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# Theory of diffusions applied to stochastic flow in porous media *

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**Abstract**

Contaminant transport by liquid flow in a porous medium is modeled by the addition of a stochastic term to Darcy's flow equation. The resulting stochastic differential equation is studied using results from the theory of diffusions as embodied in the Dynkin formula.

The resulting integral equation for the probability distribution of fluid elements is solved for the case of a spatially homogeneous medium without microdiffusion. This distribution is shown to also solve a deterministic transport equation containing an effective diffusion constant, analogous to the hydrodynamic dispersion equation. This relates the stochastic and deterministic approaches to the contaminant transport problem. The case of a non-homogeneous medium is discussed, leading to a tentative conclusion that the stochastic description will not reduce to a dispersion equation in general.

## 1 Introduction

The modelling of contaminant transport by the flow of water in natural aquifers is of considerable interest, e.g. for ecological studies and resource planning. To set up a mathematical model for this problem it is firstly necessary to understand the underlying flow of fluid through a porous medium, and secondly to superimpose on this a description of the transport process.

The overall flow rate can be obtained from Darcy's law (Fetter [6])

$$\mathbf{v}(\mathbf{x}) = -\frac{\kappa(\mathbf{x})}{\varphi(\mathbf{x})}\nabla\phi(\mathbf{x},t) \tag{1}$$

Here $\mathbf{v}(\mathbf{x})$ is the fluid velocity at position $\mathbf{x}$ and $\phi$ is the gravitational potential (i.e., hydraulic head). The material properties are the hydraulic conductivity $\kappa$ and

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the porosity $\varphi$, the latter being the fraction of the total volume occupied by voids that can be filled by fluid. In what follows it will be assumed for simplicity that the flow is 1-dimensional so that the position reduces to a scalar variable $x$, and that there is a constant piezometric gradient $h$, i.e. $\phi(x) = -hx$. Also, at first we assume that the medium is homogeneous so that $\kappa$ and $\phi$ are independent of $x$. These simplifications reduce Darcy's law to a constant velocity $v_0 = \kappa h/\varphi$.

Solute transport in a free flowing liquid can be described by deriving a continuity equation for the solute concentration $c(x,t)$ in the form

$$\partial c/\partial t \;=\; -\nabla(c\,\mathbf{v} - \mathbf{D_m}\cdot\nabla c) \tag{2}$$

The flux density in the brackets consists of (i) the convection term representing solute carried along by the fluid flow, and (ii) the diffusion term determined by a diffusion tensor $\mathbf{D_m}$ that in simple cases reduces to a scalar coefficient. This term is an expression of Fick's law and represents molecular scale or microdiffusion.

In a porous medium, microdiffusion e.g. in a stationary fluid is suppressed by the inreased path length of a diffusing particle as it travels around the grains of the medium, giving rise to an effective diffusion coefficient $D^*$. Despite this, experimental observation (Bear [1],Rashidi et al [10]) shows that for flow in the presence of a porous medium the diffusion of dissolved contaminants is enhanced beyond that in free flow. The reason is evidently that the pore structure deflects the fluid elements into tortuous flow paths, producing additional mixing of liquid carrying different solute concentrations. The implication is that a more detailed description of the flow than that contained in Darcy's law is needed to model solute transport. This introduces a statistical element into the description, since it is clearly not feasible to know or model the mechanics of the flow in a natural medium that has an unlimited variety of pore shapes and sizes.

The continuum (deterministic) approach (e.g. Bear [1], [2], [3]) is to split the fluid velocity into averaged and fluctuation contributions. Since fluctuations by definition average to zero, they can only produce net solute transport when they represent fluid exchange between points at different concentrations. Hence a net fluctuation solute flux proportional to the concentration gradient is plausible.

By making this Fickian assumption, the explicit inclusion of statistical terms is avoided and equation (2) may still be used if the velocity is reinterpreted as the averaged velocity and $D^*$ is augmented by adding a dispersion coefficient D to it. The resulting equation is known as the advection-dispersion equation (Fetter [6]).

It is also plausible to assume that dispersion is proportional to the average flow velocity, so the relation $D = \alpha v$ is used to extract a pure materials constant $\alpha$ called the dispersivity. The dispersivity has the dimensions of a length and by length scale arguments (Bear [2]) can be expressed as proportional to the pore size with a coefficient of order 1.

