

Lagrangian-Eulerian statistics and numerical modeling of transport in homogeneous random media

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Abstract

Relationships between statistical properties of Eulerian velocity (in a fixed reference frame) and Lagrangian velocity (i.e. the velocity of marked molecules) are examined for the case of diffusion in velocity fields described by random space functions. Assuming a constant diffusion coefficient and a divergence-free homogeneous Eulerian random field, we give simple proofs of the statistical homogeneity of the Lagrangian velocity field and of the equality between the Lagrangian and Eulerian one-point marginal probability densities. Further, we analyze numerical simulations using velocity fields generated with a classical randomization method. The numerical Eulerian velocity is homogeneous within a reasonably small confidence interval. Surprisingly, at early times the Lagrangian mean velocity still depends on the starting point of the trajectory and shows small oscillations which, however, are well beyond the confidence interval for the Eulerian mean velocity. We demonstrate that the lack of strict statistical homogeneity of the Lagrangian velocity induces a dependence of the second moment of the ensemble averaged concentration on the initial concentration distribution. At large times, the simulated Lagrangian mean velocity tends to the Eulerian mean velocity and the second moment of the mean concentration loses the memory of the initial conditions.

1 Introduction

We consider the diffusive transport of solute molecules in a spatially heterogeneous fluid flow. The flow velocity is modeled as a random space function $\mathbf{V}(\mathbf{x})$.

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For a given realization $\mathbf{V}(\mathbf{x})$ of a time independent random velocity field and a constant diffusion coefficient D , the trajectories of the local advection-dispersion process starting at $t = t_0$ from $\mathbf{X}_0$ are the solutions of the integral Itô equation

$$X_l(t) = X_{0l} + \int_{t_0}^t V_l(\mathbf{X}(t')) dt' + \int_{t_0}^t dW_l(t'), \quad (1)$$

where $l = 1, 2, 3$ and $W_l(t) = \int_{t_0}^t dW_l(t')$ is a stochastic integral which defines a Wiener process with the properties $\langle W_l \rangle_D = 0$, $\langle W_l \rangle_D^2 = 2D(t - t_0)$.

The velocity $\mathbf{V}(\mathbf{x})$ described in a fixed reference frame is referred to as “Eulerian velocity”, while the velocity sampled on the trajectory of the molecule $\mathbf{V}(\mathbf{X}(t))$ is the “Lagrangian velocity”. The latter consists of observations of the random field $\mathbf{V}(\mathbf{x})$ at random locations $\mathbf{X}(t)$ which depend on $\mathbf{V}(\mathbf{x})$ [Zirbel, 2001]. In this context, “Lagrangian” only refers to statistics of such observations and has nothing to do with the Lagrangian description, as for instance that used in the case $D = 0$. The latter is based on a one-to-one change of coordinates between $\mathbf{X}(t)$ and $\mathbf{X}_0$, which does not exist in the case $D > 0$ because the trajectories of the Itô process (1) are not differentiable.

In the following, the random Eulerian velocity $\mathbf{V}(\mathbf{x})$ will be stationary, statistical homogeneous, i.e.

$$\text{Prob}\{\mathbf{V}(\mathbf{x}_1) \in B_1 \cdots \mathbf{V}(\mathbf{x}_n) \in B_n\} = \text{Prob}\{\mathbf{V}(\mathbf{x}_1 + \mathbf{L}) \in B_1, \cdots \mathbf{V}(\mathbf{x}_n + \mathbf{L}) \in B_n\}$$

for arbitrary space translations $\mathbf{L}$ and Lebesgue-measurable sets $B_1, \cdots, B_n \in \mathbb{R}^3$, and incompressible, $\text{div} \mathbf{V}(\mathbf{x}) = 0$.

The transport in random velocity fields depends on diffusion (D), initial distribution of molecules (X_0), and velocity realization (V). Various averages to be used in the following will be labeled with the corresponding subscripts, e.g. $\langle \cdot \rangle_D$, $\langle \cdot \rangle_{X_0}$, $\langle \cdot \rangle_V$, $\langle \cdot \rangle_{D, X_0 V}$, a.s.o.

2 Lagrangian homogeneity

Since the trajectory (1) has an intricate nonlinear dependence on velocity, the probability distribution for Lagrangian velocity depends on the entire infinite-dimensional probability distribution on the function space of all possible Eulerian velocity fields (see also [Monin and Yaglom, 1971]). Even when this functional probability can be constructed (for instance in the non-diffusive case $D = 0$), the functional integration can be carried out only in particular simple cases for which the results can be obtained directly [Lumley, 1962a].

