Development of a Stochastic Solute Transport Model

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Development of a Stochastic Solute Transport Model

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1.0 The purpose of the report

The purpose of this document is to summarise the research conducted to date according to the subcontract to FRST bid 95-LVL-517-4317 (Objective 2). It was agreed to conduct research in stochastic modelling of contaminant transport in aquifers with the specific objective of developing a model for the aquifers which are being built by Lincoln Ventures Ltd. Prior to and during the term of this contract, a study of mathematical theories and applications of stochastic differential calculus was undertaken in order to formulate numerical models which characterise the flow in heterogeneous porous media. A preliminary model was developed using Mathematica® and computational experiments are being carried out to make further improvements to the model.

2.0 Flow in porous media

Flow in porous media has been a subject of active research for the last four to five decades. Wiest et. al. (1969) reviewed mathematical developments used to characterise the flow within porous media prior to 1969. He and his co-authors concentrated on natural formations found in the soil in which matrix and aquifers. Study of fluid and heat flow within porous media is also of significant importance in many other fields of science and engineering, such as drying of biological materials and biomedical studies. But in these situations we can study the micro-structure of the material and understand the transfer processes in relation to the micro-structure even though modelling such transfer processes could be mathematically difficult. Simpler mathematical models can be used to understand and predict behaviour of transport phenomena in such situations and in many cases direct monitoring of the system variables such as pressure, temperature and fluid flow is feasible. So the problem of prediction can be simplified with the assistance of the detailed knowledge of the system and real-time data. However, the nature of porous formation in underground aquifers is unknown and monitoring the flow is prohibitively expensive. This forces scientists and engineers to rely heavily on mathematical and statistical methods in conjunction with computer experiments of models to understand and predict, for example, the behaviour of contaminants in aquifers. In this report, we confine our discussion to porous media saturated with water, which is the case in real aquifers.

Past experience shows that a tracer, which is a labeled portion of water which may be identified by its colour, electrical conductivity or any other distinct feature, introduced into a saturated flow in a porous medium gradually spreads into areas beyond the region it is expected to occupy according to the Darcy's law. As early as 1905 Stlicher studied the behaviour of a tracer injected into a groundwater movement upstream of an observation well and observed that the tracer, in a uniform flow field, advanced gradually in a pear-like form which grew longer and wider with time. Even in a uniform flow field given by Darcy's law, an unexpectedly large distribution of tracer concentration showed the influence of the medium on the flow of the tracer. This distribution of tracer particles is termed hydrodynamic dispersion, and Bear (1969) described this phenomenon in detail.

Hydrodynamic dispersion is the macroscopic outcome of a large number of particles moving through the pores within the medium. If we consider the movement of a single tracer particle in a saturated porous medium under a constant piezometric head gradient in the x direction, we can understand the phenomenon clearly (Figure 1). In the absence of a porous
medium, the particle will travel in the direction of the decreasing pressure (x direction) without turbulence but with negligibly small Brownian transverse movements. (Average velocity is assumed low and hence, the flow field is laminar.) Once the tube in Figure 1 is randomly packed with, for example, solid spheres with uniform diameter, the tracer particle is forced to move within the void space, colliding with solid spheres and traveling within the velocity boundary layers of the spheres.

Figure 1. A possible traveling path of a tracer particle in a randomly packed bed of solid spheres.

As shown in Figure 1, a tracer particle travels in the general direction of x but exhibits local transverse movements, the magnitude and direction of which depend on a multitude of localised factors such as void volume, solid particle diameter and local fluid velocities. It can be expected that the time taken for a tracer particle to travel from one end of the bed to the other is greater than that taken if the solid particles are not present. If a conglomeration of tracer particles are introduced, one can expect to see longitudinal and transverse dispersion of concentration of particles with time. Bear (1969) attributed hydrodynamic dispersion in natural formations to (a) external forces acting on the liquid; (b) variation of the microscopic geometry of the pore structure; (c) molecular diffusion caused by tracer concentration gradients; (d) variations of liquid properties such as density and viscosity which affect the flow patterns; (e) changes in concentration of the tracer due to chemical and physical processes; and (f) interaction between the liquid and the solid phases. In essence, hydrodynamic dispersion is the continuous subdivision of tracer mass into finer ‘offshoots’ due to the microstructure of the medium when carried by the liquid flowing within the medium. Because the velocities involved are low, one can expect molecular diffusion\(^1\) to have a significant impact on the concentration distribution of the tracer. If the effects of chemical reactions within the porous medium can be neglected, convection of tracer particles due to local random velocity fields and molecular diffusion due to concentration gradients are the primary mechanisms which drive the hydrodynamic dispersion.