Many authors have studied alternative approaches in which the statistical description is more explicitly incorporated. In the work of Dagan [4],[5] random variations in the variables such as velocity and concentration are treated as perturbation terms. However, a more profound way is to allow random variations of the material properties, as that adresses the source of randomness more directly. Being coefficients in the differential equations such as (1) the material properties are the driving terms, and this leads to stochastic differential equations (SDE's) as used, for example, by Unny [11].

This article deals mainly with the SDE approach obtained by modeling the deflection of fluid trajectories by individual grains, as random fluctuations of the materials coefficients that produce a stochastic displacement term in the flow equation (1):

$$dx = -u(x,t)dt + \gamma\, dB(x,t,\theta) \tag{3}$$

Here $u(x,t)$ is the righthand side of (1), and reduces to $v_0$ in the case of a stationary homogeneous problem. $B(x,t,\theta)$ represents a Wiener process with $\theta$ labeling individual realisations and $\gamma$ is an amplitude that regulates the extent to which the path is perturbed.

The addition of the stochastic term to the flow equation somewhat complicates the allocation of units of measurement, since according to the principles of Ito calculus a dimension $T^{\frac{1}{2}}$ has to be allocated to $B$. This is avoided by introducing the convention that all coordinates and times are henceforth to be interpreted as dimensionless ratios having been divided by a length scale $x_0$ and time scale $t_0$. The proper scaling will be restored in the final results when appropriate criteria for choosing the scaling constants will also become clear.

In the porous flow problem, fluid element displacements at neighbouring points (e.g. while traversing a pore) are not independent, and so the finite pore size can be modeled by introducing a spatial covariance function $C(x_1,x_2)$ as

$$< B(x_1,t_1,\theta)B(x_2,t_2,\theta) > = C(x_1,x_2)\int_0^{min(t_1,t_2)} q(s)ds \tag{4}$$

Here, the angular brackets signify averaging over all representations, the spatial and time correlations have been assumed to be independent and the time correlation factor is the expression for a generalised Wiener process, i.e. for $q(s) = 1$ it reduces to the standard Wiener process as associated with Brownian motion.

A functional form for the spatial covariance must be chosen that is mathematically tractable and reflects the physical properties of the porous medium. A plausible choice might be an exponentially peaked function, $C(x_1,x_2) = exp(-|x_1 - x_2|/\lambda)$ in which $\lambda$ is the correlation length and would be chosen to be some average pore diameter. The detailed functional form is not important for the purpose of this article.

The chosen spatial correlation is implemented by making a Karhunen-Loeve (KL) expansion [8] for the coordinate dependence of the $B(x,t,\theta)$. This means that the covariance function is used as the kernel in an integral eigenfunction equation which is solved for the eigenfunctions $f_n(x)$ and eigenvalues $e_n$, and then used to transform (3) into

$$dx = -u(x,t)dt + \gamma \sum_n \sqrt{e_n}\, f_n(x) dB_n(t,\theta) \tag{5}$$

The result of the KL expansion is that the Wiener process in space and time has been replaced by a sum of simpler independent Wiener processes $B_n(t,\theta)$ in time only. The sum over $n$ in principle runs over the infinite set of eigenfunctions of the covariance function, but is for practical reasons truncated at a cutoff value typically of the order of 10.

# 2 Expectation values for the concentration profile

In a straightforward approach, Ito calculus ( see Kloeden et al [7]) may be used to generate numerical solutions in the form of individual realisations of the flow path from (5). The resulting flow velocity may be substituted in (2) and by averaging a large number of realisations, an expected concentration profile can be generated.

