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

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Abstract 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 Hibert 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 Karhunnen-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 it describes 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 dispersion coefficient (Fetter, 1999). The hydrodynamic dispersion 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), φ is the porosity of the material 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).
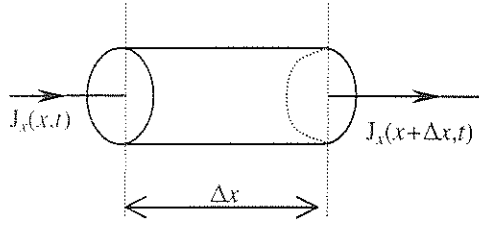
Figure 1 An infinitesimal cylindrical object within the porous medium having the solute concentration of C(x,t)

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

$$\Delta C(x,t)\,\varphi A\,\Delta x = \left(J_x(x,t) - J_x(x+\Delta x,t)\right)\varphi A\,\Delta t$$

$$\left(\frac{\Delta C}{\Delta t}\right)_{x,t} = \frac{\left(J_x(x,t) - J_x(x+\Delta x,t)\right)}{\Delta x} \qquad (1)$$

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,

$$J_{x+\Delta x} - J_x = \frac{1}{1!}\frac{\partial J_x}{\partial x}\Delta x + \frac{1}{2!}\frac{\partial^2 J_x}{\partial x^2}(\Delta x)^2 +$$

$$\frac{1}{3!}\frac{\partial^3 J_x}{\partial x^3}(\Delta x)^3 + R(\varepsilon)$$

where R(ε) 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

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

where,

$$R_r(x,t) = -\frac{1}{6}\frac{\partial^3 J_x}{\partial x^3}(dx)^2 -$$

$$\frac{1}{24}\frac{\partial^4 J_x}{\partial x^4}(dx)^3 -$$

Substituting $dx = h_x$

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

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

$$dC = -\left(\frac{\partial J_x}{\partial x} + \frac{h_x}{2}\frac{\partial^2 J_x}{\partial x^2}\right)dt + R_r(x,t)\,dt$$

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

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

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

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

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.

$$V(x,t) = \overline{V}(x,t) + \xi(x,t) \qquad (6)$$

where:

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

$K(x) =$ 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

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

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

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

Substituting (6) into (5),

$$J(x,t) = \left(\overline{V}(x,t) + \xi(x,t)\right)C(x,t) \qquad (9)$$

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

Substituting (10) into (5),

$$dC = -\frac{\partial}{\partial x}\left[\overline{V}(x,t)\,C(x,t) + C(x,t)\,\xi(x,t)\right]$$
$$-\frac{h_x}{2}\frac{\partial^2}{\partial x^2}\left[\overline{V}(x,t)\,C(x,t) + C(x,t)\,\xi(x,t)\right]$$
$$= -\left(\frac{\partial}{\partial x} + \frac{h_x}{2}\frac{\partial^2}{\partial x^2}\right)* \qquad (11)$$
$$\left[\overline{V}(x,t)\,C(x,t) + C(x,t)\,\xi(x,t)\right]$$

Let us define the operator in space,

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

Then:

$$dC = S\left(\overline{V}(x,t)\,C(x,t) + C(x,t)\,\xi(x,t)\right)dt$$

$$dC = S\left(\overline{V}(x,t)\,C(x,t)\right)dt +$$
$$S\left(C(x,t)\left(\xi(x,t)\,dt\right)\right) \qquad (12)$$

(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:

$$dC = S\left(\overline{V}(x,t)\,C(x,t)\right)dt + S\left(C(x,t)\,d\beta(t)\right) \qquad (13)$$

$$C(x,t) = \int_o^t S\left(\overline{V}(x,t)\,C(x,t)\right)dt +$$
$$\int_o^t S\left(C(x,t)\,d\beta(t)\right) \qquad (14)$$

where S is the differential operator given above.