2.1 Models of hydrodynamic dispersion

Since Navier-Stokes equations for flow in porous media are impossible to apply to explain hydrodynamic dispersion mainly due to the complex geometry of pore structure, different approaches to model the dispersion have been described in literature (e.g. Taylor, 1953; Daniel, 1952; Bear and Todd, 1960; Chandrasekhar, 1943). These approaches can broadly be classified into two categories: deterministic and statistical. In the deterministic models the porous medium is modelled as a single capillary tube (Taylor, 1953), a bundle of capillary

---

\(^1\) The molecular diffusion (microdiffusion) is the transport phenomenon observed when a substance, A, with high concentration is surrounded by another non-moving substance, B. The concentration of A is observed to increase in B with time and described by the Fick’s law (Crank, 1990).
tubes (Daniel, 1952), and an array of cells and associated connecting channels (Bear and Todd, 1960). These models were mainly used to explain and quantify the longitudinal dispersion in terms of travel time of particles and were confined to simple analytical solutions (Bear, 1969). They have been applied to explain the data from laboratory scale soil column experiments in soil science. Statistical models, on the other hand, use statistical theory extensively to derive ensemble averages and variances of spatial dispersion and travel time of tracer particles. It is important to note that these models invoke an ergodic hypothesis of interchanging time averages with ensemble averages after sufficiently long time, and the law of large numbers. By the law of large numbers, after a sufficiently long time, the time averaged parameters such as velocity and displacement of a tracer particle may replace the averages taken over the assembly of many particles moving under the same flow conditions. Bear (1969) questioned the validity of this assumption arguing that it was impossible for a tracer particle to reach any point in the flow domain without taking the molecular diffusion into account.

In statistical models, the problem of a cloud of tracer particles traveling in a porous medium is reduced to a problem of a typical single particle moving within an ensemble of random porous media. Characteristic features of these models are: (a) assumed probability distributions for the properties of the ensemble; assumptions on the microdynamics of the flow, such as the relationships between the forces, the liquid properties and velocities during each small time step; laminar flow; and assumed probability distributions for events during small time step within the chosen ensemble. The last assumption usually requires correlation functions between velocities at different points or different times, or joint probability distributions of the local velocity components of the particle as functions of time and space, or a probability of an elementary particle displacement (Bear, 1969).

Another modelling approach that has been used widely is to consider the given porous medium as a continuum and apply mass and momentum balance over a representative elementary volume (REV) (Bear et al., 1992). Once the assumption is made that the properties of the porous medium, such as porosity defined as the ratio of the void volume to the volume of the REV, can be represented by average values over the REV, then the mass and momentum balances can be applied to a REV to derive the governing partial differential equations which describe the flow in the medium. Since the concept of the REV is central to this development, it is important to summarise a working model based on this approach.

2.2 Modelling macroscopic behaviour

2.2.1 Representative elementary volume

Bear et al. (1992) showed that representative values of the properties of a porous medium such as porosity can be obtained by averaging those values over a sufficiently large volume within the medium. The size of the representative elementary volume (REV) is such that it is the basis of statistically valid averages of properties that are insensitive to small variations in the size of the volume. The variation of porosity with the size of REV is illustrated in Figure 2 (Bear et al., 1992).
Porosity is defined as the ratio between the void volume and the volume occupied by the solid particles within the REV. The fluctuation in porosity values in region A shows that the REV is not sufficiently large to neglect the microscopic variations in porosity. If the porous medium is homogeneous, porosity is invariant within the region B which can be considered as the operational region of REV for mass and momentum balance equations. Porosity fluctuations still exist for a heterogeneous porous medium and are independent of the size of REV (Region C). Once the size of REV in the region B is established for a given porous medium, macroscopic models can be developed for the transport of tracer (solute). However, variables, such as velocity and concentration, are defined to have volume-averaged components and small perturbations, and these small perturbations play a significant role in model formulations (Gray, 1975; Gray et al., 1993; Hassanizadeh and Gray, 1979; Whitaker, 1967).