Some information can be nevertheless obtained under the assumption that the velocity realizations are analytical space functions. In the following, we extend the argument of [Lumley, 1962b] to the case $D > 0$ and prove the statistical homogeneity of the Lagrangian velocity for analytical Eulerian velocity realizations.

By the Itô formula the velocity on the trajectory (1) can be expressed as

$$V_l(\mathbf{X}(t)) = V_l(\mathbf{X}(t_0)) + \sum_{m=1}^3 \left\{ \int_{t_0}^t [V_m(\mathbf{X}(t')) \partial_{x_m} + D \partial_{x_m}^2] V_l(\mathbf{X}(t')) dt' + \int_{t_0}^t \partial_{x_m} V_l(\mathbf{X}(t')) dW_l(t') \right\} \quad (2)$$

Strongly convergent Itô-Taylor expansions can be obtained by iterations of (2) [Kloeden and Platen, 1995, Chap. 5]. Since the average (with respect to D) of the multiple Itô integral vanishes if it contains at least one integration with respect to the Wiener process [Kloeden and Platen, 1995, Lemma 5.7.1], the average velocity for given realization of the velocity field and deterministic initial position $\mathbf{x}_0 = \mathbf{X}(t_0)$ is given by

$$\langle V_l(\mathbf{X}(t)) \rangle_D = V_l(\mathbf{x}_0) + \sum_{n=1}^{\infty} [\mathbf{A}^n V_l](\mathbf{x}_0) (t - t_0)^n, \quad (3)$$

where $\mathbf{A}$ is an operator defined by $\mathbf{A} = \sum_{m=1}^3 [V_m(\mathbf{X}(t)) \partial_{x_m} + D \partial_{x_m}^2]$.

If the fields $\mathbf{A}^n V_l$ are statistically homogeneous, then the ensemble average Lagrangian velocity $\langle \langle V_l(\mathbf{X}(t; \mathbf{x}_0, t_0)) \rangle_D \rangle_V$ is statistically homogeneous as well (i.e. independent of $\mathbf{x}_0$).

For statistical homogeneous Eulerian fields $\mathbf{V}(\mathbf{x})$, the statistical homogeneity of $\mathbf{A}^n V_l$ can be shown by using the Fourier representation of the velocity and the convolution theorem. But this does not yet imply the equality of Lagrangian and Eulerian mean velocity. This can be proved under supplementary conditions, which ensure the equality of the Lagrangian and Eulerian one-point distributions (see next Section). However, for analytical forms of V_l like those used in most of randomization methods, both the Lagrangian stationarity and the equality of Lagrangian and Eulerian means can be shown directly. Let us consider, the 1-dimensional problem and the velocity field $\mathbf{V}(\mathbf{x}) = \mathbf{U} + \mathbf{v}(\mathbf{x})$,

$$\mathbf{v}(\mathbf{x}) = \mathbf{a}(\mathbf{k}) \sin(\mathbf{k}\mathbf{x} + \varphi), \quad (4)$$

where $\mathbf{U}$ is a constant which represents the Eulerian mean velocity, $\mathbf{k}$ is a Gaussian distributed random variable, $\mathbf{a}(\mathbf{k})$ is a random amplitude chosen

under the restriction of incompressibility, and φ is a random phase uniformly distributed in $[0, 2\pi]$. The Kraichnan generator used by simulations presented in this paper is just a superposition of many periodic modes (4).

For the sake of simplicity, we analyze in the following only the 1-dimensional case. The ensemble average velocity is obtained by averaging with respect to the distribution of the random numbers k and φ : $\langle v(x) \rangle_V = \langle v(x) \rangle_{k\varphi}$. The latter average is given by $\langle v(x) \rangle_\varphi = \frac{1}{2\pi} \int_0^{2\pi} a \sin(kx + \varphi) d\varphi = 0$ for all x . The first two coefficients of the series in (3) are obtained by successive applications of the operator $A = [v(X(t))\partial_x + D\partial_x^2]$ to (4),

$$\begin{aligned} Av &= a^2 k \sin(kx + \varphi) \cos(kx + \varphi) - ak^2 \sin(kx + \varphi) \\ A^2 v &= a^3 k^2 [\sin(kx + \varphi) \cos^2(kx + \varphi) - \sin^3(kx + \varphi)] \\ &\quad - 5a^2 k \sin(kx + \varphi) \cos(kx + \varphi) + ak^3 \sin(kx + \varphi), \end{aligned}$$

and both have the mean zero: $\langle Av \rangle_\varphi = 0$, $\langle A^2 v \rangle_\varphi = 0$. By mathematical induction, one shows that for all orders n the coefficients $A^n v$ are composed by terms of the form $\sin(x+\varphi)^\alpha \cos(x+\varphi)^\beta$, where the exponents α and β are either both odd or α odd and β even. It follows that $\langle A^n v \rangle_\varphi = 0$ for all n . By inserting this result in (3) we obtain: $\langle \langle V(X(t)) \rangle_D \rangle_V = \langle \langle \langle V(X(t)) \rangle_D \rangle_\varphi \rangle_k = U = \langle V(x) \rangle_V$. We note that this proof of the equality of Eulerian and Lagrangian mean velocity did not use the incompressibility property, accounted for by the random variable $a(k)$.

