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Research Report 01/2002
April 2002

ISSN 1174-6696

RESEARCH REPORT

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Solute Dispersion in Porous Flow with a Constant Velocity Gradient

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Abstract:

In a previous paper, we have shown that stepwise changes in the macroscopic flow velocity of a carrier fluid through a porous medium, substantially affects the dispersion of solutes that it carries. This paper extends the work to the case of a continuously changing flow velocity. The stochastic model used to describe pore deflection of the flow path, is reduced by the use of Dynkin's formula to the formulation of a deterministic differential equation. An exact solution is found for the case of a flow velocity that varies linearly with position, and the resulting integral equation for the solute probability distribution is also solved exactly. This is applied to the case of a solute concentration plume represented by an initially Gaussian concentration peak. The modulated Gaussian that is calculated shows that the time evolution of the plume differs fundamentally from that predicted by the standard diffusive model. Implications of this conclusion for modelling dispersion in a variable flow velocity are further explored.

Keywords: Mathematical modelling; contaminant dispersion; stochastic differential equation; solute transport

1. INTRODUCTION

A straightforward approach to modelling solute transport by the flow of a carrier fluid through a porous medium, is to split the carrier fluid velocity into averaged and fluctuating contributions. This is the basis of the advection-dispersion equation (ADE) [Fetter, 1993] that is widely used to model the dispersion of contaminants by water in an underground aquifer. Using plausibility arguments, a Fickian assumption is made to represent the transport of solutes that result from the fluctuations. This leads to a diffusion-like transport equation but with the diffusion constant replaced by a medium-dependent dispersion constant D. It is well known that D, as measured e.g. from real world aquifers, turns out to be scale dependent.

Many authors have suggested that this is due to inhomogeneity of the hydraulic conductivity and other properties of real porous media. An up to date review of work in this field has been done by Li, McLaughlin and Liao [2002], and identifies as a major issue the fact that the mean flow in field scale aquifers is not uniform. For example, Adams and Gelhar [1992] found that at the Columbus site, the groundwater flow accelerates due to a 2-order increase in mean conductivity. A large body of work by McLaughlin, Li and other

authors has studied the interplay between small-scale heterogeneity and large-scale nonuniformity. For example, a numerical simulation by Ruan [1997] studying transport in a nested two-scale conductivity field showed significant effects of the large scale variation, on dispersion due to the small scale heterogeneity.

To improve understanding of such phenomena, we study a model where stochasticity is introduced at the fundamental level of the path that a fluid element follows through a porous medium, rather than stochastic variations of medium properties as done in most of the literature referred to.

Hence, we describe the stochastic path followed by a single fluid element through the porous medium, by the equation:

$$dx = u(x)dt + \gamma\, dB(x,t,\theta) \tag{1}$$

Here u(x) is the macroscopic carrier fluid velocity, as derived from an appropriate flow equation such as Darcy's law, and will in general depend on the hydraulic head differential as well as medium properties such as hydraulic conductivity and porosity. The second term represents the pore-scale (microscopic) stochastic perturbation of the fluid velocity; $B(x,t,\theta)$ is a Wiener process with θ labelling individual realisations and γ is an amplitude that regulates the extent to which the path is modified. Only 1-dimensional flow is modelled at this stage.

Equation (1) is a stochastic differential equation (SDE) and needs to be solved by using Ito calculus and other methods from SDE theory as set out, for example, by Øksendal [1998]. Each individual realisation of the solution represents a possible path of a fluid element through the porous structure, and macroscopic dispersion is described by calculating statistics over all realisations.

Instead of numerically calculating individual realisations, our approach is to calculate expectation values over all realisations, of a suitably chosen function. Using Dynkin's formula [Øksendal, 1998] this in effect replaces the SDE by a deterministic partial differential equation. From the expectation value expression, a probability distribution for the position of a fluid element as function of time is calculated. Finally, neglecting microdiffusion, this can be used to calculate the evolution of an initial solute concentration.

In the first study we undertook using these methods [Verwoerd and Kulasiri, 1999] it was shown that for a constant velocity u of the carrier fluid, this evolution reduces to the same diffusion-like behaviour (with the variance of the concentration growing proportional to time) that solution of the ADE also produces.

However, in real aquifers, macroscopic variations in the velocity are to be expected because of flow geometry and variations in media properties.

It is known from simple examples of SDE's, that the effects of stochastic variations of a driving coefficient (the role played by velocity in (1)) can go beyond the predictions of a model that superimposes perturbations on the solution of a deterministic differential equation (which is the implicit basis of the ADE approach). So the question arises whether a changing velocity would modify the evolution of solute dispersion away from a simple diffusion-like behaviour, and if so whether this modification can explain the observed scale dependence of dispersivity.