2.2.2 Review of a macroscopic continuum transport model

Consider a cylindrical column of internal radius $R$ with the Cartesian coordinate system as shown in Figure 3. The column is filled with a solid granular material and it is assumed that the typical grain diameter $l_d \ll R$. Assuming that the porous matrix is saturated with a liquid of density $\rho$, the local flow velocity of the liquid with respect to the stationary porous structure and the local concentration of a neutral solute in the fluid are denoted by $v(x,y,z,t)$ and $c(x,y,z,t)$, respectively. The averaging volume ($\delta V$) for this system is a cross sectional volume of the column of some width, $\Delta z$. It is assumed that $\delta V$ is sufficiently large to form statistically valid averages that are insensitive to small variations in $\delta V$. (The notation for the model is adopted from Rashidi et al. (1996).)
Figure 3. Configuration for the model

The volume average of a pore scale quantity, $\psi$, associated with the liquid phase is defined by

$$\langle \psi \rangle(z, t) = \frac{1}{\delta A} \int_{-\Delta \zeta/2}^{\Delta \zeta/2} \int \psi(x, y, z + \zeta, t) \gamma(x, y, z + \zeta) d\zeta$$

where $\delta A$ represents the cross-sectional area of the column and $\gamma$ is an indicator function which equals to 1 if the point $(x, y, z + \zeta)$ lies in the void space and zero otherwise. The cross sectional porosity, $\phi(z)$ is obtained by setting $\psi=1$ in equation (1). The volume of the fluid momentum is given by

$$\langle \rho v \rangle = \rho q = \rho k,$$

where $k$ is a unit vector along the z-axis and $q$ is the specific volumetric flux. The total volumetric flux through the cross section is given by

$$Q = q_z (\pi R^2),$$

and the mean velocity can be defined by,

$$\bar{v} = q_z k / \phi.$$

The following one-dimensional macroscopic mass balance for the solute can be derived using averaging theorems (Thompson et al., 1986):

$$\frac{\partial (\phi c)}{\partial t} + \frac{A}{\partial z} + \frac{B}{\partial z} \frac{\partial (\phi J_z)}{\partial z} - \frac{\partial}{\partial z} \left( \phi D_m \left( \frac{\partial c}{\partial z} + \tau_z \right) \right) = 0$$

[5]
The rate of change of the intrinsic volume average concentration \( \langle \bar{c} \rangle \) is balanced by the spatial gradients of the terms, A, B, and C respectively. The term A represents the average volumetric flux of the solute transported by the fluid in the z-direction at a given point in the porous matrix, \((x,y,z)\). But the total solute flux at a given point is the sum of the average flux and the fluctuating component due to the velocity fluctuation above the mean velocity, \(\bar{v}_z\). The fluctuating component of the flux is expressed in terms of perturbation terms of velocity \(\langle v'_z \rangle\) and concentration \(\langle c' \rangle\), each of which represents the difference between the microscopic quantity evaluated at \(x,y,z+\zeta\) within a REV and the corresponding intrinsic average evaluated at \(z\):\[
J_z(z,t) = \bar{v}_z c'. \tag{6}
\]

The terms A and B are called the mean advective flux and the mean dispersive flux, respectively, and the latter is often expressed in terms of the spatial gradient of the mean concentration:
\[
J_z(z,t) = -\alpha_t \bar{v}_z \frac{\partial \bar{c}}{\partial z} \tag{7}
\]

where \(\alpha_t\) is defined as the dispersivity which depends on a typical particle diameter. The product \(D = \alpha_t \bar{v}_z\) is called the standard dispersion coefficient.

The term C in Equation 5 is the modified Fick’s law for microdiffusion of solute to accommodate the increased diffusion when a high degree of tortuous paths are present within the porous media. The term C is called the diffusive tortuosity and it is approximated by,
\[
\tau_z(z,t) = -B \frac{\partial \bar{c}}{\partial z}, \tag{8}
\]

where \(B\) is a material coefficient ranging from 0 to 1. Again the diffusive tortuosity is expressed in terms of concentration gradient as in the Fick's law for microdiffusion. The traditional working model for solute transport in porous media can be obtained by combining Equations 5, 7 and 8.

\[
\frac{\partial}{\partial t} (\phi \bar{c}) + \frac{\partial}{\partial z} (\phi \bar{v}_z \bar{c}) - \frac{\partial}{\partial z} \left( (\phi D + \phi D_m (1 - B)) \frac{\partial \bar{c}}{\partial z} \right) = 0 \tag{9}
\]

The sum \(D_H = D + D_m(1-B)\) is called the coefficient of hydrodynamic dispersion. In many cases, \(D >> D_m\) such that \(D_H \approx D\) (Rashidi et al., 1996).