3 Lagrangian and Eulerian velocity fields with the same one-point statistics

Lumley [1962b] proved, in the purely advective case $D = 0$, that for analytical velocity realizations $V(x)$ of an incompressible homogeneous random field the Lagrangian velocity is statistically homogeneous, has stationary time autocorrelation and the same one-point marginal distribution as the Eulerian field. Port and Stone [1976] supplied a different proof for these properties and extended them to the case $D > 0$, by relaxing the analyticity requirement to the continuity of the velocity and of its first spatial derivatives. The issue of Lagrangian-Eulerian relationship was formulated in a unified framework and complemented with new results, in terms of random mappings on the physical space (which generalize incompressibility), by Zirbel [2001]. The state of the art and applications in turbulence are presented in [Kramer and Majda, 2007]. In the following we shall use the general result for the case $D = 0$ stated by Proposition 4.2 of [Kramer and Majda, 2007]:

Suppose the Eulerian velocity field $V(x, t)$ is incompressible, statistically homogenous and stationary, and continuously differentiable. Then:

a. The Lagrangian velocity field $V(X(x, t), t)$ is statistically homogenous for any fixed t and statistically stationary for any fixed value of x .

b. The one-point probability distributions of the Eulerian and Lagrangian velocity fields coincide.

Note that while the one-point probability distributions for the Eulerian and Lagrangian velocity fields coincide, the multi-point probability distributions will generally differ [Lumley, 1962b; Zirbel, 2001; Kramer and Majda, 2007].

We show in the following how the above proposition can be used to prove that the same conclusions hold for the case $D > 0$. The idea is to fix a realization of the Wiener process and to define an Eulerian field which satisfies the conditions of the proposition (P. R. Kramer, unpublished manuscript, 2007). Here we apply this principle to the simpler case of one-dimensional diffusion in a time independent velocity field.

We consider the 1-dimensional integral form of the Itô equation (1) and the deterministic initial condition $X(0) = x_0$,

$$X(t) = x_0 + \int_0^t V(X(t'))dt' + W(t), \quad (5)$$

for a fixed realization $W(t) = \int_0^t dW(t')$ of the Wiener process starting from $W(0) = 0$, and we assume conditions for the existence and uniqueness of the solution. We define the function $Y(t) = X(t) - W(t)$, which according to (5) verifies the equation

$$Y(t) = x_0 + \int_0^t V(Y(t') + W(t'))dt'. \quad (6)$$

Inspired by (6), we define a new velocity field $U(y, t) = V(y + W(t))$, for arbitrary y . The random field U is homogeneous and incompressible because it inherits these properties of V . Furthermore, because it depends on time only via the Wiener process with stationary increments $W(t) = W(t) - W(0)$, and V is statistically homogenous, U is also a stationary random field. Using (6), we find that $Y(t)$ verifies the equation for the trajectory of the new field U ,

$$Y(t) = x_0 + \int_0^t U(Y(t'), t')dt', \quad (7)$$

with the initial condition $Y(t = 0) = x_0$. For a fixed realization of the Wiener process, $U(Y(t), t)$ is the Lagrangian velocity observed at the point $(Y(t), t)$

which is determined by the incompressible, statistically homogenous and stationary Eulerian field $U(y, t)$. Then, the proposition for the case $D = 0$ applies and the Lagrangian and Eulerian fields have the same one-point statistics. Using the definition of U , one obtains $U(Y(t), t) = V(Y(t) + W(t)) = V(X(t))$, from where we conclude that the Lagrangian field $V(X(t))$ has the same one-point statistics as the Eulerian field $U(x_0, t = 0) = V(x_0)$, is homogeneous, and is stationary.