A first step in answering this question was taken in a subsequent application of the method [Verwoerd and Kulasiri, 2001] that investigated the effect of stepwise changes in the macroscopic fluid velocity. It was found that there are kinematic effects on a solute plume penetrating a step, which interact with the dispersion mechanism. While the kinematic effects themselves are reversible at subsequent steps in the opposite direction, their effects on dispersion are not. As a result, velocity fluctuations tend to increase dispersion beyond that produced by flow at the same average constant velocity. Moreover, it was found that a varying velocity causes dispersion to assume a time dependence that is different from the linear one characterising the diffusive model of the ADE.

This paper explores the phenomenon further by investigating the propagation of a plume in a flow with a constant spatial gradient of the flow velocity. We are concerned in particular with a longitudinal velocity gradient (the only kind relevant in a 1-dimensional model); variations transverse to the flow direction have previously been shown [Gelhar, Gutjahr and Naff, 1979] to enhance dispersion. However, our focus is on the fact that as the velocity plays the role of a driving coefficient in equation (1) its variation can change the nature of the solutions to the SDE in a fundamental way, a fact already hinted at by the non-linear time dependence found for stepwise changes.

In section 2 the mathematical model is formulated. An exact solution of the model is presented and shown to reduce to the simple diffusive dispersion model in the limit where the flow velocity becomes constant. The last section is devoted to a discussion of the limits of applicability and the significance of the results that were derived.

2. MATHEMATICAL FORMULATION

Dynkin's formula [Øksendal, 1998, theorem 7.4.1] asserts that the expectation value at time τ of a function f of a stochastic variable X_t can be calculated as

$$E^x[f(X_\tau)] = f(x) + E^x\left[\int_0^\tau A f(X_s)\,ds\right] \tag{2}$$

where the expectation value is taken over all realisations of the stochastic process that starts from the initial value x. The symbol A represents a partial differential operator called the generator, and its form is derived from that of the SDE equation that the stochastic process satisfies. By requiring f to simplify $A\ f$ appropriately, equation (2) becomes tractable. In the case of equation (1), this gives rise to the following deterministic DE for f:

$$\frac{1}{2}\gamma^2\frac{\partial^2 f}{\partial x^2} + u(x)\frac{\partial f}{\partial x} = \frac{\partial f}{\partial t} \tag{3}$$

In order to obtain a solution in a form that will allow progress as detailed below, it is necessary to choose an explicit form for $u(x)$. In fact, such progress has only proven possible so far if u is chosen to depend linearly on position, i.e.

$$u(x) = v_0 \pm \mu^2 x \tag{4}$$

Here, v_0 and μ are simply parameters that characterise the macroscopic flow velocity; if $\mu = 0$ we have a constant flow at a velocity v_0, which is the case shown in a previous article [Verwoerd and Kulasiri, 1999] to reduce to the ADE equation. Solution of equation (3) is facilitated by transforming to the dimensionless variable pair

$$z = \pm\frac{\mu}{\gamma}(x \pm \frac{v_0}{\mu^2}); \qquad T = \mu^2 t \tag{5}$$

The cases of accelerating and decelerating flow are explicitly distinguished by the choice of $\pm$. As can be confirmed by back substitution, the following expressions are solutions of equation (3) in each of these cases:

$$\begin{aligned} f_+(z,T) &= \exp\left[-T - z^2 - aze^{-T} - \tfrac{1}{4}a^2\left(1 - e^{-2T}\right)\right] \\ f_-(z,T) &= \exp\left[-aze^{-T} + \tfrac{1}{4}a^2\left(1 - e^{-2T}\right)\right] \end{aligned} \tag{6}$$

Here, a is an arbitrary constant. Substituting equation (6) into equation (2), we obtain expectation values for the two distinct functions $exp\left(-z^2 - az\right)$ and $\exp(-az)$ for accelerating and decelerating flows respectively.

However, an alternative expression for the expectation values can be written down by defining the probability density function $P_t(x \mid x',t')$ as the spatial x-domain probability density function, for finding a fluid element at position x at time t, given that it was at position x' at the earlier time t'. Setting these two expressions for the expectation value equal gives for decelerating flow the integral equation

$$\int_{-\infty}^{\infty} P_T(z \mid z_0, 0)\exp(-az)\,dz = \exp\left[-az_0e^{-T} + \tfrac{1}{4}a^2\left(1 - e^{-2T}\right)\right] \tag{7}$$

and an analogous equation for accelerating flow. These integral equations are similar in structure, although more complicated, to the one solved in the constant velocity case [Verwoerd and Kulasiri, 1999], and by analogy a gaussian trial solution for P allows the integration to be done by completing squares in the exponent. The resulting solutions for both equations can be combined into

$$P_T(z \mid z_0, 0) = \frac{1}{\sqrt{\pi}\sqrt{\pm\left(e^{\pm 2T} - 1\right)}}\exp\left[\frac{-\left(z - z_0e^{\pm T}\right)^2}{\pm\left(e^{\pm 2T} - 1\right)}\right] \tag{8}$$