The following observations can be made from the above discussion:

1. The division of solute flux into advective and dispersive components is a result of the mathematical division of velocity and concentration into mean and perturbation terms.

2. The coefficient of dispersion depends upon the velocity fluctuations induced by the pore structure; therefore, it can be expected to be scale dependent.

3. A Fickian type assumption is made for diffusive tortuosity and this assumption has not been justified as in the case of microdiffusion.
4. There are only two physical phenomena involved in the solute transport in a porous medium: the solute is carried by the flowing fluid (convection) and, if the velocities are very small, microdiffusion can occur as described by the Fick’s law.

5. The working model described above can only be applied to homogeneous porous media where a representative elementary volume can be defined.

Rashidi et al. (1996) experimentally investigated the solute transport in a bed of packed polymethylmethacryle (PMMA) plastic spherical beads of 0.31 cm diameter contained in a cylindrical column having 4.5 cm diameter. They have used the Fluorescene imaging technique to measure and compute the velocity and concentration fields, and other associated parameters such as dispersion coefficient and dispersivity. Their results are reproduced in Table 1.

Table 1. Summary of measured or estimated dispersivities and dispersion coefficients (Rashidi et al., 1996)

<table>
<thead>
<tr>
<th>Method</th>
<th>Dispersivity $\alpha_L$ (cm)</th>
<th>Dispersion Coefficient $D$ (cm$^2$/min)</th>
<th>Assumptions and comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct experiment</td>
<td>0.12</td>
<td>0.018</td>
<td>Rashidi et al. (1996); Constant velocity experiments to get $\alpha_L$; $D$ found directly.</td>
</tr>
<tr>
<td>Length-scale arguments</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha_L=0.5 \ell_d$</td>
<td>0.15</td>
<td>0.023</td>
<td>$Pe = \frac{\bar{v} \ell_d}{D_m} = 75$</td>
</tr>
<tr>
<td>$\alpha_L=1.8 \ell_d$</td>
<td>0.54</td>
<td>0.081</td>
<td>Bear (1972) pp 609</td>
</tr>
<tr>
<td>$\alpha_L= \ell_d$</td>
<td>0.30</td>
<td>0.045</td>
<td></td>
</tr>
<tr>
<td>Breakthrough slope</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>methods</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Numerical curve fits:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Square IC</td>
<td>0.20</td>
<td>0.030</td>
<td>Constant velocity; constant porosity; square Initial Conditions (IC); averages over 28 locations</td>
</tr>
<tr>
<td>Slope IC</td>
<td>0.12</td>
<td>0.018</td>
<td>Constant velocity; porosity</td>
</tr>
</tbody>
</table>

Values of dispersivity and dispersion coefficient obtained from different approaches for the same porous medium vary considerably as shown in Table 1. Assuming that the values reported by the direct method are ‘correct’ values, which is a reasonable assumption given the advanced laser beam measurement techniques employed in the method (Rashidi et al., 1996),
the length scale argument that the dispersivity can be approximated by the half of the typical particle diameter, and the numerical curve fitting technique with slope IC gave the most accurate values for the dispersivity and the dispersion coefficient. It is interesting to note that the dispersivity, which is the volumetric flux per unit average concentration gradient and per unit average velocity (Equation 7), is better related to the half of the typical particle size. Higher the typical diameter, higher the dispersivity, hence higher the dispersion coefficient. A high dispersion coefficient is a result of a relatively high velocity perturbations, i.e. increased randomness in the velocity field. The random component in velocity field plays a significant role in determining the concentration field even in a homogeneous porous medium tested under laboratory conditions.