Furthermore, the time-independence of the Eulerian field, the equality of one-point Lagrangian and Eulerian probability distributions, and a Taylor expansion in time, for the same fixed realization $W(t)$ of the Wiener process in (5), imply the stationarity of the Lagrangian auto-correlation $\langle V(X(t))V(X(t) + \tau) \rangle_V$ [see e.g., Lumley, 1962b, p. 21]. Since the coefficients of the Taylor expansion are Eulerian averages and the Eulerian random field is homogeneous, the Lagrangian auto-correlation is also independent of initial position x_0 .

An alternative proof of these results, using random mappings, is outlined in [Zirbel, 2001, Remark 6.7]. A proof which is not based on a fixed Wiener process uses a “spatially correlated noise” described by a martingale jointly homogeneous with V , which replaces the Wiener process W in (5) [Zirbel, 2001, Section 7]. The diffusion in random velocity field (5) is then retrieved as a limit case, when the noise correlation length goes to zero. Another idea is followed by Brouwers [2002], who derives a Fokker-Planck equation for the probability density of the particle position by applying a rigorous asymptotic analysis for small velocity fluctuations to a kinematic equation of form (7). This approach leads to general relations for the ensemble averaged Lagrangian functions, in a second order approximation. In particular, the leading term of the mean Lagrangian velocity is the mean Eulerian velocity, and for incompressible flows and spatially constant diffusion coefficients (e.g. in the case of homogeneous turbulence) it was shown that the mean values of the Lagrangian and Eulerian velocity coincide up to the third order in velocity fluctuations [Brouwers, 2002, equation (46)].

Even though the model of transport in a random velocity field and a fixed realization of the Wiener process used to derive the results presented above is not physically satisfying for the motion of all solute particles [Zirbel, 2001, p. 824], it proves to be useful in investigations on homogeneity of the transition probability of the transport process, viewed as a random quantity depending on velocity realization, as well as in analyses of the solute dispersion. This will be illustrated in the next sections.

4 Ensemble average transition probability

The density of the transition probability $p(x, t|x_0, 0)$ for the Itô process (5) is the solution of the Fokker-Planck equation

$$\partial_t p(x, t|x_0, 0) + \partial_x (V(x)p(x, t|x_0, 0)) = D\partial_x^2 p(x, t|x_0, 0), \quad (8)$$

with the initial condition $p(x, 0|x_0, 0) = \delta(x - x_0)$ (i.e. it is a Green's function).

In terms of trajectories described by (5), the transition probability is given by

$$p(x, t|x_0, 0; V(\cdot)) = \langle \delta[x - X(t)] \rangle_D, \quad (9)$$

where the “argument” $V(\cdot)$ is used to show the dependence of p on the random velocity field. Equation (5) can also be written as

$$\tilde{X}(t) = X(t) - x_0 = \int_0^t V(X(t')) dt' + W(t) = \int_0^t V(\tilde{X}(t') + x_0) dt' + W(t), \quad (10)$$

and the initial condition $X(t = 0) = x_0$ implies $\tilde{X}(t = 0) = 0$. With $X(t) = \tilde{X}(t) + x_0$ in (9), one obtains for the transition probability

$$p(x, t|x_0, 0; V(\cdot)) = \left\langle \delta[(x - x_0) - \tilde{X}(t)] \right\rangle_D = p(x - x_0, t|0, 0; V(\cdot + x_0)), \quad (11)$$

which is the solution of the Fokker-Planck equation corresponding to the Itô equation (10),

$$\partial_t p(x - x_0, t|0, 0) + \partial_x (V(x)p(x - x_0, t|0, 0)) = D\partial_x^2 p(x - x_0, t|0, 0), \quad (12)$$

for the initial condition $p(x - x_0, 0|0, 0) = \delta(x - x_0)$.

Based on relations (11) one can conclude that for translation-invariant statistics of the Eulerian velocity the ensemble average transition probability is translation-invariant as well

$$\langle p(x, t|x_0, 0; V(\cdot)) \rangle_V = \langle p(x - x_0, t|0, 0; V(\cdot + x_0)) \rangle_V = \bar{p}(x - x_0, t). \quad (13)$$

Arguments based on (13) and (12) implicitly assume that the translation invariance of the velocity implies the translation invariance of an arbitrary function of velocity. In general this statement is true for an arbitrary function of a single variable $p(V)$ [see e.g. Yaglom, A. M., Correlation theory, Springer, 1987, p.51]. It is also true for a Gaussian p which depends only on the constant mean velocity, on t , and on $x - x_0$. The construction of the average transition probability (13) is still formal. It shows indeed that p depends on

$x - x_0$ but, because the functional dependence on velocity is not known, we cannot conclude that p depends on space variables only via $x - x_0$.