If we neglect molecular scale diffusion, solute is transported by motion of fluid elements only. Hence the evolution of a given initial solute concentration $C(x,t_0)$, can be calculated from the probability density by formulating an integral form of the solute mass conservation law (equivalent to the differential form that is the basis of the ADE equation) as follows:

$$C(x,t) = \frac{1}{u(x)} \int_{-\infty}^{\infty} dx' C(x',t_0) u(x') P_{t_0}(x' \mid x,t) \tag{9}$$

Here $P_{t'}(x' \mid x,t)$ is the x'-domain probability density, that a fluid element which is found at the position x at time t, originated from position x' at the earlier time $t'<t$. It is related to the probability density in equation (8) by an appropriate variable transformation, which turns out to merely add a factor exp(±T) to the numerator of the coefficient on the right hand side of equation (8).

In the absence of stochastic perturbations of the path (i.e. deterministic flow), and neglecting microdiffusion, the probability distribution is a Dirac delta function given for the simple case of flow at a constant speed v_0 by:

$$P_{t'}(x' \mid x,t) = \delta(x' - x + v_0(t - t')) \tag{10}$$

Substituting this into (9) clearly reduces it to a statement of solute mass conservation, confirming that equation (9) is merely the generalisation of the conservation law to stochastic flow.

The integral in (9) becomes particularly simple to do if we take $t_0 = 0$ and choose a Gaussian form for the initial concentration plume:

$$C(x,0) = \mathcal{G}(\xi,s) \tag{11}$$

where $\mathcal{G}$ is the normalised Gaussian

$$\mathcal{G}(\xi,\sigma) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{(x-\xi)^2}{2\sigma^2}\right) \tag{12}$$

Using these expressions for the initial concentration and probability density, the integrand in (9) becomes the exponential of a quadratic expression in x' which after some tedious but straightforward algebra can be evaluated by completion of squares as before. The result is that the evolving concentration takes the form of a modulated Gaussian

$$C(x,t) = M(x - X,T)\,\mathcal{G}\left[X, s^2 e^{2T} \pm \tfrac{1}{2}\left(e^T - 1\right)\varphi\right] \tag{13}$$

Here *X(t)* is the position that the concentration peak would have in a deterministic (i.e. plug) flow at velocity *u(x)*, and (13) shows that the Gaussian part of the plume still propagates at the deterministic (but changing) velocity.

However, there is a very significant change in the way that the plume disperses with time. This information is contained in the time dependent variance of the Gaussian:

$$\sigma(t) = s^2 e^{2T} \pm \tfrac{1}{2}\left(e^T - 1\right)\varphi \qquad (14)$$

The hallmark of the diffusion-like spreading of a plume that holds in constant velocity flow (and predicted by the ADE equation) is that the variance of a Gaussian input plume increases linearly with time. By contrast, equation (14) shows that for a linearly changing flow velocity, the variance changes exponentially with time. Hence, dispersion in the presence of a gradient in the carrier fluid velocity is a more complex phenomenon, which cannot be adequately described by a diffusive model.

The parameter φ in (14) is defined as γ^2/μ^2, and essentially measures the scale of stochastic displacements, relative to the scale over which the carrier velocity changes.

The modulation factor M in (13) is a complicated rational expression and has the qualitative effect of introducing skewness into the peak. Except near stagnation points of the flow it is slowly varying with x compared to the exponential variation of the peak, and can be taken to a first approximation as the fixed value at the peak position. This turns out to be $M(0,T) = 1$.

In the work on transmission of a plume through a discrete velocity step, we showed [Verwoerd and Kulasiri, 2001] that part of the effect of a velocity change on dispersion is simply a kinematic effect needed to satisfy solute mass conservation. The same is true in the smoothly changing velocity. In fact, the stochastic contribution can be removed mathematically by taking the limit $\varphi \rightarrow 0$. Hence, from equation (14) the first term $s^2 e^{2T}$ in the variance is easily identified as the kinematic contribution. This may be confirmed by performing a strictly deterministic calculation using the δ-function probability of equation (10) instead of the stochastic one (8) when calculating equation (9).

The second term in the variance expression may consequently be identified as the "intrinsic" dispersion as a result of stochastic perturbation of the pore-scale flow path.

It is of interest to consider the intrinsic dispersion in the constant flow velocity limit, represented by $p \rightarrow 0$. It is easily shown that

$$\pm\varphi\left(e^{2T} - 1\right) \xrightarrow[0]{\mu} 2\gamma^2 (t - t_0) \qquad (15)$$

hence recovering the standard diffusive behaviour of constant flow.

