The Effects of Variable Flow Velocity on Contaminant Dispersion in Porous Flow

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Abstract: The diffusion-like behaviour of contaminant dispersion that underlies the commonly used advection-dispersion equation (ADE), has been previously shown to follow rigorously from a model that uses stochastic displacements to represent porous flow in a homogenous medium. This paper extends the model, as in a realistic aquifer the velocity will vary due to flow geometry and inhomogeneity of the medium. An integral formulation of the solute mass conservation law involving the probability distribution of fluid elements is presented. This is first applied to several numerical examples involving transmission of a gaussian contaminant plume through discrete velocity steps. A net increase in dispersion is found even when the average velocity is maintained. This is the result of the interaction of kinematic effects and dispersion. Some results from an analytical calculation are also presented, which show that the effects of a velocity step decay away from the step location. This leads to an expression for a scaling length, and the conclusion that dispersion is only sensitive to velocity fluctuations on a similar length scale as that of the dispersion itself.

Keywords: Contaminant dispersion; Stochastic modelling; Solute transport; Heterogeneous porous medium

1. INTRODUCTION

The advection-dispersion equation (ADE) [Fetter, 1993] that is widely used to model the dispersion of solutes in fluid flow through porous media, is based on splitting the carrier fluid velocity into averaged and fluctuating contributions. Using plausibility arguments, a Fickian assumption is made to represent solute transport as a result of 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.

Studies by many authors suggest 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 and McLaughlin [2001], 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.

With the purpose of improving 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:

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

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,θ) 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.

Using these methods, we have shown in a previous paper [Verwoerd and Kulasiri, 1999] that an expression can be derived for the time evolution of the probability distribution of fluid element positions. Neglecting microdiffusion, this can be used to calculate the evolution of an initial solute concentration. Moreover, we showed that for a constant velocity u , 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. This result establishes the equivalence of the stochastic model to the more conventional ADE description in the case of a homogeneous medium, where the assumption of a constant fluid velocity is plausible.

The large scale variation of the mean velocity in real aquifers, raises the question whether a changing velocity in the SDE 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.

To fully answer this question requires elaborate study of solutions of equation (1) for variable u, and this will be presented elsewhere. In this paper, however, a far simpler approach is presented. The simplest possible way to approximate a variable u is as a piecewise constant velocity, where all the variation is contained in isolated discrete velocity steps separating regions of constant u. The only aspect that needs to be explicitly included in extending our constant velocity model [Verwoerd and Kulasiri, 1999], is that the law of solute mass conservation is formulated in terms of a probability integral rather than a differential equation. This is discussed in detail below.

After formulating the method in section 2, numeric results are presented in section 3 to illustrate the effects of velocity steps on an assumed initial solute concentration profile. These show that single steps produce both kinematic and dispersal effects; although there is partial cancellation between upwards and downwards steps, a velocity fluctuation produces a net increase of the dispersion compared to flow at the same average velocity. Section 4 presents analytical calculations to investigate this further and establishes a maximum length scale for fluctuations that significantly affect dispersion. The final section summarises conclusions and puts them in a wider context.

2. MATHEMATICAL FORMULATION

Assuming a given initial solute concentration $C(x,t_0)$, we calculate the concentration at a later time t as

$$C(x,t) = \frac{1}{u(x)} \int_{-\infty}^{\infty} dx' C(x',t_0) u(x') P_{t_0}(x' \mid x,t) \tag{2}$$

Here $P_{t'}(x'|x,t)$ is the probability density w.r.t x', that a fluid element which is found at the position x at time t, originated from position x' at the earlier time $t'<t$. 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 u_0 by:

$$P_{t'}(x' \mid x,t) = \delta(x' - x + u_0(t-t')) \tag{3}$$

Substituting this into (2) clearly reduces it to a statement of solute mass conservation; equation (2) is merely the generalisation of the conservation law to stochastic flow and variable flow velocity.