To proceed, let us consider the Fourier transform of p (i.e. the characteristic function) expressed as a series of moments $\mu_k = \langle X(t)^k \rangle_D$,

$$\phi(s) = \int_{-\infty}^{\infty} e^{isx} p(x) dx = \sum_{k=0}^{\infty} \frac{(is)^k}{k!} \mu_k. \quad (14)$$

The transition probability $p(x)$ is uniquely specified by its characteristic function $\phi(s)$. Because of the linearity of the expansion (14), the ensemble average $\bar{p}$ is also determined by $\bar{\phi}$ and $\bar{\mu}_k$. The ensemble average moments $\bar{\mu}_k$ computed from Itô equation (1) depend on velocity statistics only through k -order moments of the Lagrangian velocity, evaluated on trajectories starting from the same initial position x_0 ,

$$\int_0^t \cdots \int_0^t \langle V(X(t_1)) \cdots V(X(t_k)) \rangle_V dt_1 \cdots dt_k.$$

Itô-Taylor expansions, similar to those used in Section 2, and the equality of the one-point probability distributions of Lagrangian and Eulerian velocity fields, proved in Section 3, can be used to show that these moments of the Lagrangian velocity are independent of x_0 . Finally, by (14) it follows $\bar{p}$ does not change under translations of its space variables.

In a similar way, it is possible to prove the translation invariance of the joint Lagrangian probability in the position-velocity state space p^L , i. e. the probability that $\tilde{X}(t)$ takes the value $x - x_0$ and $V(\tilde{X}(t) + x_0)$ takes the value v , provided that at $t = 0$ they had the values 0 and $v_0 = V(x_0)$, respectively,

$$p^L(x - x_0, v, t | 0, v_0, 0) = \left\langle \delta[(x - x_0) - \tilde{X}(t)] \delta[v - V(\tilde{X}(t) + x_0)] \right\rangle_V, \quad (15)$$

defined for a fixed realization of the Wiener process.

We note that the statistical homogeneity of the velocity random field alone is not sufficient to infer the translation invariance of the averaged transition probabilities (9) and (15) from the equality of one-point probability distributions of Lagrangian and Eulerian velocity fields. As shown in Section 3, smoothness conditions, necessary to ensure the existence of a unique solution of Itô or Fokker-Planck equation, and incompressibility of the velocity field have to be assumed as well.

5 Solute dispersion

In terms of trajectories X_l , $l = 1, 2, 3$, the second moment s_{ll} of the actual concentration is given by the dispersion (or the mean-square displacement) of

the solute molecules

$$s_{ll} = \langle [X_l - \langle X_l \rangle_{DX_0}]^2 \rangle_{DX_0}. \quad (16)$$

Equivalent forms of the actual dispersion s_{ll} are obtained if we add and subtract in (16) the ensemble averaged center of mass $\langle X_l \rangle_{DX_0V}$:

$$\begin{aligned} s_{ll} &= \sigma_{ll} - r_{ll}, \\ \sigma_{ll} &= \langle [X_l - \langle X_l \rangle_{DX_0V}]^2 \rangle_{DX_0}, \\ r_{ll} &= [\langle X_l \rangle_{DX_0} - \langle X_l \rangle_{DX_0V}]^2. \end{aligned} \quad (17)$$

With $\tilde{X}_l = X_l - X_{0l}$ (displacement relative to the initial position X_{0l}), we get

$$\begin{aligned} s_{ll} &= S_{ll}(0) + \tilde{x}_{ll} + m_{ll} - r_{ll} \\ \tilde{x}_{ll} &= \langle [\tilde{X}_l - \langle \tilde{X}_l \rangle_{DX_0V}]^2 \rangle_{DX_0}, \\ m_{ll} &= 2\langle [X_{0l} - \langle X_{0l} \rangle_{X_0}] \tilde{X}_l \rangle_{DX_0}. \end{aligned} \quad (18)$$

The term $S_{ll}(0) = \langle [X_{0l} - \langle X_{0l} \rangle_{X_0}]^2 \rangle_{X_0}$ in (18) is the deterministic initial second moment.

The ensemble average dispersion $S_{ll} = \langle s_{ll} \rangle_V$ has the same form,

$$S_{ll} = S_{ll}(0) + \tilde{X}_{ll} + M_{ll} - R_{ll} = \Sigma_{ll} - R_{ll}, \quad (19)$$

where $\tilde{X}_{ll} = \langle \tilde{x}_{ll} \rangle_V$, $M_{ll} = \langle m_{ll} \rangle_V$. The term $R_{ll} = \langle r_{ll} \rangle_V$ is the variance of the center of mass and $\Sigma_{ll} = \langle \sigma_{ll} \rangle_V = S_{ll}(0) + \tilde{X}_{ll} + M_{ll}$ is the dispersion of the ensemble averaged concentration.