However, SDE theory (Oksendal [9]) makes powerful tools available for the calculation of expectation values without explicit sampling. In particular, the theory of diffusions is relevant here. It is based on Dynkin's formula (Oksendal [9], theorem 7.4.1):

$$E^x[f(X_\tau)] = f(x) + E^x[\int_0^\tau Af(X_s)ds] \tag{6}$$

Here $X_\tau$ is a stochastic variable evaluated at a stopping time $\tau$, $E^x$ is the expectation value over all realisations that start at an initial value $x$, and $f$ is an arbitrary function. The symbol $A$ in the integral represents a partial differential operator called the generator, and it can be constructed from an SDE provided that the latter takes the form of a diffusion. A diffusion is defined as a set of 1-st order equations

$$dX_t = b(X_t)dt + \sigma(X_t)dB(t,\theta) \tag{7}$$

where $X_t$ and $B$ may be vectors of variables, and the coefficients $b$ and $\sigma$ correspondingly matrices. The generator $A$ is a 2-nd order deterministic differential operator with coefficients formulated in terms of $b$ and $\sigma$:

$$A\, f(x) = \sum_i b_i(x)\frac{\partial f}{\partial x_i} + \frac{1}{2}\sum_{i,j}(\sigma\sigma^T)_{ij}(x)\frac{\partial^2 f}{\partial x_i \partial x_j} \tag{8}$$

To apply Dynkin's formula, one chooses $f$ as the solution of an equation chosen to simplify the integral, such as $Af = 0$. Then the expectation value of that particular function is directly given by the formula.

The contaminant transport problem is specified by equations (2) and (5). The second of these is already in the desired diffusions form. The first, the transport equation, does not conform in general. However, for many systems it is adequate (Rashidi et al [10]) to neglect microdiffusion by putting $D_m = 0$ in (2) to obtain

$$\frac{dc}{dt} = -c(x,t)\frac{du}{dx} \tag{9}$$

for 1-dimensional flow. Equations (5) and (9) together are in the appropriate form in the pair of variables (x,c), to allow construction of the generator

$$A\,f = u(x)\frac{\partial f}{\partial x} - \frac{du}{dx}\,c(x,t)\,\frac{\partial f}{\partial c} + \frac{1}{2}\gamma^2\,\mathcal{C}(x)\,\frac{\partial^2 f}{\partial x^2} \tag{10}$$

To derive (10), it is noted that $\sigma(x)$ is in the case of (5) a row vector with components $(\sqrt{e_n}\,f_n(x))$ and use has been made of the identity

$$\mathcal{C}(x_1,x_2) = \sum_n e_n f_n(x_1) f_n(x_2) \tag{11}$$

which follows directly from the eigenfunction equation, and $\mathcal{C}(x) \equiv \mathcal{C}(x,x)$.

Equation (10) already contains the first significant result from the application of SDE theory. While the details of the covariance function contained in its eigenfunctions and -values determines the behaviour of an individual realisation through equation (5), only the diagonal value $\mathcal{C}(x)$ remains in the generator that eventually determines all expectation values. In a homogeneous medium it is in fact plausible to assume that $\mathcal{C}(x) \equiv \mathcal{C}$, i.e. constant, so that the covariance function is apparently averaged out completely on taking expectation values. This is not quite accurate, as the correlation length will reappear when proper scaling of variables is restored in the final results. Nevertheless, a major simplification of the dependence on microscopic media properties is contained in the reduction to $\mathcal{C}(x)$.

In the case of a homogeneous medium $u(x) = v_0$ and the middle term in (10) falls away leaving a generator independent of the concentration, and in fact identical to that obtained from the flow equation on its own. This implies that all statistical information is contained in the fluid element position, which is plausible in the absence of microdiffusion. It is noted that this simplification only applies for a homogeneous medium.

The expectation value of most interest in the flow problem, is that of the position of a fluid element after an elapsed time $t$. This can be obtained from a slight elaboration of the Dynkin formula, called Kolmogorov's backward equation (Oksendal [9], theorem 8.1.1). This requires solution of the partial differential equation

$A\,f = (\partial f/\partial t)$. Using the appropriate simplifications of (10) for a homogeneous medium, we find a solution to be

$$f(x,t) \;=\; e^{-a(x+v_0 t)}\; e^{\frac{1}{2}a^2\gamma^2 \mathcal{C} t} \tag{12}$$

where a is the arbitrary constant arising from separation of position and time variables. Substituting this in the Kolmogorov equation yields

$$E^0[e^{-aX_t}] \;=\; e^{-av_0 t}\; e^{\frac{1}{2}a^2\gamma^2 \mathcal{C} t} \tag{13}$$