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

$$d\beta_m(t) = \sum_{j=1}^{m} f_j\sqrt{\lambda_j}\,db_j(t) \qquad (15)$$

where m is the number of terms used, $db_j(t)$ is the increments of standard Wiener processes, f_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 Karhunnen-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:

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

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 (f_n) and eigen values (λ_n) of $q(x_1, x_2)$ are obtained as the solution to the following integral equation:

$$\int_0^a q(x_1, x_2) f_n(x_2) \, dx_2 = \lambda_n f_n(x_1) \tag{17}$$

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

$$\lambda_n = \frac{2\theta\sigma^2}{\omega_n^2 + \theta^2} \tag{18}$$

where $\theta = \frac{1}{b}$ and ω_n's are roots of the following equation[1]

$$\tan \omega_n a = \frac{2\omega_n \theta}{\omega_n^2 - \theta^2} \tag{19}$$

$$f_n(x) = \frac{1}{\sqrt{N}} \left(\sin \omega_n x + \frac{\omega_n}{\theta} \cos \omega_n x \right) \tag{20}$$

where:

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

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 ($\underline{N}$-1) equidistant and small intervals of Δx, and the interval from 0 to t on the time axis into ($\underline{K}$-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)
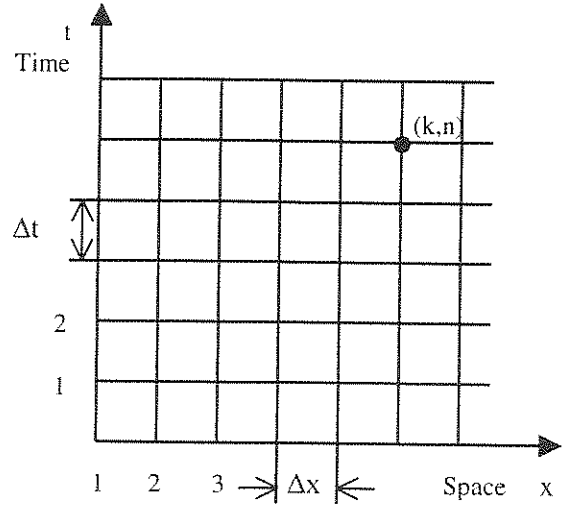

Figure 2 Space-time grid used in the computational scheme with respect to x.

The first derivative of a variable U can be written as

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

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

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

The operator S can be written as,

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

In the difference form

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

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

$$(SU)_k^n = -\left(\frac{1}{2\Delta x} \right) *$$

$$\left[3U_k^n - 4U_{k-1}^n + U_{k-2}^n \right] \tag{23}$$

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

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

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

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

$$C_k^{n+1} = C_k^n -$$

$$\left(\frac{\Delta t.v}{2\Delta x}\right)*$$

$$\left[3C_k^n - 4C_{k-1}^n + C_{k-2}^n\right] - \qquad (25)$$

$$\left(\frac{1}{2\Delta x}\right)*$$

$$\left[C_k^n \beta_k^n - 4C_{k-1}^n \beta_{k-1}^n + C_{k-2}^n \beta_{k-2}^n\right]$$

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 $a = 1.0$m correlation length, b = 0.05m (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 Platen (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.
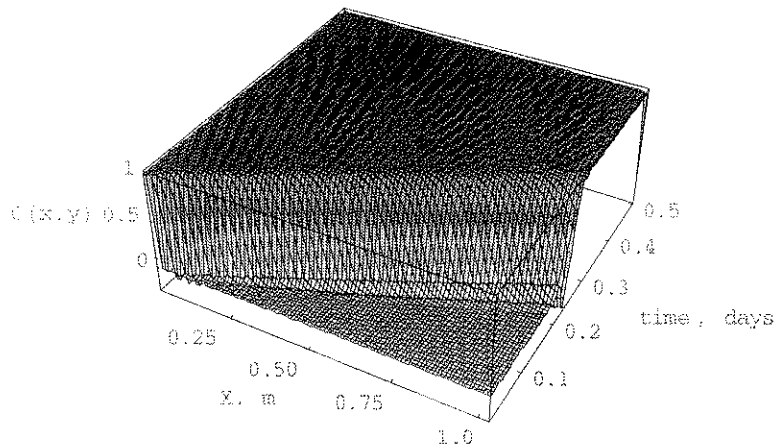

Figure 3 A realisation of the solution of (13)

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 CONCLUSIONS

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.