3.0 Flow in aquifers

3.1 Transport in heterogeneous natural formations

Field experiments show that spatial heterogeneity is the most significant factor effecting dispersion of solute in natural formations such as aquifers (Anderson, 1979; Gelhar et al., 1985; Freyberg, 1986). Dagan (1988) referred to the experimental results depicting large scale spatial distribution of hydraulic conductivity at the Borden site. Large scale irregular variations in hydraulic properties, such as hydraulic conductivity and porosity, lead to high degree of uncertainty of parameters in transport equations based on the continuum approach, whose application to solute transport in natural formations is questionable (Dagan, 1988). Dagan (1988) concluded that the concentration of a solute can be considered as a random variable, which can be described by its statistical moments; ergodic hypothesis can not be applied except in a limited sense in describing some gross features such as the motion of the centre of gravity and the second order spatial moment of the solute body; it is extremely difficult to predict accurately the point value of concentration in an irregularly distributed body of solute within the natural formations; the expected value of concentration does not necessarily satisfy a convection-dispersion type equation, such as Equation 9, based on the continuum approach; and even if the latter is satisfied, the dispersion coefficient increases with the travel time reaching an asymptotic value. In other words, the flow is non-Fickian during the preasymptotic period.

Dagan (1988, 1990) developed a mathematical formulation to predict the spatial moments of concentration plumes in aquifers introducing perturbation terms to describe random variations of variables such as concentration and velocity. It is usually assumed that a solute is transported by convection described by the Darcian steady velocity and by pore scale diffusion. The governing equation is a modified form of Equation 9 and is given by,

$$\frac{\partial C}{\partial t} + V_j \frac{\partial C}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_{d,jl} \frac{\partial C}{\partial x_l} \right)_{j,l = 1,2,3}$$

[10]

where \( x(x_1,x_2,x_3) \) is the coordinate vector; \( V=(K/\phi)V\phi \) is the Eulerian velocity according to the Darcy's law; \( K \) is the hydraulic conductivity; \( \phi \) is the effective porosity; \( \phi \) is the piezometric head; and \( D_{d,jl} \) is a diffusion tensor representing the effect of pore scale dispersion (Dagan, 1988). Here the summation convection for repeated indices is used.

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2 When the flow can be described by a convection-dispersion type equation, the transport is said to be Fickian.
Dispersive flux due to velocity variations is lumped into the right hand term in Equation ?? through a pore scale diffusion tensor and the mean velocity given by the Darcy’s law is used in the convection term whereas Equation 9 models a dispersive flux due to velocity fluctuations and microdiffusion is modelled by the Fick’s law. Dagan (1988) assumed constant components for the pore scale dispersive tensor, $D_{d,j}$, and the expected values of the spatial second moments of a solute plume within a stationary heterogeneous porous structure were derived by starting with introducing perturbation terms to velocity and concentration and after a non-trivial mathematical analysis.

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 spatial distribution of hydraulic conductivity in many studies Serrano (1988). However, Serrano (1988) has cited other researchers' work which mentioned the inconsistencies of the approaches to solve the transport equation in their review article. They have concluded that the advective-convective model neither explained the scale effect of the dispersion process nor elucidated the transient behaviour of solute concentration. In addition, Serrano (1988) summarised the main difficulties with the existing solutions:

1. The assumption that the perturbations are small random variations in the perturbation expansion solutions (Gelhar and Axness, 1983; Dagan, 1984) is not valid in a differential equation unless the variables have small variance. 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).

2. The assumption that hydraulic conductivity is the only source of uncertainty in many existing solutions has to be challenged. Dispersion in natural formations can not only be explained by the variability of hydraulic conductivity; and if this is feasible the large-scale hydraulic conductivity can safely be described by well defined deterministic functions.

3. Some of the solutions are valid in the steady state of the concentration field.

4. The assumed ergodicity in the hydraulic conductivity field in some solutions does not necessarily imply that the concentration field is ergodic.

The above discussion leads to a hypothesis that mathematically sound and realistic modelling of the transport phenomenon in natural formations can be accomplished when the variables and parameters involved in the processes are treated as stochastic variables each having its own probability distribution, and when they satisfy conservation laws, subsequent differential equations have to be solved by using theories of stochastic differential calculus and numerical methods. A comprehensive review of stochastic differential equations and related mathematical development is given by Kloeden and Platen (1994), and their definitions, which are mathematically precise, and notation are extensively used in this report.
3.2 Stochastic velocity in natural formations

Since the velocity of a solute particle is central to formulating a model of transport processes, it is important to develop a stochastic model to describe the motion of a particle in a porous medium. Assuming the velocity and fluxes associated with the flow are stochastic processes\(^3\), the velocity can be described in 2-dimensional Cartesian coordinates by the average Darcian velocity and a random component accounting for uncertainty due to pore structure:

\[
V(x,t) = -\frac{K(x)}{\phi(x)} \nabla \phi(x,t) + W(x,t) \tag{11}
\]

Here \(K\) is hydraulic conductivity, \(\phi\) is porosity, \(\phi\) 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 \(\delta\)-correlated in time. This assumption has some practical significance and provides a method to obtain stochastic differential equations having separable time and space related differential equations (Unny, 1989). \(W(x,t)\) is assumed to be a Weiner process (in some literature it is called a Brownian process) in time and in space.

