# ON TRANSPORT IN FORMATIONS OF LARGE HETEROGENEITY SCALES

Gedeon Dagan
Faculty of Engineering, Tel Aviv University, Israel

Abstract

It has been recently suggested that in transport through heterogeneous aquifers, the effective dispersivity increases with the travel distance since plumes encounter heterogeneity of increasing scales. This conclusion is underlain, however, by the assumption of ergodicity. If the plume is viewed as made up from different particles, this means that these particles move independently from a statistical point of view. To satisfy ergodicity the solute body has to be of a much larger extent than heterogeneity scales. Thus, if the latter are increasing for ever and the solute body is finite, ergodicity cannot be obeyed. To demonstrate this thesis we relate to the two-dimensional heterogeneity associated with transmissivity variations in the horizontal plane. First, the effective dispersion coefficient is defined as half the rate of change of the expected value of the solute body second spatial moment relative to its centroid. Subsequently the asymptotic large time limit of dispersivity is evaluated in terms of the logtransmissivity integral scale and of the dimensions of the initial solute body in the direction of mean flow and normal to it. It is shown that for a thin plume aligned with the mean flow the effective dispersivity is zero and the effect of heterogeneity is a slight and finite expansion determined solely by the solute body size. In the case of a solute body transverse to the mean flow the effective dispersivity is different from zero, but has a maximal value which is again dependent on the solute body size and not on the heterogeneity scale. It is concluded that from a theoretical standpoint and for the definition of dispersivity adopted here for non-ergodic conditions, the claim of ever-increasing dispersivity with travel distance is not valid for the scale of heterogeneity analyzed here.

## 1. Introduction

It is generally accepted nowadays that the mechanism of spreading of solutes in groundwater is dominated by the large scale aquifer heterogeneity and mainly by the spatial variability of the hydraulic conductivity. Under certain conditions to be discussed in the sequel, transport may be described with the aid of effective dispersivities (also coined as field scale or macrodispersivities). Furthermore, if the travel distance of a solute body or plume is large compared to the heterogeneity correlation scale, the effective dispersivity tends to a constant value and transport is said to be "Fickian". Then, the effective dispersivity becomes proportional to the heterogeneity scale.

It has been suggested recently in the hydrologic literature (Philip, 1986, Wheatcraft and Tyler, 1988, Neuman, 1990) that in natural formations plumes encounter heterogeneities of ever-increasing scale and therefore the effective dispersivity does not reach a constant value, but it also grows with the travel distance. Furthermore, models to describe this growth have been suggested. These developments have been motivated by a few findings which are examined briefly and critically herein.

(i) *Inspection of outcrops.* Field geologists find sometimes that outcrops of consolidated formations display a kind of self-similar increase of heterogeneity features, as the dimension of the sample is expanded. This qualitative finding has led to the hypothesis that larger and larger scales are encountered as the size of the formation scanned by the plume grows. I find this extrapolation quite questionable for the simple reason that there is a natural upper bound to this type of heterogeneity, namely the formation thickness. Indeed, aquifers are generally shallow, with thickness of the order of tens to hundreds of meters while the horizontal extent is of kilometers to tens of kilometers. While the regional scale of transmissivity variation in the plane may be quite large, the scale of heterogeneity showing up in outcrops is limited as a fraction of the thickness.

(ii) *Summary of field experiments.* Numerous field experiments of transport have been conducted in the past. Unfortunately, in most of them neither the aquifer heterogeneous properties nor the concentration distribution have been monitored in sufficient detail to permit determining the relationship between them. It is only recently that carefully monitored experiments have been conducted at the expense of considerable efforts and it is precisely one of the aims of the present conference to review these tests. At any rate, Gelhar et al (1985) have compiled the various values of dispersivities in the literature, determined by different methods. Their main finding is represented in their Figure 2-6 (also reproduced by Gelhar, 1986) in which the effective longitudinal dispersivity $\alpha_L$ is plotted against the travel distance L. This important work, summarizing findings in tens of aquifers over the world, indicates a trend of increase of $\alpha_L$ with L. One may be tempted to draw a kind of universal curve relating $\alpha_L$ to L through the points of the figure of Gelhar et al, as suggested by Neuman (1990). It seems that such an attempt is speculative for the following few reasons. First, to assume that dispersivities compiled from various aquifers apply to transport in each aquifer separately seems to be quite far-reaching. Secondly, the points in Gelhar et al (1985) display a large spread in the large L zone. Thus, for $L \simeq 10^4$ m, $\alpha_L$ varies between a few meters to hundreds meters. Thirdly and most important, as pointed out by the authors, many of the findings are of low reliability. To illustrate this point I shall discuss briefly the article by Wood (1981), which produced the extreme point of the figure, for $L=10^5$ m. The dispersivity was calibrated for the transport of a natural tracer (Na) in the Aquia aquifer in Southern Maryland. The following assumptions were adopted: (i) the transport process started around $8 \times 10^4$ years ago, (ii) the source location was hypothesized at the zone of contact with sea water, (iii) transport takes place in a hypothetical one-dimensional column, (iv) the flow is steady and uniform with velocity determined from present head and transmissivity measurements, (v) the concentrations were taken as uniform over the depth and measured at a few points and interpolated in the plane and (vi) the solute is assumed to be conservative. Under these assumptions a best fit between the theoretical solution and the measured concentrations is achieved for longitudinal dispersivities between 5600 m and 40000 m (the latter value has not been plotted by Gelhar et al, 1985). The author himself (Wood, 1981) expresses serious reservations about the results for a few reasons: possible solute transfer to the low conductivity formations adjacent to the Aquia aquifer is neglected and exchange sites are assumed to be uniformly distributed "which is very unlikely" and "this fails to separate hydrodynamic dispersion from nonhomogeneous distribution of exchange sites". These question marks and the assumption of 1D steady and uniform flow for a period of around $10^5$ yrs, on one hand, and the huge disparity of inferred $\alpha_L$ values, make them questionable at best.