The expression for the probability density derived from SDE theory for constant flow speed [Verwoerd and Kulasiri, 1999], is

$$P_{t'}(x' \mid, x,t) = \frac{1}{\sqrt{2\pi \gamma^2 (t-t')}} \exp\left(-\frac{(x-x'-u_0(t-t'))^2}{2\gamma^2(t-t')} \right) \tag{4}$$

The integral in (2) becomes particularly simple to do if we choose a Gaussian form for the initial concentration, and take $t_0 = 0$:

$$C(x,0) = \frac{1}{\sqrt{2\pi}\, s} \exp\left(-\frac{x^2}{2s^2} \right) \tag{5}$$

It is easily seen by completion of squares in the exponent that (2),(4) and (5) gives

$$C(x,t)=\frac{1}{\sqrt{2\pi(s^2+\gamma^2 t)}}\exp\left(-\frac{(x-u_0 t)^2}{2(s^2+\gamma^2 t)}\right) \tag{6}$$

This shows that a gaussian input concentration peak propagates at the constant flow velocity, maintaining its gaussian peak shape, but spreads and has a variance increasing linearly with time. This is a well known solution of the ADE equation, allowing identification [apart from scale factors, Verwoerd and Kulasiri, 1999] of the macroscopic dispersion constant D with the microscopic stochastic amplitude γ^2.

In the case of a flow velocity that is piecewise constant in a number of adjoining regions, (4) applies in each of these separately by taking an appropriate value for u in each region. For simplicity, we assume that u remains positive throughout. Let u_i indicate the flow velocity in region i, defined by its entrance boundary x_{i-1} and exit boundary x_i.

To describe the transmission of a peak from one region to the next, we need to formulate the solution of a boundary value problem, rather than the initial value problem discussed so far. The underlying notion is that transmission of a peak from region i to region $i+1$, delivers solute concentration at the boundary x_i as a time profile $C(x_i,t)$; and this is equivalent (inside region $i+1$) to injecting the same time profile from an external source at $x = x_i$. It seems straightforward to modify (2) appropriately:

$$C_{i+1}(x,t)=\frac{u(x_i)}{u(x)}\int_{-\infty}^{t} dt'\, C_i(x_i,t')P_{x_i}(t'\mid x,t) \tag{7}$$

where the time-dependent probability density used in the boundary value problem is obtained from the spatial density in (2) by an appropriate transformation of variables. Equation (7) is indeed equivalent to (2) as a formulation of solute mass conservation in the case of deterministic flow, as may be confirmed by use of the appropriate δ-function expression for P.

However, in the stochastic case, the situation is more subtle. The time profile of an external source injecting solute at position x_i ,is not the same any more as the time profile in the flow at position x_i. This is because there is a finite probability of solute dispersing upstream from the injection point as well as downstream. There is also a mathematical difficulty in extrapolating the injection profile backwards in time, as required by the lower integration limit of equation (7). This necessitates the introduction of a time cutoff, t_c. The effect of these difficulties is illustrated by noting that (7), applied to the trivial case when $u_i = u_{i+1}$, does not reduce to transmission thorough the non-existent step according to (6), as it should. To rectify the matter, we introduce a modifying factor $g(x',t',x,t,u)$ by which a desired concentration profile in the flow, needs to be multiplied in order to find the required injection profile. It turns out that it is possible to solve for this function, in the case of a gaussian peak propagating through a step, by requiring conformation to equation (6) for the case of a non-existent step; the result is

$$g(x',t',x,t,u)=\left(\frac{t-t'}{t'-t_c}\right)\left(\frac{x'-ut_c}{x-x'+u(t-t')}\right)+\frac{x-x'}{x-x'+u(t-t')} \tag{8}$$

Incorporating these modifications into (7), the final expression for the concentration in region $i+1$, given a gaussian peak in region i, is:

$$c_{i+1}(x,t)=\left(\frac{u_i}{u_{i+1}}\right)\frac{1}{4\pi\gamma^2}\int_{t_c}^{t} dt'\, g(x_i,t',x,t,u_{i+1})\times$$
$$\times\frac{x-x_i+u_{i+1}(t-t')}{(t-t')^{3/2}\sqrt{t'-t_c}}\times$$
$$\times\exp\left(\frac{\left(x-x_i-u_{i+1}(t-t')\right)^2}{2\gamma^2(t-t')}+\frac{\left(x_i-u_{i+1}t'\right)^2}{2\gamma^2(t'-t_c)}\right) \tag{9}$$

and the appropriate cutoff time is given by $\gamma^2 t_c = -s^2$.

3. NUMERICAL EXAMPLES

Before discussing analytic approximations of the rather formidable integral in (9), we present some numerical examples, for velocity step parameters chosen arbitrarily to illustrate its implications. The first example is for an upwards velocity step, and is shown in Figure 1.