Since numerical results [Suciu et al., 2006a] indicate that, for finite integral scale of the random velocity field, $\tilde{X}_{ll}$ is independent of the shape and dimensions of the source, we call it a *memory-free moment*. We call m_{ll} and M_{ll} *memory terms*. They quantify “memory effects” of initial conditions on the dispersion of the actual and ensemble averaged concentration. For point and line sources transverse to the l -axis $X_{0l} = \langle X_{0l} \rangle_{X_0}$, $m_{ll} = M_{ll} = 0$ (see (18)) and there are no memory effects.

With $\langle [\tilde{X}_l - \langle \tilde{X}_l \rangle_{DV}]^2 \rangle_{DV} = \langle [X_l - \langle X_l \rangle_{DV}]^2 \rangle_{DV} = X_{ll}$, the one-particle displacement’s variance defined by averaging for a fixed initial position X_0 , we obtain $\tilde{X}_{ll} = \langle X_{ll} \rangle_{X_0} + Q_{ll}$, where $Q_{ll} = \langle [\langle \tilde{X}_l \rangle_{DV} - \langle \tilde{X}_l \rangle_{DX_0V}]^2 \rangle_{X_0}$, and (19) takes the form

$$S_{ll} = S_{ll}(0) + \langle X_{ll} \rangle_{X_0} - R_{ll} + M_{ll} + Q_{ll}. \quad (20)$$

Relations (20) and (19) are equivalent under the only assumption that the order of averaging commutes (allowed if the trajectory X_l is continuous as a

function of X_0). Equation (20) takes the simpler form

$$S_{ll} = S_{ll}(0) + X_{ll} - R_{ll} \quad (21)$$

if and only if the relative one particle mean displacement $\langle \tilde{X}_l \rangle_{DV}$ and the one-particle displacements variance X_{ll} do not depend on X_0 . Now we show that these conditions can be satisfied, as a consequence of results presented in Sections 2 and 3, if we suppose that the Eulerian velocity field $V(x, t)$ is incompressible, statistically homogenous and stationary, and continuously differentiable. Using the Itô equation (1) and performing the ensemble average (with respect to V), one obtains the explicit forms of the terms in (20):

$$\begin{aligned} X_{ll}(t, t_0) &= 2D(t - t_0) \\ &+ \int_{t_0}^t \int_{t_0}^t [\langle V_l(\mathbf{X}(t')) V_l(\mathbf{X}(t'')) \rangle_{DV} - \langle V_l(\mathbf{X}(t')) \rangle_{DV} \langle V_l(\mathbf{X}(t'')) \rangle_{DV}] dt' dt'' \\ &+ 2 \left\langle W_l(t) \int_{t_0}^t V_l(\mathbf{X}(t')) dt' \right\rangle_{DV}, \end{aligned} \quad (22)$$

$$\begin{aligned} R_{ll}(t, t_0) &= \int_{t_0}^t \int_{t_0}^t \left[\langle \langle V_l(\mathbf{X}(t')) \rangle_{DX_0} \langle V_l(\mathbf{X}(t'')) \rangle_{DX_0} \rangle_V \right. \\ &\quad \left. - \langle V_l(\mathbf{X}(t')) \rangle_{DX_0V} \langle V_l(\mathbf{X}(t'')) \rangle_{DX_0V} \right] dt' dt'' \end{aligned} \quad (23)$$

$$M_{ll}(t, t_0) = 2 \int_{t_0}^t \langle [X_{0l} - \langle X_{0l} \rangle_{X_0}] \langle V_l(\mathbf{X}(t')) \rangle_{DV} \rangle_{X_0} dt', \quad (24)$$

$$\begin{aligned} Q_{ll}(t, t_0) &= \int_{t_0}^t \int_{t_0}^t \left[\langle \langle V_l(\mathbf{X}(t')) \rangle_{DV} \langle V_l(\mathbf{X}(t'')) \rangle_{DV} \rangle_{X_0} \right. \\ &\quad \left. - \langle \langle V_l(\mathbf{X}(t')) \rangle_{DV} \rangle_{X_0} \langle \langle V_l(\mathbf{X}(t'')) \rangle_{DV} \rangle_{X_0} \right] dt' dt''. \end{aligned} \quad (25)$$

The results of Section 3 imply that the second term of (22) is independent of X_0 and depends only on $(t - t_0)$. The third term in (22) vanishes because the averages over D and V permute, the mean Lagrangian velocity is constant, and the mean of the Wiener process is zero. The terms defined by (24) and (25) also vanish, because the Lagrangian mean velocity is constant. Thus, $\tilde{X}_{ll} = X_{ll}$ is memory-free and (19) and (20) reduce to the simple relation (21). Note that the results of Sections 2 and 3 do not lead to the cancelation of the center of mass fluctuations (23), because the product of averages with respect

to X_0 involve the 2-point spatial Lagrangian statistics. However, homogeneous fields with finite correlation range are ergodic and for widespread initial concentration distributions the space averages with respect to X_0 tends to the average with respect to V and (23) approaches zero.