3.2.1 Wiener process in time and in space

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

1. \(W(0)=0,\)
2. the random variables \(W(t_1), W(t_2), \ldots, W(t_n)\) are n-dimensional Gaussian processes whose parameters are

\[
E[W(t_i)] = 0, \quad E[W(t_i) W(t_j)] = \min(t_i, t_j). \tag{12}
\]

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

\[
E[W(t)] = 0 \quad \text{and} \quad E[W(t_i) W(t_j)] = \int_0^{\min(t_i, t_j)} q(\tau) d\tau, \quad q > 0. \tag{13}
\]

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

\[
E[W(x,t)] = 0 \quad \text{and} \quad E[W(x_i, t_i) W(x_j, t_j)] = \int_0^{\min(x_i, x_j)} \int_0^{\min(t_i, t_j)} q(\tau, \zeta) d\tau d\zeta. \tag{14}
\]

---

\(^3\)The time set under consideration is denoted by \(T\) in general and a common underlying probability space \((\Omega, \mathcal{A}, P)\) is assumed. A stochastic process \(x : T \times \Omega \to \mathbb{R}\) where \(X(t) = X(t, \omega)\) is a random variable for each \(t \in T\). For each outcome, \(\omega \in \Omega\), \(X(\cdot, \omega) : T \to \mathbb{R}\) is a realisation, a sample path or a trajectory of the stochastic process (Kloeden and Platen, 1994).
The general Wiener process, \( W(x,t) \in E^0 = L^2( \mathbb{R} ) \times [0, T] \), where \( E^0 \) is a separable Hilbert space\(^4\). Unny (1988) illustrated a procedure to replace the Wiener process increment in \( E^0 \), \( d\beta = W(x,t) \, dt \), using stochastic calculus in a Hilbert space (see also Sawaragi et al., 1978).

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

\[
    d\beta_m(t) = \sum_{j=1}^{m} e_j(d\beta(t), e_j)
\]

where the \( e_j \)'s form an orthonormal basis in the Hilbert space \( E^0 \), and can be taken as the eigenfunctions of the correlation operator \( Q \):

\[
    Qe = \omega e.
\]

Then the Wiener process increments can be written as

\[
    d\beta_m(t) = \sum_{j=1}^{m} e_j \sqrt{\omega_j} d\beta_j(t)
\]

where the \( d\beta_j \)'s are all increments of independent standard Wiener processes. The correlation operator \( Q \) has to be specified from field experiments or otherwise. Kumar et al. (1991) used a \( 4 \times 4 \) 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. In the 1-dimensional case, for example, the correlation operator is a \( 2 \times 2 \) 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 and is entirely time correlated through \( \min(t_i, t_j) \) which can be thought 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 \( 2 \times 2 \) matrix.

### 3.2.2 Movement of a solute particle in two dimensions

When Equation 11 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.

\[
    dx = -\frac{K(x)}{\varphi(x)} \nabla \nabla \psi(x, t) dt + W(x, t) dt
\]

The last term on the right hand side can be replaced by the Weiner process increment in Hilbert space, \( d\beta(t) \) for each direction; then we have ordinary stochastic differential equations

\(^4\) A Hilbert space is an inner product space which is a complete metric space with respect to the metric induced by its inner product, and a separable Hilbert space should contain a complete orthonormal sequence (Young, 1988).
for each of 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).

A program was written in Mathematica® to obtain numerical solutions for Equation 18, and several realisations are given in Figures 4, 5, 6 and 7 for $\phi=0.3$; $K=8.0$ m/day; $q_{ij}=0.001$ for each i and j; a linear piezometric gradient of 250 mm per 10 m; and for 2-dimensional space of 10m x 5 m. In each case, initial displacements are zero.

Figure 4a. A trajectory of a path of a solute particle.

Figure 4b. Same trajectory plotted against time.