The input concentration peak penetrates the 50% velocity step shown in Figure 1(a), from region 1 on the left. The concentration in region 2, calculated for a suitably chosen later time, is shown in Figures (b) and (c) as thick lines.

Figure 1(b) compares this to the peak that would result from transmission at a constant fluid velocity equal to the average over the period, shown as a thin line "background" peak. The velocity step induces some asymmetry and moreover produces additional dispersion. Part of this is merely a kinematic stretching of the peak, dictated by solute mass conservation, and is induced by the prefactor (u_i/u_{i+1}) in (9). This would be present also for purely deterministic ("plug flow") transport through a step and is reversible by a subsequent downwards step.

To gauge the extent of this kinematic effect, Figure 1(c) compares the step transmission peak, to the background peak on which kinematic stretching has been artificially superimposed. It is seen that the actual dispersion is less than expected from kinematics.

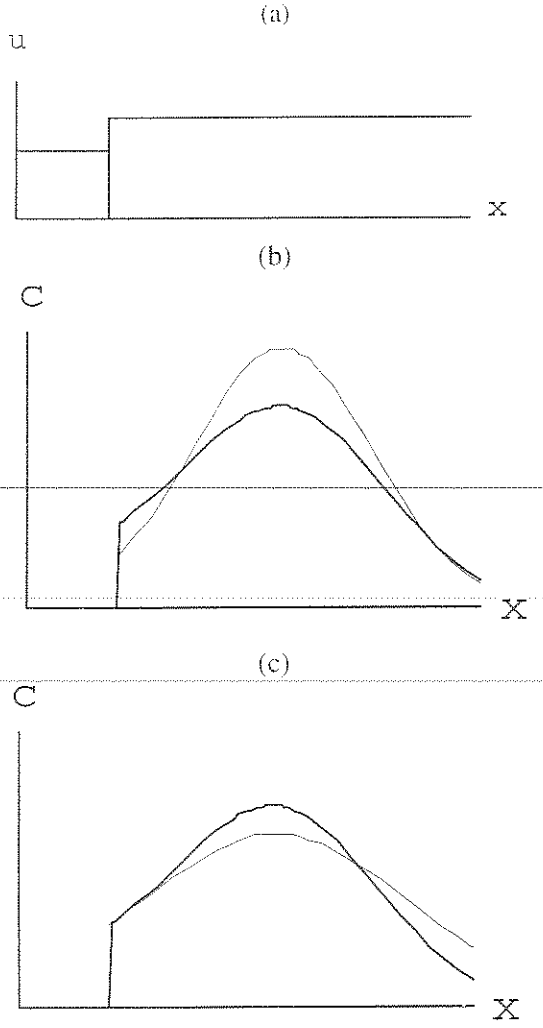

Figure 1. Spatial concentration profile after penetrating an upwards velocity step.

The interpretation of this is that because of kinematic stretching, concentration gradients are reduced in region 2 and since stochastic dispersion is effectively driven by concentration gradients, dispersion is suppressed by the upwards step.

If this is correct, a downwards velocity step should kinematically compress a contaminant peak and hence enhance dispersion. That is indeed what is observed when the calculation is repeated for that case.

When an upwards step is followed by a downwards one of the same magnitude, the kinematic effects must cancel to satisfy the conservation law. Hence the double step can be used to show irreversible effects of step changes of the velocity on dispersion. That is demonstrated by the results shown in Figure 2.

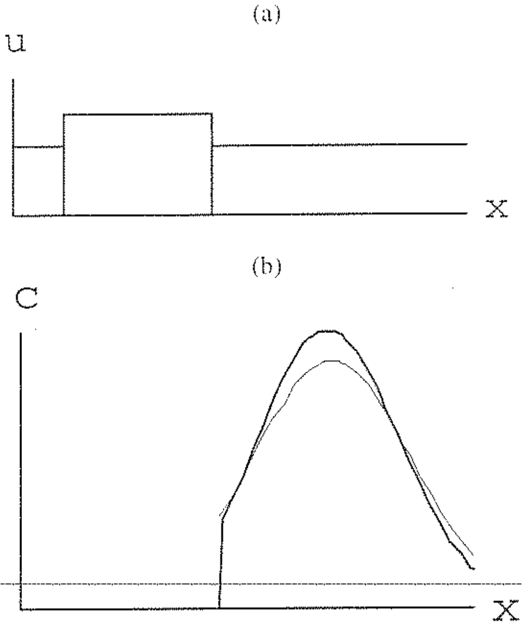

Figure 2. Spatial concentration profile after penetrating a double velocity step.