But in practice a velocity field with special properties, as assumed in Section 3, is often an idealization. This is the case of numerical simulations of transport in statistically homogeneous velocity fields as well [Suciu and Vamoş, 2007]. A numerical illustration for non-vanishing M_{ll} shall be given in the next section.

6 Numerical simulations

In the following we present some results based on simulation data presented in [Suciu et al., 2006a] and in the manuscript 2007WR006740 submitted to Water Resources Research (where mean and fluctuations of memory terms for different initial conditions are presented in more detail).

We considered an isotropic two-dimensional aquifer system, with log-hydraulic conductivity with variance 0.1, and exponentially decaying correlation with correlation length $\lambda = 1$ m. Incompressible velocity fields were approximated numerically by Gaussian fields. This was achieved with the Kraichnan method, using 6400 periodic modes (4), as in example presented in Section 2. The mean flow velocity was $U = 1$ m/d. The local dispersion was described as an isotropic diffusion process with a constant coefficient $D = 0.01$ m²/d (Péclet number $Pe = U\lambda/D = 100$). Ensembles of 256 realizations of transport were simulated with the “global random walk” algorithm [Vamoş et al., 2003], by tracking simultaneously in every velocity realization 10^{10} particles that were initially uniformly distributed in rectangular domains $L_1\lambda \times L_2\lambda$ or released from the origin of the computational grid. It was shown that this numerical approach reproduces the self-averaging behavior of dispersion in Gaussian fields [Eberhard et al., 2007].

Figures 1 and 2 show that the mean velocity varies with the initial position $\mathbf{X}_0$ of the simulated advection-dispersion processes. The differences between $\langle V_l(\mathbf{X}(t; \mathbf{X}_0)) \rangle_{DV}$, $l = 1, 2$, are mainly significant at less than 100 dimensionless times. In the pre-asymptotic regime, the average of $\langle V_l \rangle_{DV}$ over $\mathbf{X}_0$ (solid line in Figures 1 and 2) is still different from the estimated Eulerian mean velocity components $V_1 = 1.00214 \pm 0.00033$ m/d, $V_2 = -0.00051 \pm 0.00021$ m/d [Suciu et al., 2006a, Table B1]. A comparison of the curves presented in Figure 2 indicate that the term Q_{22} , which according to (25) depends on the spatial variance of the ensemble mean velocity, is about two orders of mag-

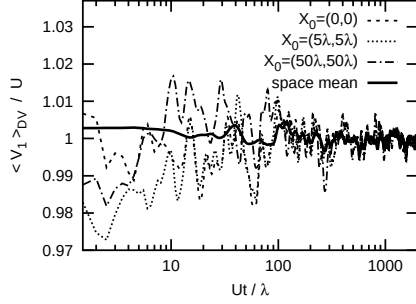


Figure 1. Ensemble average longitudinal Lagrangian velocity for different initial positions $\mathbf{X}_0$; the solid line represents the space average of $\langle V_1 \rangle_{DV}$ with respect to $\mathbf{X}_0$ for a square source with dimensions $(10\lambda, 10\lambda)$.

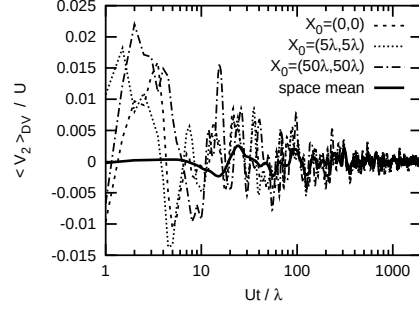


Figure 2. Ensemble average transverse Lagrangian velocity for different initial positions $\mathbf{X}_0$; the solid line represents the space average of $\langle V_2 \rangle_{DV}$ with respect to $\mathbf{X}_0$ for a square source with dimensions $(10\lambda, 10\lambda)$.

