and eigen values of the covariance function of the velocity, respectively

2.1. Covariance Kernel For Velocity

Ghanem and Spanos (1991) describe the mathematical details of expressing the noise term of a stochastic variable (e.g. velocity in this case) as a Karhunen-Loeve expansion. The central to this expansion is the choice of the covariance function (Covariance Kernel) which models the spatial correlation of the 'noise' term ($\xi(x,t)$ in (6)). We assume an exponential covariance kernel in this work to illustrate the model development. The exponential covariance kernel is frequently used in modelling the correlation of geographical data.

The exponential covariance kernel can be given as

$$q(x_1, x_2) = \sigma^2 e^{-\frac{|x_1 - x_2|}{b}} \quad (16)$$

where $y = |x_1 - x_2|$, b is the correlation length and σ^2 is the variance (Ghanem and Spanos, 1991). x_1 and x_2 are any two points within the range $[0, a]$. The eigen functions (σ^2) and eigen values (λ_n) of $q(x_1, x_2)$ are obtained as the solution to the following integral equation

$$\int_0^a q(x_1, x_2) e_n(x_2) dx_2 = \lambda_n e_n(x_1) \quad (17)$$

The solutions to (17) assuming σ^2 is a constant over $[0, a]$ are given by,

$$\lambda_n = \frac{2C\sigma^2}{\omega_n^2 + C^2} \quad (18)$$

where $C = \frac{1}{b}$ and ω_n 's are roots of the following equation¹

$$\tan \omega_n a = \frac{2\omega_n C}{\omega_n^2 - C^2} \quad (19)$$

$$e_n(x) = \frac{1}{\sqrt{N}} \left(\sin \omega_n x + \frac{\omega_n}{C} \cos \omega_n x \right) \quad (20)$$

where

$$N = \frac{1}{2} a \left(1 + \frac{\omega^2}{C^2} \right) - \frac{1}{4\omega} \left(1 + \frac{\omega^2}{C^2} \right) \sin 2\omega a - \frac{1}{2C} (\cos 2\omega a - 1) \quad (20a)$$

3. COMPUTATIONAL SOLUTION

3.1. Numerical Scheme

The differential operator A in (12) can be expressed as a difference operator using a backward difference scheme. By dividing the interval from 0 to a on x axis into $(N-1)$ equidistant and small intervals of Δx , and the interval from 0 to t on the time axis into $(K-1)$ equidistant and small intervals of Δt , we can write the derivatives for any variable U at (k, n) point on the space-time grid (Figure 2).

¹ The derivation of the solution can be obtained from the authors.

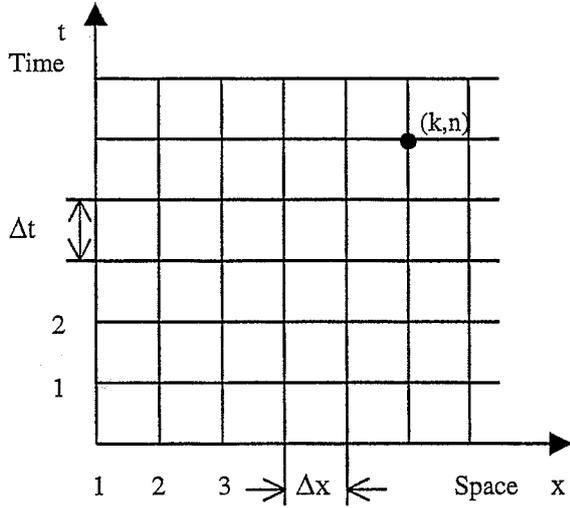


Figure 2 Space-time grid used in the computational scheme with respect to x .

The first derivative of a variable U can be written as

$$\left(\frac{\partial U}{\partial x}\right)_k^n = \frac{U_k^n - U_{k-1}^n}{\Delta x} \quad (21)$$

where U_k^n indicates the value of U at the grid point, (n,k) . The second derivative can be written as

$$\left(\frac{\partial^2 U}{\partial x^2}\right)_k^n = \frac{U_k^n - 2U_{k-1}^n + U_{k-2}^n}{\Delta x^2} \quad (22)$$

The operator A can be written as,

$$AU = -\left(\frac{\partial U}{\partial x} + \frac{h_x}{2} \frac{\partial^2 U}{\partial x^2}\right)$$