As in Figure 1(b), Figure 2(b) shows the calculated concentration in comparison to a thin line that represents the peak propagation at the same constant average velocity. The net effect of the pair of steps is to produce less dispersion, because during the time spent in the intermediate region 2, the peak was kinematically stretched and dispersion was reduced .

Our final example applies the same procedure to a velocity fluctuation, represented by a sequence of three velocity steps. The step sizes and positions are chosen in such a way that the average velocity is exactly equal to the constant velocity value in regions 1 and 4. This allows a direct comparison between a contaminant peak propagated at a constant velocity, and one that arrives simultaneously at the same position after having been subject to a velocity fluctuation. This example corresponds most directly to the effects of neglecting inhomogeneities in real porous media. The result is presented in Figure 3.

The main interest of this example, is whether the enhancement of dispersion when the speed is lowered initially on entering region 2, is compensated by the suppression of dispersion caused by the velocity increase when region 3 is entered. The comparison with the background peak shown as a thin line in Figure 3(b), shows that it is not the case. There is a small but noticeable net increase in dispersion caused by the velocity fluctuation. This calculation was repeated for the case were the high speed region is encountered first, and shows an identical overall increase in dispersion. A plausible explanation of the fact that the enhancement of dispersion in the low speed region dominates, is that more time is spent traversing this region than the high speed region.

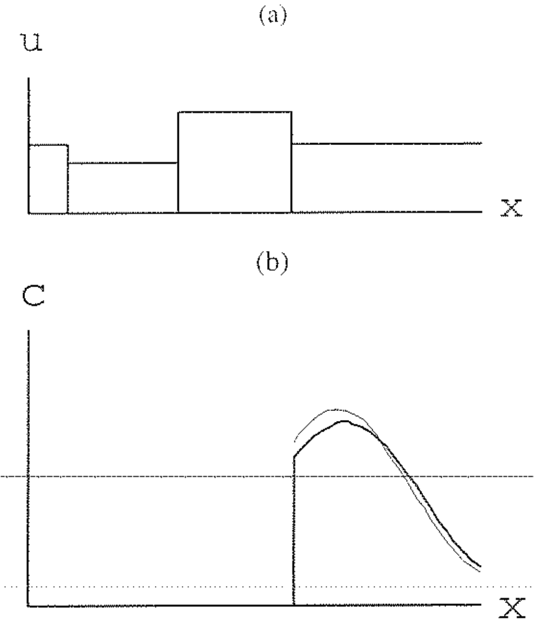

Figure 3. Spatial concentration profile after penetrating a 3-step velocity fluctuation.

Although the effect for a single fluctuation may be small, it is additive for a sequence of fluctuations as may reasonably be expected in a real aquifer. This will result in additional dispersion proportional to the elapsed time, compared to transport in a homogeneous medium with the same average flow velocity.

By itself, this effect represents an increase of the dispersivity, but does not explain a scale dependent D. To investigate that, a more quantitative understanding of how step parameters determine the additional dispersion is required.

4. ANALYTICAL RESULTS

A full description of the approximations and procedures used to solve the integral in (9) analytically, is beyond the scope of the present paper. Some salient points arising from the analysis of a gaussian input peak undergoing a velocity change from V_1 to V_2 are as follows:

- The functional form of the contaminant peak after step penetration, consists of a gaussian factor multiplied by a slowly varying modulation factor.
- The peak of the gaussian still translates at the constant speed V_2
- The time dependence of the variance of the Gaussian is modified. The diffusion-like factor $\gamma^2(t-t_c)$ as in (6), is multiplied by a factor $b^2(t) = 1/a(t)$
- The time dependence of a is given to a good approximation by the expression

$$a(t) = 1 + c\frac{\theta_1 - t_c}{t - t_c} + d\frac{(\theta_1 - t_c)^2}{(t - t_c)(t - \theta_1)} \tag{10}$$

Here $\theta_1 = x_1 / V_1$ is the time taken for the peak to reach the step at $x = x_1$, and c and d are time independent coefficients proportional respectively to Δ and Δ^2, where Δ is a measure of the relative size of the step given by $\Delta = (V_2 - V_1)/(V_2 + V_1)$.