6. REFERENCES

Fetter, C.W., Contaminant hydrogeology, Second Edition, Prentice Hall, 1999.

Ghanem, R.G., and P.D. Spanos, Stochastic finite elements: a spectral approach, Springer-Verlag, 1991.

Kloeden, P.E. and E Platen, Numerical solution of stochastic differential equations, Springer-Verlag, 1991.

Unny, T. E., Stochastic partial differential equations in groundwater hydrology. Part 1: *Theory, Stochastic Hydrology and Hydraulics*, 3, 135-153.

Modelling Deep Drainage Under Different Land Use Systems. 1. Verification and Systems Comparison

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Abstract Drainage beyond the root zone contributes to water table rise and salinity in some parts of the Liverpool Plains catchment in northern NSW. The effect of land use on deep drainage was investigated by comparing the traditional long fallow system with more intense 'opportunity cropping'. Long fallowing (two crops in three years) is used to store rainfall in the soil profile but risks substantial deep drainage. Opportunity cropping seeks to lessen this risk by sowing whenever there is sufficient soil moisture. Elements of the water balance and productivity were measured under various farming systems in a field experiment in the southern part of the Liverpool Plains. The APSIM (Agricultural Production Systems Simulator) model was parameterised for the site using soil and water data (soil moisture, runoff, climate), and crop data (phenology, biomass, leaf area). Model performance was tested against four years of measured data on the site. Good agreement between model predictions and measurements indicated that the model captures the main hydrological and biological processes. The verified model was used in long-term (41 years) simulations to predict deep drainage under different systems and extrapolate experimental results. The results showed large differences between agricultural systems mostly because differences in evapotranspiration caused different profile moisture at the time of rain. Opportunity cropping resulted in greater water use, significantly reduced deep drainage and increased production compared to long fallowing. Modelling also indicated that continuous sorghum might be a better alternative for reducing deep drainage, than continuous wheat.

1. INTRODUCTION

Dryland salinity caused by shallow water tables is a major concern in the Liverpool Plains catchment in northern NSW, one of the most fertile agricultural areas in Australia. The catchment has a total area of 1.2 million ha which is predominantly under agricultural production. Large areas of the alluvial plains within the catchment are at risk of production loss due to high water tables and salinity [Broughton, 1994]. Deep drainage, which is the amount of water draining below the root zone, can potentially become recharge and contribute to rising water tables and salinity. The effect of farm scale management strategies on long-term deep drainage was investigated using both field experimentation and modelling. The APSIM (Agricultural Production Systems Simulator) model was parameterised with data measured on the experimental site. This paper describes model verification using measured and simulated results. The verified model was used in long-term simulations to extrapolate the results of the water balance and productivity in time to examine the capacity of alternative cropping systems to reduce deep drainage. It builds on previous studies [eg. Keating et al., 1995] by using more extensively tested and more accurately parameterised modelling tools. A second paper in these proceedings [Ringrose-Voase et al., 1999] describes how the model can be applied over the whole catchment taking into account soil and climate variability.

2. METHODS

2.1. Site Description

The experimental site was established in the foothills of the Liverpool Ranges on the 'Hudson' property in 1993 and is typical of the highly productive farming country in the catchment. The average annual rainfall is 678 mm, with most falling during summer. Average annual potential evapotranspiration is 1718 mm. The site is representative of areas previously identified as being significant contributors to groundwater recharge. The site is situated across two contour bays on a slope of approximately 2%. The soil is a Self-mulching Black Vertosol [Isbell, 1996], with a clay content of about 75% of which 90% is smectite. This gives the soil marked shrink/swell potential (linear shrinkage coefficient of 0.21) and a self-mulching surface. The available moisture holding capacity of the soil is large (505 mm to 3 m depth). Groundwater occurs 15 m below the surface above basalt bedrock.

The experiments were designed to compare water balance and production of cropping systems with varying lengths of fallow and perennial pastures. Only the cropping systems results are discussed here. The 'long fallow' system of one wheat and one sorghum crop in three years (see Table 1) is