In the difference form

$$(AU)_k^n = -\left(\left(\frac{\partial U}{\partial x}\right)_k^n + \frac{h_x}{2} \left(\frac{\partial^2 U}{\partial x^2}\right)_k^n\right)$$

Substituting from (21) and (22) and taking $h_x = \Delta x$,

$$(AU)_k^n = -\left(\frac{1}{2\Delta x}\right)^* \left[3U_k^n - 4U_{k-1}^n + U_{k-2}^n\right] \quad (23)$$

The first derivative of U with respect to time can be expressed using a forward difference scheme.

$$\frac{\partial U}{\partial t} = \frac{U_k^{n+1} - U_k^n}{\Delta t} \quad (24)$$

Applying (23) and (24) to (13) and for the case of the mean velocity being constant (v),

$$C_k^{n+1} = C_k^n - \left(\frac{\Delta t \cdot v}{2\Delta x}\right)^* \left[3C_k^n - 4C_{k-1}^n + C_{k-2}^n\right] - \left(\frac{1}{2\Delta x}\right)^* \left[C_k^n \beta_k^n - 4C_{k-1}^n \beta_{k-1}^n + C_{k-2}^n \beta_{k-2}^n\right] \quad (25)$$

The difference equation (25) gives the future value of a stochastic variable in terms of past values. In addition this possesses the properties of Ito definition of integration with respect to time.

4. AN EXAMPLE

We have solved (19) with $a = 1.0\text{m}$ correlation length, $b = 0.05\text{m}$ ($c = 20$) and obtained 11 roots: $\omega_1 = 2.85774$; $\omega_2 = 5.72555$; $\omega_3 = 8.6116$; $\omega_4 = 11.2511$; $\omega_5 = 14.4562$; $\omega_6 = 17.4166$; $\omega_7 = 23.4054$; $\omega_8 = 26.4284$; $\omega_9 = 29.4669$; $\omega_{10} = 32.5187$ and $\omega_{11} = 35.5871$.

With these roots we have constructed the basis functions using (20). With $\sigma^2 = 1.0$ we have calculated the eigen values λ_n to construct the increments of Wiener processes in the Hilbert spaces using (15). The standard Wiener process increments were generated for $\Delta t = 0.0001$ days for a total time of 1 day (see Kloeden and Platan (1991)). The value of 50.0 m/day was used for the hydraulic conductivity and piezometric head

gradient of 0.020 m/m was used to obtain the mean velocity of 4.0 m/day for a porous medium having porosity of 0.25. A realisation of the solution is given in Figure 3.

The statistical nature of the computational solution changes as σ^2 and b changes. This allows us to model hydrodynamic dispersion without the need for a scale dependent diffusion coefficient. The characterisation of σ^2 and b still needs to be investigated for different porous media, and much work is still remaining to be done.

5. SUMMARY AND CONDITIONS

We have developed a model for solute transport in saturated porous media without using the dispersion coefficient and Fikian assumption that leads to the coefficient. We have considered the variables involved (concentration, velocity, and flux) as stochastic variables and developed a numerical scheme to solve the stochastic

differential equation formulated in space and time. We have shown that it is possible to formulate a model which closely reflects the natural phenomenon that occurs when a solute disperses in a saturated porous medium.

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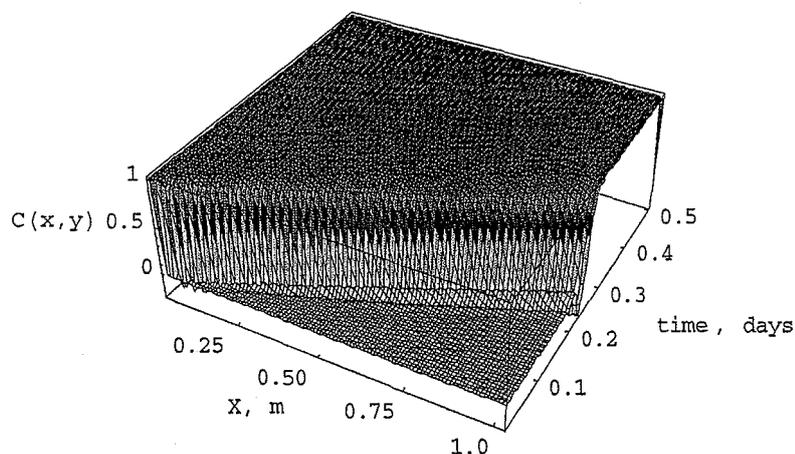


Figure 3 A realisation of the solution of (13).