(iii) *Theoretical considerations.* From a theoretical standpoint it is possible to arrive at the conclusion that dispersivity is increasing with travel distance if unbounded correlation scales are present in the system or even if they are finite, but large compared to the travel distance of the plume.

Such large correlation scales, of the order of $10^4$ m, are the ones encountered at the regional scale, i.e. the ones characterizing the spatial variability of transmissivity (see Sect. 3). Our main criticism about the conclusions based on this argument is that they rest upon the assumption of *ergodicity*, which roughly speaking implies that the solute body is made up from parts which move independently in a statistical sense. In turn, this condition is satisfied if the initial size of the plume $\ell$ is large compared to the heterogeneity scale $I_Y$. I submit that these two requirements, of ever-increasing scale on one hand, and of a large solute body size compared to $I_Y$, on the other, are contradictory and cannot be satisfied at least for "point source" plumes originating from repositories or landfills.

The present paper concentrates solely on the theoretical aspects of the problem. In Sect. 2 we review briefly the theoretical background of the recent literature, to derive the dependence of $\alpha_L$ upon $I_Y$. Sect. 3 reexamines the concept of effective dispersion coefficient in light of our recent study (Dagan, 1990). The original contribution of the present article is in Sect. 4 in which we actually derive the effective dispersivity and its dependence upon both heterogeneity scale $I_Y$ and initial plume size $\ell$ and demonstrate that for large $I_Y/\ell$ the dispersivity is *bounded* and independent of travel distance and it is controlled by $\ell$ rather than $I_Y$.

## 2. Theoretical background.

We review here briefly the Lagrangian approach to transport (for a detailed derivation and discussion of various assumptions see, for instance, Dagan, 1989). We model $Y(\mathbf{x}) = \ln K(\mathbf{x})$ as a stationary random function, i.e. $\langle Y\rangle$ is constant and the covariance $C_Y = \langle Y'(\mathbf{x})\, Y'(\mathbf{y})\rangle$ is a function of $\mathbf{r}=\mathbf{x}-\mathbf{y}$. Here $\mathbf{x}(x_1,x_2)$ is a Cartesian coordinate in the plane, K is the transmissivity, $Y'=Y-\langle Y\rangle$ is the residual and $\langle\rangle$ stands for an ensemble average. With $\sigma_Y^2$ the variance of Y and with $\rho_Y(r)$ the auto-correlation, assumed to be isotropic for simplicity, the linear integral scale is defined by $I_Y= \int_0^\infty \rho_Y(r_1,0)\, dr_1$. For steady flow conditions, for an uniform average flow and for a flow domain of large extent compared to $I_Y$, the Eulerian velocity field $\mathbf{V}(\mathbf{x})$ is also stationary and can be related to Y through Darcy's Law and the continuity equation. We may write, therefore, $\mathbf{V} = \mathbf{U} + \mathbf{u}(\mathbf{x})$, where $\mathbf{U}=\langle\mathbf{V}\rangle$ is constant, whereas the covariance tensor $u_{ij}=\langle u_i(\mathbf{x})u_j(\mathbf{y})\rangle$ is depending on $\mathbf{r}=\mathbf{x}-\mathbf{y}$.

If Y is normal and a first-order approximation in $\sigma_Y^2$ is adopted, the theory shows that $\langle C\rangle$, where $C(\mathbf{x},t)$ is the concentration of a conservative solute, satisfies a transport equation

$$\frac{\partial\langle C\rangle}{\partial t} + U_i \frac{\partial\langle C\rangle}{\partial x_i} = [D_{ij}(t) + D_{d,ij}]\, \frac{\partial^2\langle C\rangle}{\partial x_i \partial x_j} \qquad (i,j = 1,2) \qquad (1)$$

where the index summation convention is adopted here and in the sequel. In (1) $D_{ij}$ is the tensor of effective dispersion coefficients, representing the effect of velocity variation in space, and t is the travel time form the source. The constant $D_{d,ij}$ incorporates in an approximate manner the effect of local heterogeneity, which is characterized by a correlation scale *much smaller* than $I_Y$, the transmissivity integral scale. Besides the various aforementioned assumptions underlying (1), it also implies *ergodicity*, to be discussed later on.