By expanding both sides as power series in $a$, it is easy to see that the average position propagates at a constant speed $v_0$ while the variance increases proportional to $t$. A more complete description of the statistics is obtained by defining $p(x,t)$ as the probability density, for a fluid element that starts at $(0,0)$ to arrive at $(x,t)$. Then (13) may be written as an integral equation for $p(x,t)$

$$\int_{-\infty}^{\infty} e^{-ax} p(x,t)dx \;=\; e^{-av_0 t}\; e^{\frac{1}{2}a^2\gamma^2 \mathcal{C} t} \tag{14}$$

When microdiffusion is neglected, the solute concentration is simply carried along with the fluid element so that at time t its expectaion value is easily calculated from the injection profile at $x = 0$ and a known probability distribution:

$$E[c(x,t)] \;=\; \int_0^t c(0, t-\tilde{t})p(x,\tilde{t})d\tilde{t} \tag{15}$$

In particular, for a $\delta$-function injection pulse at $t = 0$ the expected concentration and probability distribution become identical.

The remarks above about the time developement of low-order moments of the distribution suggests that a reasonable trial solution of the integral equation (14) would be a propagating Gauss peak, with width $\sigma(t)$ starting at 0 and increasing with time:

$$p(x,t) \;=\; \frac{1}{\sqrt{\pi}\sigma}\, e^{-\frac{(x-v_0 t)^2}{\sigma^2}} \tag{16}$$

Substituting this in (14) shows that (16) is in fact an exact solution provided that

$$\sigma(t) \;=\; \sqrt{2\gamma^2 \mathcal{C} t} \tag{17}$$

The result just derived, that a concentration pulse injected into the fluid is spread by stochastic perturbation at a rate proportional to $\sqrt{t}$, is reminiscent of the classical

theory of diffusion. In fact, for 1-dimensional stationary flow the diffusion equation is

$$\frac{\partial c}{\partial t} + v_0 \frac{\partial c}{\partial x} - D \frac{\partial^2 c}{\partial x^2} = 0 \tag{18}$$

and it is easily shown by substitution of (16) in (18) that the former solves the latter provided that

$$\sigma(t) = 2\sqrt{Dt} \tag{19}$$

Comparing (17) and (19) it is concluded that in the absence of microdiffusion and in a homogeneous porous medium, the effects of stochastic scattering by the pore structure is equivalent to that of introducing a macroscopic diffusion with an effective diffusion coefficient $D$. This proves the basic heuristic assumption made in the traditional deterministic theory of contaminant transport, for the rather simple case under discussion.

Moreover, the derivation allows us to express the macroscopic parameter $D$ in terms of microscopic medium properties. Eliminating $\sigma$ from (17) and (19) and bearing in mind that $\gamma$ and $\mathcal{C}$ are defined as coefficients in dimensionless equations and hence themselves dimensionless, we can write the properly dimensioned equation

$$D = \frac{1}{2}\gamma^2 \mathcal{C}\left(\frac{x_0^2}{t_0}\right) \tag{20}$$

It remains to choose the scaling constants. In Darcy's equation, there is only one physical quantity that can determine a scale, namely the homogeneous flow velocity $v_0$. As only the ratio $x_0/t_0$ appears in that solution it is sufficient to identify the ratio with $v_0$. Equation (20) shows that when a stochastic term is added this is no longer true and two separate scaling constants must be chosen.

Evidently the second scale must be supplied by the stochastic term. Again, there is only one plausible candidate: the correlation length $\lambda$ introduced in defining the covariance function. If we choose $x_0 = \lambda$, and for consistency with the deterministic limit let $x_0/t_0 = v_0$, the time scale $t_0$ represents the average time for a fluid element to traverse a pore. This is also plausible if we consider that in using a Wiener process to model any physical phenomenon, there is an inherent time scale that determines how quickly the Brownian variable wanders away from an initial value. In the fluid flow application, the stochastic variation is intended to model the scattering of fluid elements by the grains that form the pores, so that the pore traversal time is indeed the relevant time scale.