Figure 5. Another simulated trajectory.
Figures 4 to 7 show different possible paths a particle can take in a porous medium having a constant porosity and a constant piezometric head gradient. 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 the correlation operator $Q$ and the time, $t$ (Equation 16). It has been observed that the spatial second moment of concentration of a solute body grows with a travel time, and a stochastic differential equation similar to Equation 18 can be used to model the dispersion in natural formations. In these particular examples, porosity and hydraulic conductivity are taken as constants, but they can either be deterministic functions reflecting their distributions of the spatial domain or be random functions if their changes are highly irregular or 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 (Kloeden and Platen, 1994).

When values of the correlation operator are increased to 0.01 for all $q_{ij}$'s, some of the resulting trajectories are given in Figures 8 to 9 to illustrate the effect of the random component in Equation 18.
Figure 8a. A simulated trajectory giving x-y displacements.

Figure 8b. Same trajectory as in Figure 8a plotted against time.

Figure 9. Another trajectory showing larger movement in y direction.

A ten-fold increase in the correlation operator produced sample paths with a large dispersion in the y direction, sometimes closer to 1 m. This suggests that the correlation operator can be used to model the dispersion in porous media, and a convection term based on stochastic velocity can be used to model the effects of both the advective and the dispersive terms in Equation 5.
4.0 A stochastic solute transport model

4.1 Governing equations

The development of a stochastic solute transport model based on stochastic variables is briefly described here. The following assumptions are made:

1. The solute has similar density and viscosity to those of water.

2. Representative values of effective porosity \( \phi(x,y) \) and hydraulic conductivity \( K(x,y) \) can be assigned to specific points in a 2-dimensional domain using either random or deterministic spatially distributed functions.

3. Piezometric head \( \phi(x,y) \) is given or can be calculated for a specific point.

4. The velocity at a given point is given by Equation 11.

For the sake of simplicity, consider a small cylindrical section having a cross-sectional area of \( A \) and length \( \delta x \) in the \( x \) direction. Solute flux\(^5\) at \( X=x \) is \( J_x \left( \frac{M}{L^2T} \right) \) and that at \( X=x+\delta x \) is \( J_{x+\delta x} \).

\[
\text{Figure 9. A small cylindrical element for mass balance}
\]

During a small time duration \( \delta t \),

solute mass entering the element = \( J_x (A\phi(x)) \delta t \), and

solute mass leaving the element = \( J_{x+\delta x} (A \phi(x+\delta x)) \delta t \) where \( J_{x+\delta x} = J_x + \frac{\partial J_x}{\partial x} \delta x \).

Change of solute mass within the element = \( J_x A \phi(x) \delta t - \left( J_x + \frac{\partial J_x}{\partial x} \delta x \right) A \phi(x + \delta x) \delta t \)

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

\[
= - J_x A \delta \phi \delta t - \frac{\partial J_x}{\partial x} A \phi \delta x \delta t - \frac{\partial J_x}{\partial x} A \delta \phi \delta x \delta t.
\]

\(^5\) Solute flux is defined as the mass flow rate of solute per unit void cross-sectional area perpendicular to the flow. Dimensions are given in M (mass), L (length) and T (time).
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 \( \delta x \). Then the change in solute mass within the element during \( \delta t \) can be written in terms of concentration.

\[
\text{Change in solute mass within the element} = \delta C \varphi A \delta x.
\]

Therefore,

\[
\delta C \varphi A \delta x = -J_x A \delta \varphi \delta t - \frac{\partial J_x}{\partial x} A \varphi \delta x \delta t - \frac{\partial J_x}{\delta x} A \delta \varphi \delta x \delta t
\]

Simplifying we obtain

\[
\varphi \frac{\partial C}{\partial t} = -J_x \frac{\partial \varphi}{\partial x} - \varphi \frac{\partial J_x}{\partial x}
\]

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

\[
\varphi \frac{\partial C}{\partial t} = -J_x \frac{\partial \varphi}{\partial x} - \varphi \frac{\partial J_x}{\partial x}
\]  \[19\]

Equation 19 can be simplified further if we can neglect the gradient of the effective porosity within certain regions. In those cases, Equation 19 reduces to,

\[
\frac{\partial C}{\partial t} = -\varphi \frac{\partial J_x}{\partial x}.
\]  \[20\]

Even though the porosity does not appear in Equation 20 it is intrinsically contained in the concentration term.