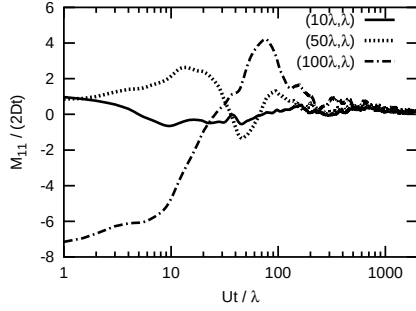


Figure 3. Longitudinal memory terms for slab sources oriented along the mean flow, $(L\lambda, \lambda)$, with increasing L .

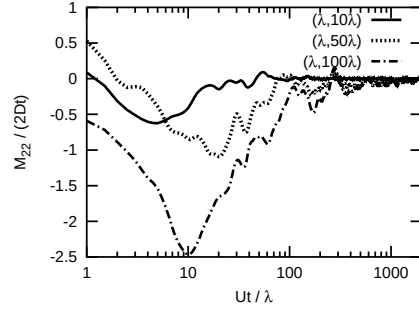


Figure 4. Transverse memory terms for slab sources oriented across the mean flow, $(\lambda, L\lambda)$, with increasing L .

nitude smaller than the local dispersion $2Dt$, with $D = 0.01$. Therefore, we can approximate $\tilde{X}_u = X_u + Q_u \approx X_u$, which was shown in Section 5 to be independent of initial conditions if the velocity field is statistically homogeneous. This explains why the term $\tilde{X}_u$ derived from simulations is practically independent of initial conditions [see e.g. Suciú et al., 2006a, Figure 11].

With $\tilde{X}_u = \Sigma_u - S_u(0) + M_u = \Sigma_u - S_u(0)$ estimated numerically for a point source, for which according to (18) the memory term M_u vanish, we use (19) to derive M_u for slab sources oriented along the l -axis. The results for longitudinal and transverse mean memory terms presented in Figures 3 and 4 indicate that the mean memory terms increase with the source dimension. This is at variance with the theoretical result in Section 5 which shows that

mean memory terms should vanish for homogeneous, incompressible and continuously differentiable velocity fields. Figures 1 and 2 help us to explain the numerical result. Indeed, the significant variations of the Lagrangian velocity with the initial position at early times, multiplied by $[X_{0l} - \langle X_{0l} \rangle_{X_0}]$ in (24), can be the source of the large mean memory terms shown in Figures 3 and 4.

7 Conclusions

We provided simple proofs that for smooth, homogeneous, stationary, and incompressible random velocity fields, the mean Lagrangian and Eulerian velocities and their one-point statistics are the same. Under these conditions, it can be shown that the ensemble average Green function of the transport problem is translation-invariant.

Numerical simulations based on the Kraichnan method, which fulfils the above requirements for the random velocity field, also indicate the equality of the mean Lagrangian and Eulerian velocities within an acceptable range of errors (see Figures 1, 2). Similar results were previously obtained by Gleeson [2002]. But the small differences between the Lagrangian and Eulerian mean velocities produce memory effects shown by the solute dispersion in the case of large asymmetric sources (Figures 3, 4). Such mean memory effects seem to be inherent in numerical simulations, where the equality of Lagrangian and Eulerian mean velocity is always an approximation [Suciu and Vamos, 2007]. These findings have also implications for practical applications of stochastic modeling to real life systems, for which the velocity field does not fulfill strictly the restrictions assumed in Sections 2-4.

Since the numbers of particles and velocity realizations were large enough to ensure reliable simulations [Suciu et al., 2006a; Eberhard et al., 2007], the mean memory terms can be a consequence of the overshooting errors in the numerical integration of trajectories [Suciu et al., 2006b]. It should be also noted that exponentially correlated fields, as considered in our simulation, are not differentiable in the mean-square sense and there is no guarantee that the sample velocities are differentiable [Yaglom, 1987, p. 67]. Since the sample differentiability is a prerequisite for the divergence-free condition to make sense, there is also no guarantee that Lagrangian and Eulerian one-point statistics coincide. The larger the number of harmonics in the Kraichnan routine, the closer the behavior of the numerically generated velocity field is to that of a Gaussian field with exponential correlation. It was shown that for a coarser approximation, with 640 harmonics instead of 6400 used in simulations presented here, the mean memory were negligible small [Suciu et al., 2007].

Another important remark is that in the limit of large times the Lagrangian velocity loses the memory of initial state (Figures 1, 2) and the mean memory effect is averaged out (Figure 3, 4). This behavior is consistent with theoretical and numerical results on the convergence for $t \rightarrow \infty$ of Lagrangian observations made in velocity fields with finite correlation lengths to up-scaled Eulerian quantities [Suciu et al., 2006a].

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