The expression for the pore induced hydrodynamic diffusion (i.e. dispersion) constant $D$, now becomes

$$D = \frac{1}{2}\gamma^2 \mathcal{C} v_0 \lambda \tag{21}$$

This equation incorporates two key features also arrived at by heuristic arguments in the advection-dispersion treatment of porous flow: i) that dispersion is proportional to the Darcian flow velocity, allowing the calculation of dispersivity as a materials property, and ii) that the dispersivity is a length of the order of the pore size (Bear [2],Rashidi et al [10]). The latter remark presupposes that $\gamma$ and $\mathcal{C}$ are both of order 1; for $\gamma$ that follows because the tortuous path in a porous medium can only be reproduced if the perturbing term in (3) is of similar magnitude as the Darcian displacement, while we have $\mathcal{C} = 1$ for a standard Wiener process and values of similar magnitude is appropriate if the model is generalised to use general Wiener processes.

# 3 Discussion

Having shown the essential equivalence of the stochastic and deterministic approaches in the case of stationary flow without microdiffusion in a homogeneous porous medium, it is of interest to consider whether the equivalence survives if the restrictions are relaxed. For example, will a variable correlation length $\lambda$ lead to a variable dispersion coefficient? There is one special case in which the answer is yes. If it is assumed that $\lambda$ is time dependent so that $\mathcal{C} = \mathcal{C}(t)$, substituting

$$f(x,t) \;=\; e^{-a(x+v_0 t)}\, e^{\frac{1}{2}a^2\gamma^2 s(t)} \tag{22}$$

into the generator equation produces an easily soluble differential equation for $s(t)$. Equation (16) still solves the integral equation (14) by allowing completion of the square in the exponent, so that $\sigma(t)$ can be expressed in terms of $s(t)$. Finally, subtituting the resulting expression for $p(x,t)$ into the diffusion equation (18) gives rise to a second differential equation for $s(t)$ that happens to be identical to the first, if a time dependent dispersion constant is introduced as

$$D(t) \;=\; -\frac{1}{2}\,\gamma\,\mathcal{C}(t) \tag{23}$$

. So consistency between the solutions to the generator equation, the probablity distribution integral equation and the diffusion equation has been regained.

The assumption of a time-dependent correlation length may appear contrived, as it is not obvious how that will come about physically. However, it may be a consequence of an approximation made to exploit the fact that it is easier to handle a time-dependent than a position-dependent $\lambda$. For example, since in a homogeneous medium the concentration plume is at first highly concentrated about the moving position $x = v_0 t$, the correlation length encountered by a plume moving through a slowly varying medium might be approximated by the value at the centre of the plume. It is also interesting to note that the resulting time dependent dispersion displays one form of scale dependence: a laboratory experiment measuring flows over a short time span would obtain a different value from a field experiment covering a longer period.

However, the main purpose in discussing the time dependent case is to illustrate how fragile the equivalence between the stochastic and deterministic approaches is. If only a minor further relaxation is introduced, namely to assume that $\lambda$ also depends on position, the chain of reasoning that connects them breaks down at several points. It would require that $s = s(x,t)$, and then the two differential equations for $s$ obtained from the generator equation and the diffusion equation respectively, no more coincide. A trial solution of the form of (16) does not give a tractable solution to the integral equation any more. Furthermore, in such a case it is reasonable to assume that both $u$ and $D$ will also depend on x, and then both the generator equation and the diffusion equation acquire additional terms making the equations for $s$ diverge in form even more.

It is therefore conjectured that the stochastic description does not reduce to the simpler advection-dispersion model in the case of a non-homogeneous medium. While it is not logically impossible that new solutions to the new set of equations might again agree, it seems highly unlikely that such a happy coincidence can recur. A full resolution of this point will require a solution of the generator equation (10) in its stated form, under assumption of functional forms for $u(x)$ and $\mathcal{C}(x)$ and this may necessitate numerical rather than analytical procedures.

# 4 Conclusions

To summarise, the main results derived in this article are

1. Expectation values over all realisations, depend only on general features of the covariance function such as its diagonal value and the correlation length. This is in contrast to individual realisations that depend on the detailed functional form of the covariance function.

2. An equivalence between the stochastic and deterministic descriptions was derived in the case of flow in a homogeneous porous medium. This allows the macroscopic dispersion constant to be expressed in terms of microscopic parameters.

Further investigation is required for the case of non-homogeneous media.

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