$D_{ij}$ has been determined theoretically (Dagan, 1982, 1984) by using the Lagrangian approach, i.e. Taylor (1921) theory of dispersion by continuous motion. In this approach a solute particle is followed in its motion and its trajectory $\mathbf{x} = \mathbf{X}_t(t,\mathbf{a}) = \mathbf{X}(t,\mathbf{a}) + \mathbf{X}_d$ is defined by

$$\frac{d\mathbf{X}}{dt} = \mathbf{V}(\mathbf{X}_t) \tag{2}$$

where $\mathbf{X}_t$ is the coordinate vector of a particle at time t that was at $\mathbf{x}=\mathbf{a}$ at time t=0 and $d\mathbf{X}_d$ represents a "Brownian motion" or Wiener process such that $\langle \mathbf{X}_d\rangle=0$ and $X_{d,ij} = 2\, D_{d,ij}\, t$. The theory aims at deriving the covariance $X_{ij}(t) = \langle X_i'(t,a)\, X_j'(t,a)\rangle$ where $\mathbf{X}' = \mathbf{X} - \langle \mathbf{X}\rangle$, $\langle \mathbf{X}\rangle = \mathbf{U}t$ and $X_{t,ij} = X_{ij} + 2D_{d,ij}t$. The effective dispersion coefficient is defined by $D_{ij}(t) = (1/2)\, dX_{ij}/dt$ and it can be shown that for a Gaussian $\mathbf{X}$ $\langle C\rangle$ satisfies (1), with $D_{ij}$ given by the preceding relationship. $D_{ij}$ has been computed by adopting a first-order approximation in $\sigma_Y^2$ (Dagan, 1982, 1984). The main result for the longitudinal component, in the direction of mean flow, is that it first increases with t from zero and eventually, for a travel distance L=Ut of a few tens $I_Y$, and for large $Pe = UI_Y/D_d$, it tends to the constant, asymptotic, value

$$D_L = \sigma_Y^2\, U\, I_Y \tag{3}$$

At this limit the transport is said to be Fickian and an effective dispersivity may be defined by $\alpha_L = D_L/U$. The same results has been obtained by a different approach by Gelhar and Axness (1983) and extended for arbitrary Pe by Neuman et al (1987). For the case of large Pe considered here $D_L$ (3) is generally much larger than $D_d$ and the latter, representing pore-scale or local effects, can be neglected. The results are somewhat different for the transverse components of $D_{ij}$, but we shall limit the discussion here to the longitudinal component solely.

An exception to these results is the case of the three-dimensional stratified formations with flow *parallel* to the bedding. If pore-scale dispersion is neglected it can be easily shown (Mercado, 1967) that $D_L=(\sigma_K^2/\langle K\rangle^2)\, U^2\, t$, i.e. $D_L$ increases linearly with time or with the travel distance L = Ut. Matheron and De Marsily (1980) have shown, however, that transverse pore-scale dispersion has a profound effect upon transport and then, for large t $D_L$ grows like $t^{1/2}$ rather than t. By using more refined models of stratification (Hewett, 1986), various powers of t may be obtained. There is no contradiction between these results and (3), since a stratified formation is characterized by an infinite correlation scale in the plane of the layers. An important point set forth by Matheron and De Marsily (1980) is that in the case of a flow tilted with respect to the bedding, $D_L$ tends again to a constant limit and the transport is asymptotically Fickian.

Returning to the result (3) it is worthwhile to mention that the parameter which is the most difficult to estimate is $I_Y$. Indeed, U can be inferred from head measurements and from the average transmissivity while $\sigma_Y^2$ is estimated from a few transmissivity measurements by simple statistical methods. In contrast, $I_Y$ requires inferring the covariance $C_Y$ and its integration, which is an involved process.

An essential point of the analysis is that (3) as well as the results for stratified formation imply ergodicity. Putting it in a simple way, the ensemble mean $X_{ij}$, representing the spread of a particle around its mean position, is equated with the second spatial moment $S_{ij}$ of the solute body in any realization. Thus one writes

$$D_{ij} = \frac{1}{2}\frac{dS_{ij}}{dt} \quad ; \quad S_{ij} = \frac{1}{M}\int n\,(x_i - R_i)\,(x_j - R_j)\,C(\mathbf{x},t)\,d\mathbf{x} \tag{4}$$

where $M = \int nC d\mathbf{x}$ is the total mass of a finite solute body and n is the porosity. In the simple case of an initial constant $C_0$, $M = C_0 V_0$, where $V_0$ is the initial volume (area). The vector **R** is the trajectory of the centroid, i.e.

$$\mathbf{R}(t) = (1/M)\int n\,\mathbf{x}\,C(\mathbf{x},t)\,d\mathbf{x} \tag{5}$$

and under the assumed ergodic conditions, $\mathbf{R} = \langle \mathbf{R} \rangle = \mathbf{R}_0 + \mathbf{U}\,t$.

The exchange between $D_{ij}$ (3) and **U** and the one-realization $(1/2)\ dS_{ij}/dt$ (4) and $d\mathbf{R}/dt$ (5), respectively, can be justified if the scale $\ell$ of $V_0$ is much larger than $I_Y$, so that the solute body may be viewed as made up from many particles which move independently in space. A similar ergodic effect may be achieved by the spreading associated with the component $X_{dij} = 2\ D_{d,ij}\ t$. However, due to the smallness of $D_d$ the required time is exceedingly large and this mechanism cannot be considered to be effective for regional flows.

As we have mentioned in Sect. 1, a few models have been suggested recently (Philip, 1986, Neuman, 1990) to express $D_L$ as an increasing function of L for media of unbounded $I_Y$. It is seen that there is no contradiction of principle between such models and (3), since for an infinite $I_Y$ the conditions which warrant (3) are never achieved. But even if $I_Y$ is finite but large, (3) shows that the effective dispersivity may become very large. We discuss next the validity of this conclusion for the stratified aquifer and for regional scale heterogeneity separately.