The difference between the expressions on both sides of relation (15), in the case that $\mu \neq 0$, represents the effect of interaction between velocity changes and intrinsic dispersion. As argued in connection with step penetration [Verwoerd and Kulasiri, 2001], the underlying mechanism of this interaction is that kinematic stretching or compression of the solute plume that results from a velocity change, alters concentration gradients and hence affects dispersion. To demonstrate the significance of the interaction, we show in the figure below a comparison for chosen numerical parameters, between the actual dispersion and the value that is obtained when the interaction is ignored, i.e. when a simple diffusive dispersion is superimposed on the kinematic part of the dispersion.

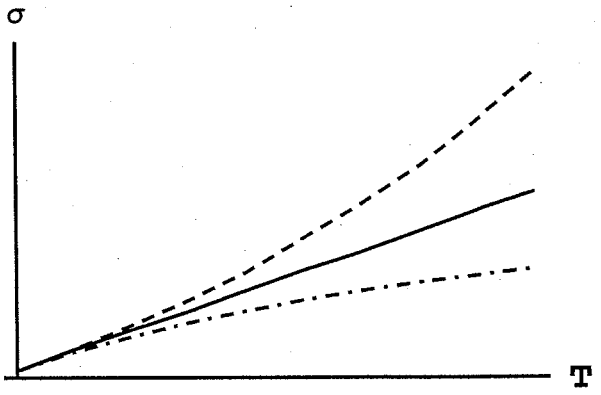

Figure 1: Evolution of actual dispersion with time for accelerating flow (dashed line) and decelerating flow (dash-dot line) in comparison to diffusive dispersion superimposed on kinetic dispersion (solid line)

DISCUSSION

The exponential terms in equation (14) appear somewhat alarming, especially in the case of accelerating flow where this means an exponential growth rather than decline. However, their appearance is merely a reflection of the fact that even in simple deterministic flow, the displacement of a fluid element grows exponentially with time if the fluid velocity increases linearly in space. The unrealistic aspect of the mathematical treatment presented so far, is the implicit assumption that equation (4) holds over the entire x-axis.

Clearly it is only realistic to apply equation (4) over a finite interval; or, more generally, any arbitrary continuous macroscopic spatial variation of the flow velocity can be approximated by a sequence of finite length intervals within which the velocity varies linearly. Unfortunately it is far from trivial to perform this generalisation in practice because of the care that is needed in describing the transition from one subinterval to the next. That point is amply illustrated by the complications arising in the much simpler case treated in the previous paper [Verwoerd and Kulasiri, 2001] of subintervals with constant velocity and diffusive dispersion.

Bearing these reservations in mind, significant insights about dispersion in a varying flow velocity can still be gained from the results presented in the previous section.

Many of the conclusions reached in the previous paper using numerical examples and approximations, are confirmed and sharpened by the analytical treatment here. For example, the distinction between kinematic and intrinsic dispersion observed already for the discrete steps, are here given analytic expression by the separate terms appearing in equation (14) for each of these.

Moreover, the reversible nature of the kinematic dispersion is clearly shown by the functional form of the first term in equation (14). A Gaussian peak that starts from an initial variance s^2 and propagates for a time τ in a flow with acceleration coefficient μ^2 in the absence of stochastic effects, attains a variance value of $s^2e^{2\mu^2\tau}$ according to (14). If at that moment the acceleration is reversed, the variance after a further time interval τ will by the same argument be given by $\left(s^2e^{2\mu^2\tau}\right)e^{-2\mu^2\tau} = s^2$, i.e the stretching of the peak during the first phase is exactly reversed in the second phase. On the other hand, the functional form of the intrinsic dispersion term does not allow the same manipulation, showing explicitly that that part is not reversible.

The fact shown in figure (1) that a continuous increase of the flow velocity enhances dispersion beyond the value expected from the diffusive model whereas a decrease inhibits dispersion in the same comparison, also agrees with the results found in the previous paper for a discrete velocity step. However, we now have an explicit analytic expression for the magnitude of this effect.

The most significant general conclusion reached is that the time dependence of dispersion is drastically altered away from linearity by the presence of flow velocity variation.

The dispersion coefficient D that is customarily used to characterise the dispersive properties of a porous medium, is in essence the coefficient of a linear growth of dispersion with time. Hence a non-linear time dependence implies that this characterisation, implicit in the standard ADE equation, is not adequate any more when the flow velocity varies.

As mentioned in the introduction, empirical evidence has led many authors to describe D as scale dependent. Instead, it is our view that it is the basic assumption that dispersion is linear, that needs to revised. The results above give an indication of the direction that such a revision might take, and will be pursued in our further work.

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