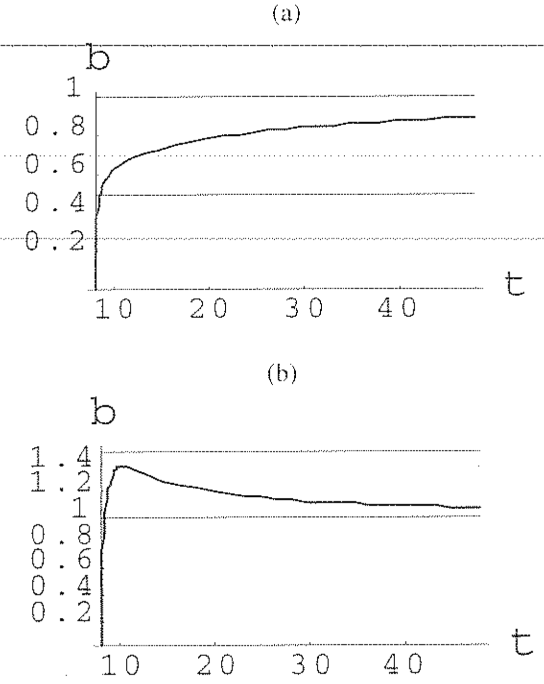

Figure 4. Time development of the factor that multiplies diffusive dispersion, after penetration of (a) an upwards, and (b) a downwards velocity step.

The time dependence of the multiplicative factor in the standard deviation, is illustrated in Figure 4 for the cases of a 50% upwards and downwards velcocity step respectively. Shown as thin lines in these figures, are the values corresponding to a diffusive model (i.e., =1) and the kinematic values 1.5 and 0.5 respectively.

Shortly after reaching the step at $\theta_1 = 8$, the spatial extension of the peak (as measured by its standard deviation) approaches the kinematic value; after that it decays asymptotically to the diffusive value. The sharp drop to zero at the initial time θ_1 in both figures, is related to the discontinuity in the velocity at the step. A meaningful interpretation of the peak as quasi-gaussian can at any rate only be given once it has fully penetrated the step, which in the figures happens at a time value of about 10.

Of most interest is the interpretation of the decay from the kinematic to diffusive values. In the case of the upwards step, the initial kinematic compression produces larger concentration gradients than in a constant velocity, diffusive peak; consequently, it disperses faster until it has eventually reached the same extension as the diffusive peak. The opposite holds for a downwards velocity step.

This result implies that the effects of a single velocity step on dispersion, remains significant only over a limited length scale. Manipulation of (10) leads us to conclude that for b to approach unity within a tolerance ε, the spatial displacement from the step has to exceed L where

$$L = \frac{4V_2}{\gamma^2}\left|\frac{\Delta}{\varepsilon}\right|\sigma_1^{\,2} \qquad (11)$$

Here σ_1^2 is the variance of the gaussian peak as it reaches the step at $x = x_1$.

The implication of this factor in (11) is that a sequence of steps, such as in the fluctuation discussed above, will have the most noticeable effect on dispersion if their spacing is of the same order as the width of the peak. Conversely, velocity fluctuations over a length scale much larger than that of the contaminant variation, will have a negligible effect on its dispersion.

In turn, this suggests that scale dependent dispersivity can result from the fact that as a contaminant plume moves through the medium, its dispersion is initially only enhanced by small scale velocity fluctuations, but as it spreads, increasingly larger scale fluctuations also contribute. Further investigation is required to establish if this will account quantitatively for the observed scale dependence.

5. CONCLUSIONS

Tracing the evolution of a gaussian solute peak as it is transmitted across velocity steps, leads to several insights.

The primary effect that we find is a reversible, kinematic stretching or compression of the peak. In turn, this changes the concentration gradient and hence dispersion is suppressed by a velocity increase and enhanced by a decrease. This results in a residual effect on dispersion even if the kinematic change is reversed by a second velocity step. Finally, in the case of a fluctuation, the opposite effects on dispersion cancel only partly leaving a net increase of dispersion compared to transmission at the same average velocity.

The effects of the velocity change decays away from a step, introducing a maximum length scale of fluctuations to affect dispersion. The scaling is relative to the variance of the gaussian peak as it enters the fluctuation, suggesting a mechanism for dispersivity to increase with length of travel as is experimentally observed.

The feature of most general significance, is 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. Ignoring the non-linearity, inevitably leads to a time- and hence scale-dependent dispersivity. Instead, a model using a realistic non-linear dependence should still be able to be formulated in terms of constants that depend on porous medium properties only.

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