(i) *Stratified aquifer.* As mentioned above, for a perfectly stratified aquifer and for a solute body of large transverse dimension compared to the conductivity correlation scale (normal to layering), $D_L$ increases like $L^p$, where p=1 in absence of pore-scale dispersion, while p tends to 1/2 at large L if $D_d$ is accounted for. However, the prerequisite is that stratification is perfect, i.e. the layers are planar and parallel, and each layer is homogeneous in its plane. Though some formations apparently display such a structure, this does not seem to be a universal property. It is emphasized that the presence of the same sequence of layers in a few wells does not warrant perfect layering, since displacements along vertical or oblique shearing planes may be present among wells. Such events or bending of layers or conductivity variations within the layers are enough to disqualify the formation as perfectly stratified. Hence, the validation of perfect layering requires a detailed survey of conductivity measurements in order to find out whether full correlation prevails along the strata planes. In the few aquifers investigated in detail in the last few years, e.g. the Borden Site (Sudicky, 1986), this was not the case. While strong anisotropy of $C_Y$ was present, the horizontal correlation scale was finite and relatively small. A second prerequisite of the model, besides perfect stratification, is that the flow is parallel to the layers. As mentioned above, any tilt of the mean flow, caused for instance by natural recharge, leads to results similar to (3), with $I_Y$ the logconductivity integral scale in a direction parallel to the mean flow (Matheron and De Marsily, 1980). Concluding this discussion, it does not seem that the claim of universality of perfect stratification, to justify the permanent growth of $D_L$ with L, is tenable

(ii) *Regional scale heterogeneity.* As mentioned before, it manifests in variations of the transmissivity in the horizontal plane, in contrast with local variations of conductivity which are of a three-dimensional nature and of a scale smaller than the thickness. Delhomme (1979) and Hoeksema and Kitanidis (1984) have analyzed transmissivity data of many aquifers and found that they are approximately lognormal and of integral scales of the order of $10^3$ to $10^4$ meters. Unlike stratification, Y is generally isotropic in the plane and its variation causes streamlines to bend and velocities to vary from small values in regions of low transmissivity to high ones in conductive zones. This type of heterogeneity may lead to the growth of the theoretical $D_L$ with L for a long period of motion, since the travel distance maybe of the order of $I_Y$. In spite of the apparent likeliness of this mechanism, I claim that the other prerequisite for adopting $D_{ij}$ (3) as the measure of spread (4), namely ergodicity, is generally not obeyed. Indeed, the requirement is that $\ell$, the length scale of the initial volume $V_0$, is much larger than $I_Y$, and this condition is generally not obeyed for point sources. In the sequel we proceed with developing the quantitative model which supports this claim. More precisely, we shall investigate the relationship between $D_L$ as defined by (4) and the integral scale $I_Y$ and demonstrate that as the latter grows, $D_L$ is controlled by $\ell$, the length scale of $V_0$, and not by $I_Y$ anymore.

3. Effective dispersion coefficient in non-ergodic transport.

We consider two-dimensional flow and transport. We assume that the formation extent is large enough to allow for the identification of $\langle Y\rangle$ and $C_Y$, the mean and covariance of the log-transmissivity. A solute body is injected in an area $V_0$, say a rectangle of dimensions $\ell_1$, $\ell_2$ (Fig. 1). As a result of convective transport the body moves along the streamlines (Fig. 1) and due to heterogeneity it also spreads. Both $\ell_1$ and $\ell_2$ are not necessarily small compared to $I_Y$, the integral scale, and the concentration distribution is generally not Gaussian.

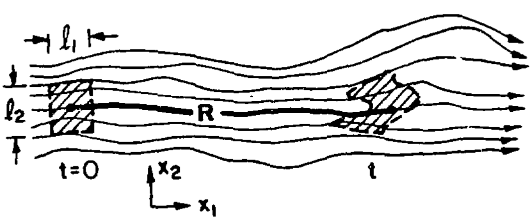


Fig. 1. Sketch of motion of a solute body in steady flow.

The first question is how to define the EDC, effective dispersion coefficient, in this case. The approach proposed by Dagan (1990) is to define first $\overline{D}_{ij}$, the actual dispersion coefficients, by Eq. (4) or in words as half the rate of change of the second spatial moment of the solute body with respect to its centroid. However, since Y and the associated velocity field V=U+u are known only statistically, we cannot predict neither **R** (5) nor $S_{ij}$ (4), which are random variables. What we can do is to estimate these variables, the best estimate being the expected value $\langle \mathbf{R} \rangle$ and $\langle S_{ij} \rangle$. Assuming uniform average flow it follows that $d\langle \mathbf{R} \rangle/dt = \mathbf{U}$. The EDC are defined (Dagan, 1990) by $D_{ij}(t,\ell) = (1/2)\ d\langle S_{ij} \rangle/dt$, i.e. $\underline{D}_{ij}=\langle \overline{D}_{ij} \rangle$. Under ergodic conditions, achieved from a theoretical standpoint for $\ell \to \infty$, we have $D_{ij} \simeq D_{ij}(t,\infty) = \mathcal{D}_{ij}(t)$, where $\mathcal{D}_{ij}=(1/2)\ dX_{ij}/dt$ is associated with one particle ensemble of trajectories (see Sect. 2). However, if $\ell/I_Y$ is not infinite, $D_{ij}$ is given by the following fundamental relationship (Kitanidis, 1988, Dagan, 1990)

$$D_{ij}(t,\ell) = \frac{1}{2}\left[ \frac{dX_{ij}(t)}{dt} - \frac{dR_{ij}(t,\ell)}{dt} \right] \quad \text{i.e.} \quad D_{ij} = \mathcal{D}_{ij} - \frac{1}{2}\frac{dR_{ij}}{dt} \tag{6}$$

where $R_{ij}$ is the covariance of **R**, the trajectory of the centroid. Its appearance in (6) makes $D_{ij}$ different from $\mathcal{D}_{ij}$ and the reason is quite simple: in the ergodic case it is assumed that $\mathbf{R} \simeq \langle \mathbf{R} \rangle$ and $R_{ij} \simeq 0$, i.e. the centroid moves in each realization along the mean path. In non-ergodic transport **R** itself is random and differs from realization to realization (Fig. 1). In other words the difference stems from the fact that $S_{ij}$ (5) is taken with respect to the actual centroid and not to its ensemble mean.