For two dimensions, Equation 19 becomes

\[
\varphi \frac{\partial C}{\partial t} = -J_x \frac{\partial \varphi}{\partial x} - J_y \frac{\partial \varphi}{\partial y} - \varphi \frac{\partial J_x}{\partial x} - \varphi \frac{\partial J_y}{\partial y}.
\]  \[21\]

It should be noted that the fluxes, concentration and porosity are stochastic variables.

### 4.2 Stochastic flux

It has been suggested previously that the dominant mode of solute transfer is convection, and if the velocities are low which is the case in aquifers, micro-diffusion plays a significant role giving highly "irregular" concentration contours, even after considerable smoothing (Dagan, 1990). The following model for the stochastic flux in heterogeneous porous media is proposed:

\[
J = VC - (D + W) \nabla C
\]  \[22\]
Here $\mathbf{V}$ is the stochastic velocity given by Equation 11, $C$ is the concentration, $\mathbf{D}$ is a diffusion coefficient matrix which gives typical values of the diffusion coefficients for microdiffusion$^6$ in the x and y directions and $\mathbf{W}$ models the random components of microdiffusion using a Wiener process in a Hilbert space. It should be noted that a Wiener process is contained in the velocity and correlation coefficients differ in both cases. Equation 22 gives the flexibility to investigate the effects of convection and microdiffusion separately. It is hypothesised that the stochastic flux has high level of randomness where concentration gradients are high.

5.0 Computer simulation

Equations 11, 19, 22 were used as governing equations to build a solute transport model which was solved numerically using a finite difference scheme for a 2-dimensional grid. Since all the equations are stochastic, Ito definition of a stochastic integral to integrate variables over time was used in the scheme (see Kloeden and Platen, 1994). The numerical scheme developed will be described in a subsequent report.

5.1 An example

The model is applied to a rectangular grid of 20 cm x 10 cm with a constant piezometric head gradient of -5.0 mm/cm. For the sake of simplicity the porosity and hydraulic conductivity are assumed to be 0.4 and 0.5556 cm/min respectively throughout the grid. The time step is taken to be 0.1 min and components of the correlation operator for velocity ($q_{ij}$'s) of 0.001 in both x and y directions were assumed; those for Wiener process for concentration are assumed to be 0.000001. The diffusion coefficient is assumed to be negligibly small and only the noise term represents the microdiffusion. A step concentration input of 10 was applied at the mid-point of the $X=0$ boundary throughout the simulation. The following figures show the status of different variables at different times.

![Figure 10. Plot of concentration after 0.1 min.](image)

$^6$ Some researchers use the term "pore scale" diffusion or dispersion to indicate the transport phenomenon which occurs when concentration gradients are present even in the absence of convection.
Figure 11. Stochastic fluxes and their contour plots in x direction (11 (a) and y direction (11 (b) after 0.1 min.

Figure 12. Stochastic velocities in x and y directions after 0.1 min.

Figure 13. Concentration distribution after 1 min.
Figure 14. Stochastic flux in x direction after 2 min.

Figure 15. Concentration distribution without peaks after 10 min.

Figure 16. Concentration distribution after 15 min.
The above figures show the spread of solute concentration in a small 2-dimensional domain subjected to a fairly high piezometric gradient. This gives a qualitative understanding of the behaviour of the model. The initial pear-like spread of concentration and the later irregular distribution of concentration confirms field observations. Irregularities increase with the introduction of a positive diffusion coefficient due to localised pore scale diffusion. Simulations of a larger domain (10m x 5 m) show similar behaviour of the model under a different time scale. Each run of the model give different realisations of concentration and other variables such as velocities and fluxes. Moments of those variables at different locations can be calculated from sufficiently large samples obtained from the model.

6.0 Future research directions

Further research and development will be conducted to build confidence in the model in predicting solute transport in heterogeneous porous media such as a confined aquifer. The following specific steps will be taken:

1. Convert the code to the C programming language in order to achieve significant improvements in computational efficiency.

2. Experiment with the model to determine regimes of correlation operator values for Fickian and non-Fickian solute transport.

3. Perform computational experiments to understand and investigate the relative role of concentration gradient-based diffusion in porous media.

4. Estimate of parameters such as correlation operators and diffusion coefficients using data from the heterogeneous and homogeneous confined aquifer being built at Lincoln University. Methodology would be similar to the maximum likelihood estimation method described by Unny (1989).

5. Extend the model to 3 dimensions and further validate the model.
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8.0 References