$R_{ij}$ has been related to the two particles trajectories covariance by Dagan (1990, Eq. 10) and the relationship stemming from (5) is

$$R_{ij} = \frac{1}{V_0^2} \int_{V_0} \int_{V_0} X_{ij}(t,\mathbf{b})\ d\mathbf{a}'\ d\mathbf{a}'' \qquad \mathbf{b}=\mathbf{a}'-\mathbf{a}'' \tag{7}$$

where $X_{ij}(t,\mathbf{a}',\mathbf{a}'') = \langle X_i'(t,\mathbf{a}')\ X_j'(t,\mathbf{a}'') \rangle$ is the covariance of the displacements of two particles originating at $\mathbf{x}=\mathbf{a}'$ and $\mathbf{x}=\mathbf{a}''$ at t=0, respectively. To simplify matters we have assumed that the initial concentration $C_0$ is constant and under the assumed stationarity of the velocity field $X_{ij}$ is a function of $\mathbf{b}=\mathbf{a}'-\mathbf{a}''$. It is seen that the previously employed $X_{ij}(t)$ for one particle is the particular case of $X_{ij}(t,0)$. $X_{ij}$ is related to the velocity field by the definition of **X** (2) and by adopting a first-order approximation of the velocity covariance (Dagan, 1984) as follows

$$X_{ij}(t,\mathbf{b}) = \int_0^t \int_0^t u_{ij}[U(t'-t'') + \mathbf{b}]\ dt'\ dt'' \tag{8}$$

and in particular

$$X_{ij}(t) = X_{ij}(t,0) = \int_0^t \int_0^t u_{ij}[U(t'-t'')]\ dt'\ dt'' = 2\int_0^t (t-t')\ u_{ij}[Ut']\ dt' \tag{9}$$

Substituting (8) and (9), into (6) and (7), we obtain the following relationship between the EDC and the velocity field

$$D_{ij}(t,\ell) = \frac{1}{V_0^2}\int_{V_0}\int_{V_0}\int_0^t [u_{ij}(Ut') - \frac{1}{2}u_{ij}(Ut'+b) - \frac{1}{2}u_{ij}(Ut'-b)]\, dt'da'da'' \tag{10}$$

Our last step is to relate the velocity covariances to that of the logtransmissivity. We refer now to the longitudinal component only and take, without loss of generality, U(U,0). The first-order approximation of $u_{11}$ is given (Dagan, 1984) by

$$u_{11}(r_1,r_2) = U^2\,[C_Y(r_1,r_2) + 2\,\frac{\partial C_{YH}(r_1,r_2)}{\partial r_1} + \frac{\partial^2\gamma_H(r_1,r_2)}{\partial r_1^2}] \tag{11}$$

where $C_{YH}(r) = \langle Y'(x)H'(y)\rangle$ and $\gamma_H(r) = (1/2)\,\langle[H'(x)-H'(y)]^2\rangle$ are the logtransmissivity-water head crosscovariance and water head variogram, respectively. To further simplify the computations, we are going to evaluate the asymptotic $D_L=D_{11}$ for large travel time t. In other words we seek the value of the EDC for a finite solute body and non-ergodic transport to replace (3), which is valid for an infinite solute body and ergodic conditions. It is seen that integration with respect to t′ in (10) is equivalent with integration with respect to $r_1$ in (11) since $r_1 \simeq Ut'$. However, it can be shown (e.g. Dagan, 1989) that $C_{YH}=0$ and $\partial\gamma/\partial r_1=0$ for $r_1=0$ and $r_1=\infty$. Consequently, substitution of (11) in (10) and integrating to t=∞ yields the final result

$$\alpha_L = D_{11}(\infty,\ell)/U = \frac{\sigma_Y^2}{V_0^2}\int_{V_0}\int_{V_0}\Big(-C_{YH}(b_1,b_2) - \frac{\partial\gamma_H(b_1,b_2)}{\partial r_1} +$$

$$+\int_0^\infty [\rho_Y(r_1,0) - \frac{1}{2}\rho_Y(r_1+b_1,b_2) - \frac{1}{2}\rho_Y(r_1-b_1,b_2)]\,dr_1\Big)da'da'' \quad (b=a'-a'') \tag{12}$$

Eq. (12) concludes the derivation of the effective longitudinal dispersivity in non-ergodic transport of a solute body which initially occupies the area $V_0$. In the next section we evaluate $\alpha_L$ in a few specific cases to demonstrate our main thesis, namely that as $I_Y$ increases $\alpha_L$ remains bounded and controlled by $\ell$, the length scale of the initial solute body.

## 4. Computation of effective longitudinal dispersivity.

The computation of $\alpha_L$ (12) for 2D flow and an initially rectangular $V_0$ involves three quadratures. To further simplify matters we examine separately the impact of each of the two dimensions $\ell_1$ and $\ell_2$, where $x_1$ is the direction of mean flow.

(i) *Thin, streamline aligned, solute body*. We assume that $\ell_2=0$, i.e. the solute body is very thin and it lies along the mean flow direction. In our first-order approximation in which the actual path is replaced by the mean trajectory (see Eqs. 8,9), this is equivalent to the solute body lying in a thin streamtube (Fig. 2a). Hence, with $b_2=0$ and $V_0=\ell_1$ and with integration in the $x_1$ direction solely, $\alpha_L$ (12) becomes

$$\alpha_L = \frac{2}{U^2\ell_1^2}\int_0^{\ell_1}\int_0^{\infty}(\ell_1-b_1)\,[u_{11}(r_1,0) - \frac{1}{2}\,u_{11}(r_1+b_1,0) - \frac{1}{2}\,u_{11}(r_1-b_1,0)]\,dr_1\,db_1 \qquad (13)$$

It is easy to ascertain by changes of variables that the integral over $r_1$ is equal to zero if $u_{11}(r)=u_{11}(-r)$, which is always the case by the definition of $u_{11}$. Hence, we have arrived at the striking result that for a "snake-like" solute body $\alpha_L=0$ and the body does not disperse at all asymptotically, *no matter how large the transmissivity integral scale is.* Hence, transport is nonergodic for such a solute body for any $\ell_1$. This result is obvious in the case of a stratified formation. Indeed, with neglect of pore-scale dispersion, the solute body translates with the velocity pertinent to the particular layer in which it lies. Hence, it does not disperse not only in the mean, but in each realization. However, from Eq. (6) with $D_{11}=0$ it is immediately seen that $dX_{11}/dt$ is balanced by $-dR_{11}/dt$, i.e. heterogeneity manifests in the uncertainty of the centroid position rather than in dispersion. The cases of 2D or 3D flow is more involved, but essentially similar. To grasp these cases we have represented in Fig. 2b in a qualitative manner the distance $s_{le}$ and $s_{te}$ covered by the leading edge and trailing edge, respectively, as functions of time. By virtue of the steadiness of the velocity field, the trailing edge follows exactly the leading one at a time lag T, where T is the time required to move by $\ell_1$. It can be shown that for $t>T$ this property leads to the constancy of $\langle[s_{le}(t)-s_{te}(t)]^2\rangle$ and furthermore to that of $S_L=S_{11}$ in the first-order approximation adopted here in which $T=\ell_1/U$.

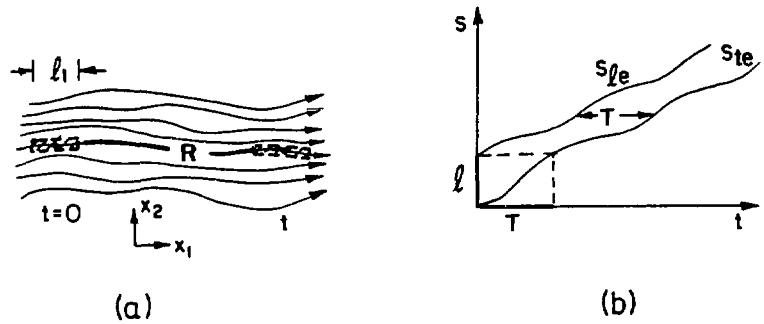


Fig. 2 Sketch of (a) the motion of a thin solute body and (b) the displacements of the leading and trailing edges.

It is seen that there are two major differences between the stratified formation and the one of 2D or 3D structure: (i) while for the stratified one $\overline{D}_L=0$ in each realization, it is only its mean $D_L$ which tends to zero in the general case and (ii) while $\overline{D}_L=0$ from t=0 in the stratified case, $D_L$ tends to zero only for sufficiently large $t>\ell_1/U$ in the multidimensional case. It follows that the second spatial moment $S_{11}(t)$ (4) grows from its initial value $S_{11}(0)=(1/12)\ell_1^2$ to a constant, asymptotic, value. The latter can be computed from its definition (4) as follows

$$\langle S_{11}(t)\rangle = S_{11}(0) + 2\int_0^t D_{11}(t')\,dt' \qquad (14)$$

By using the definition (10) of $D_{11}$ and after a change of variables it can be shown that the final result becomes

$$\langle S_{11}(\infty)\rangle - S_{11}(0) = \frac{2}{\ell_1^2}\int^{\ell_1}(\ell_1 - b_1)\,X_{11}(b_1/U)\,db_1 \qquad (15)$$

where $X_{11}(t)$ (9) is the one particle trajectory covariance. To illustrate the results we have computed $\langle S_{11}\rangle$ for the exponential $\rho_Y = \exp(-r/I_Y)$, for which $X_{11}$ has been evaluated in a close form previously (Dagan, 1982 or Dagan, 1989 Eq. 4.7.2). The results are presented in a dimensionless form in Fig. 3 after integrating numerically in (15). It is seen that the mean expansion of the solute body as measured by the second spatial moment is quite modest and is controlled entirely by its initial length when $I_Y$ becomes large.

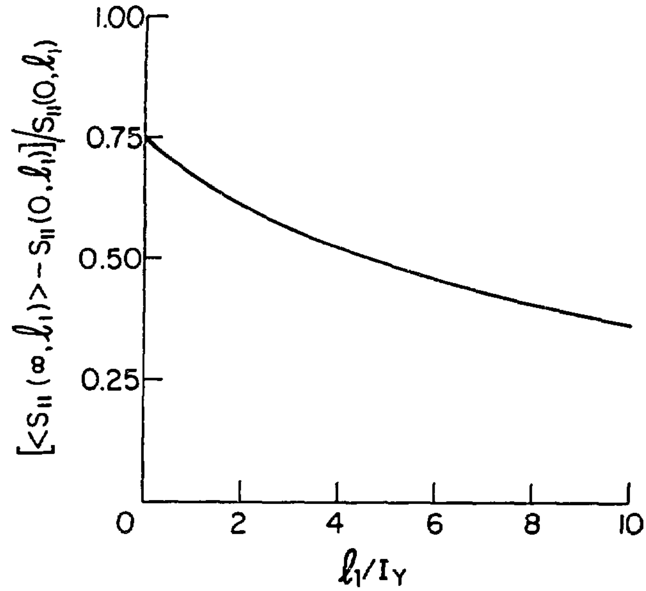


Fig. 3. The dependence of the expected value of the spatial second order moment of a thin solute body upon the ratio $\ell_1/I_Y$.

In summary we have found that convective transport is not ergodic for a thin solute body aligned with a streamline of the steady velocity field. Its second order spatial moment expands from its initial value to an asymptotic one which is reached for $t > \ell_1/U$ and remains constant. The expansion is relatively small and is controlled by $\ell_1$. In particular it tends to a constant for $I_Y \to \infty$. Hence, neither the effective dispersivity nor the second-order moment increase indefinitely with the travel distance.

(ii) *Thin, normal to the main flow direction, solute body.* We examine now the dependence of the effective dispersivity upon $\ell_2$, the transverse dimension of the solute body, which for simplicity is assumed to be of zero thickness in the mean flow direction (Fig. 4)

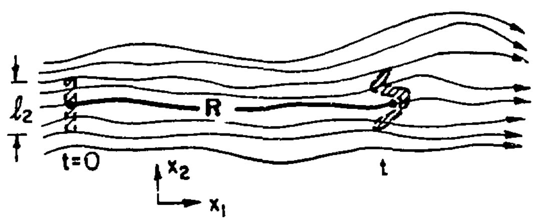


Fig. 4 Sketch of a thin body normal to the mean flow direction.

Unlike the previous case, $D_{11}$ and the associated $\alpha_L$, is now different from zero due to the shearing effect of the velocity field. Hence, there is a fundamental difference between the impact of the two dimensions, $\ell_1$ and $\ell_2$, upon ergodicity, which can be ensured only by a sufficiently large $\ell_2$. We proceed now with the computation of $\alpha_L$ (12). Because of the antisymmetry of $C_{YH}$ and of the symmetry oh $\gamma_H$, $C_{YH}(0,b_2)=0$ and $\partial\gamma_H(0,b_2)/\partial r_1=0$. Furthermore, with $b_1=0$ and $V_0=\ell_2$, $\alpha_L$ (12) becomes

$$\alpha_L = \sigma_Y^2 \left[\int_0^\infty \rho_Y(r_1,0)\, dr_1 - \frac{2}{\ell_1^2}\int_0^\infty\int_0^{\ell_2} (\ell_2-b_2)\, \rho_Y(r_1,b_2)\, db_2\, dr_1\right] \tag{16}$$

Since $\int\rho_Y(r_1,0)\, dr_1 = I_Y$, Eq. (16) reduces to

$$\alpha_L/(\sigma_Y^2\ell_2) = \frac{1}{\ell_2'}\left[1 - \frac{2}{(\ell_2')^2}\int_0^\infty\int_0^{\ell_2'} (\ell_2' - b_2')\, \rho_Y(r_1',b_2')\, db_2'\, dr_1'\right] \tag{17}$$

where $\ell_2' = \ell_2/I_Y$, $r_1' = r_1/I_Y$ and $b_2' = b_2/I_Y$.

It is easy to derive the limits of $\alpha_L/(\sigma_Y^2\ell_2)$ for $\ell_2' \to \infty$ and $\ell_2' \to 0$ and to show that in both cases it tends to zero. The first limit is the ergodic one for which $\alpha_L$ is given by (3), whereas the second one corresponds to a solute body which behaves like an indivisible particle. Consequently,

$\alpha_L/(\sigma_Y^2 \ell_2)$ has a maximum which does not depend on $I_Y$. To substantiate this picture we have computed $\alpha_L/(\sigma_Y^2 \ell_2)$ for two types of autocorrelations : exponential $\rho_Y = \exp(-r/I_Y)$ and Gaussian $\rho_Y = \exp(-\pi r^2/4I_Y^2)$. In both cases $\alpha_L/(\sigma_Y^2 \ell_2)$ could be obtained in a closed form as follows

$$\alpha_L/(\sigma_Y^2 \ell_2) = \frac{1}{\ell_2'} \{1 - \pi[K_1(\ell_2')\, L_0(\ell_2') + L_1(\ell_2')\, K_0(\ell_2')] - 2K_2(\ell_2') + 4/\ell_2'^2\} \tag{18}$$

for the exponential covariance, with $L_0, L_1$ standing for the modified Struve functions (Abramowitz and Stegun, 1965) and $K_i$ for modified Bessel functions. For the Gaussian covariance we obtain

$$\alpha_L/(\sigma_Y^2 \ell_2) = \frac{1}{\ell_2'} \{1 - \frac{2}{\ell_2'} \operatorname{erf}(\frac{\sqrt{\pi}\ell_2'}{2}) + \frac{4}{\pi \ell_2'^2} [1 - \exp(-\frac{\pi \ell_2'^2}{4})]\} \tag{19}$$

We have represented in Fig. 5 the dependence of $\alpha_L/(\sigma_Y^2 \ell_2)$ (18,19) upon $I_Y/\ell_2$. The behavior discussed before in a qualitative manner is now supported by concrete examples. The striking result is that $\alpha_L$ is bounded from above by a value around *0.15* $\sigma_Y^2 \ell_2$. *Hence, no matter how* large $I_Y$ is, the effective dispersivity is bounded and does not increase with travel distance beyond this upper limit.

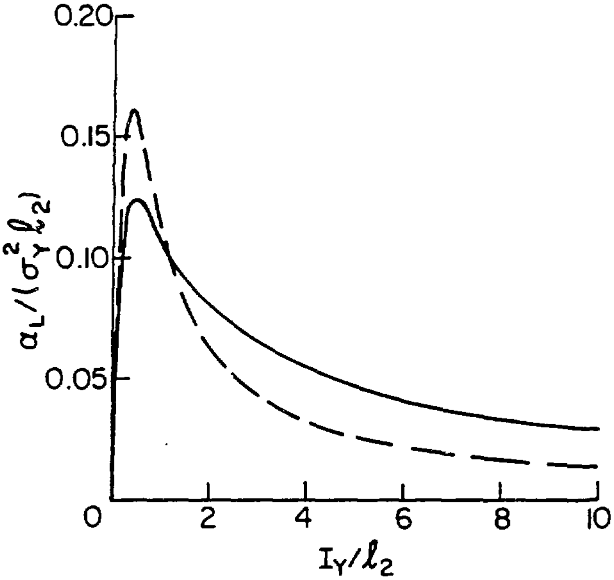


Fig. 5. The dependence of the dimensionless effective dispersivity on the ratio between the log-transmissivity integral scale and the solute body initial extent (full line Eq. 18 and dashed line Eq. 19).

To emphasize this point we have also represented in Fig. 6 the ratio $\alpha_L/(\sigma_Y^2 I_Y)$ as function of $I_Y/\ell_2$. At the ergodic limit $I_Y/\ell_2 \to 0$ this ratio is equal to unity (Eq. 3) but it drops quickly as the integral scale increases while $\ell_2$ is kept fixed. Conversely, we may interpret the result by figuring out a fixed $I_Y$ and a body of increasing size $\ell_2$. The ergodic limit is attained only for $\ell_2$ of the order of tens of integral scales.

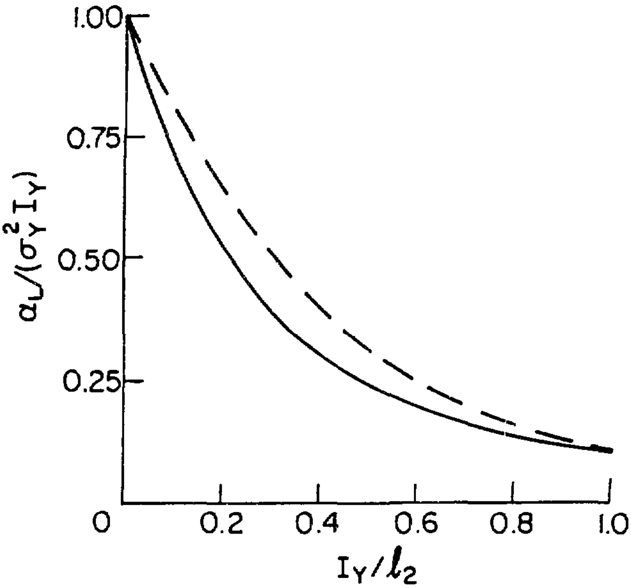


Fig. 6. The dependence of the dimensionless effective dispersivity on the ratio between the log-transmissivity integral scale and the solute body initial extent (full line Eq. 18 and dashed line Eq. 19).

We could derive the effective dispersivity for a rectangular body of finite $\ell_1$ and $\ell_2$ by using the general formulation of Eq. (12), albeit at the expense of more involved computations. It is believed that the conclusions are similar to those drawn in the partial cases.

## 5. Summary and conclusions.

In the present study we have examined transport in formations of a two-dimensional heterogeneous structure, representing for instance the spatial variability of aquifer transmissivity in the horizontal plane. Since the logtransmissivity correlation scale has been found to be of the order of $10^3$-$10^4$ meters, the theory predicts large values of the effective dispersivity if *ergodicity is obeyed*. We have demonstrated that for solute bodies or plumes of finite size, as it is the usual case, the ergodic requirements are not fulfilled. Furthermore, the effective longitudinal dispersivity is controlled by the initial size *transverse* to the mean flow rather than by $I_Y$, no matter *how large* is the latter. Ergodicity may be attained only if the initial transverse size of the solute body is large enough, say a few tens of logtransmissivity integral scales.

The main conclusion is that for this type of two-dimensional heterogeneity and for a large or unbounded integral scale, the claim that the effective dispersivity is a continuously *increasing* function of the travel distance is not valid. The main reason is that it is based on an analysis which takes ergodicity for granted, which is not necessarily the case.

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