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Effect of molecular diffusivity on turbulent diffusion in isotropic turbulence

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Abstract—Dispersion of heat or mass from a point source in homogeneous isotropic turbulence is considered. Molecular diffusion can cause thermal or molecular markers to escape from fluid particles. As a consequence, the contribution of turbulence to the dispersion decreases with increasing molecular diffusivity. This effect is explored by calculating the property autocorrelation for turbulent fields having defined Eulerian space–time correlations. The analysis uses the Corrsin independence approximation and the assumption that the distribution of the particle displacements at some time after release is defined by a Gaussian function.

1. INTRODUCTION

MOLECULAR diffusivity of heat or mass affects turbulent transport in two ways. Firstly, because the scale characterizing molecular motion is so small, molecular diffusion is independent of and additive to the turbulent diffusion; the total diffusivity is, therefore, the sum of a turbulent and a molecular component

$$\varepsilon = \varepsilon_d + \mathscr{D} \tag{1}$$

where ε_d is the eddy diffusivity and $\mathscr{D}$, the molecular diffusion coefficient. Secondly, molecular diffusion can cause thermal or molecular markers to escape from fluid particles, so as to decrease the effectiveness of turbulent motions in dispersing heat and mass.

A theoretical analysis of the effect of molecular diffusion on turbulent diffusion was presented by Saffman [1]. He generalized Taylor's Lagrangian formulation of the turbulent diffusion problem [2] by introducing the concept of a 'substance or property autocorrelation', in order to allow for molecular effects. Saffman treated the idealized case of dispersion of a dynamically passive substance from a point in a stationary, homogeneous turbulent velocity field. He showed that the total dispersion, D, represented as the mean-squared displacement of the diffusing marker, at time t can be given as

$$D(t) = 2u^2 \int_0^t (t-s)\cdot R_d^{\mathrm{L}}(s)\,\mathrm{d}s + 2\mathscr{D}t \tag{2}$$

with

$$\varepsilon_d(t) = u^2 \int_0^t R_d^{\mathrm{L}}(s)\,\mathrm{d}s \tag{3}$$

where it is assumed that the markers are released at $t = 0$. Here, u is the root-mean-square of one of the components of the fluctuating velocity field defined by $u^2 = \langle u_i \cdot u_i \rangle /3$, where the usual convention that a repeated index indicates summation is observed. The property autocorrelation R_d^{L}, is defined as

$$R_d^{\mathrm{L}}(s) \equiv \frac{1}{3}\frac{\langle v_i(\mathbf{x}_0, t_0)\cdot v_i(\mathbf{x}_0, t_0+s)\rangle}{u^2} \tag{4}$$

where $v_i(\mathbf{x}_0, t)$ is the ith component of the fluctuating fluid velocity at the position $\mathbf{X}(\mathbf{x}_0, t)$ of a marker which was at $\mathbf{x}_0$ at the time of release. It differs from the well known Lagrangian autocorrelation, $R_{\mathrm{f}}^{\mathrm{L}}$, in that it correlates fluid velocity components along the trajectory of molecular or thermal markers, and not of fluid particles. Since a marker can leak out of a fluid particle because of random molecular motion, R_d^{L}, is not purely a property of the turbulence, but depends also on molecular diffusivity. In this context, a fluid particle can be viewed as the limiting case of a marker with vanishingly small molecular diffusivity. Therefore, the Lagrangian eddy diffusivity, $\varepsilon_{\mathrm{f}}(t)$, for fluid particles is obtained by substituting the fluid Lagrangian autocorrelation, $R_{\mathrm{f}}^{\mathrm{L}}$, for the property autocorrelation in equation (3).

Even in unbounded flow, the property autocorrelation, R_d^{L}, in equation (3) vanishes at sufficiently long time delays. As a result, the eddy diffusivity, ε_d, eventually reaches a constant value which characterizes the dispersive effectiveness of the turbulent motions. The focus of this paper is the investigation of how ε_d decreases with increasing $\mathscr{D}$. The system considered is the dispersion of heat or mass from a point source in a three-dimensional, incompressible, stationary, isotropic turbulent field, with zero mean velocity. The influence of molecular diffusion on the property autocorrelation and, therefore, the turbulent diffusion coefficient defined by equation (3) is examined. Since no solidly based results are available for finite diffusion times, the main goal of the present study is to provide an understanding of the effects of molecular diffusion for all times.

The approach taken, which is described in a thesis

NOMENCLATURE

$\mathcal{D}$	molecular diffusivity
D	mean-squared displacement
f	longitudinal Eulerian velocity correlation
g	lateral Eulerian velocity correlation
L	Eulerian integral length scale (equation (13))
p	probability density of displacement
Pe	Peclet number, $Lu/\mathcal{D}$
$\mathbf{r}$	separation vector
R	velocity autocorrelation
s	time delay
S	defined in equation (21b)
t	time
T	integral time scale
u	root-mean-square Eulerian turbulent velocity
u_i	ith component of the fluctuating Eulerian turbulent velocity
v_i	ith component of the fluctuating Lagrangian turbulent velocity
$\mathbf{x}$	Eulerian coordinates
$\mathbf{X}$	Lagrangian coordinates.

Greek symbols

β	dimensionless Eulerian integral time scale (equation (31))
δ_{ij}	Kronecker delta
ε	eddy diffusivity
λ	Taylor microscale
ξ	convergence tolerance
τ	defined in equation (21a).

Subscripts

d	quantity affected by molecular diffusivity
f	quantity pertaining to fluid particles (independent of molecular diffusivity)
i	ith component
0	quantity at $t = 0$.

Superscripts

E	Eulerian
L	Lagrangian
*	dimensionless quantity.

by Kontomaris [3], is based on a generalization of the hypothesis of Corrsin [4, 5] that in homogeneous turbulence the Lagrangian property autocorrelation for a fixed time delay can be calculated as the spatial average of the Eulerian space–time velocity correlation, $R_{ij}^{\mathrm{E}}(\mathbf{r}, s)$ with the same time delay

$$R_d^{\mathrm{L}}(s) = \frac{1}{3}\iint_{-\infty}^{\infty}\int R_{ii}^{\mathrm{E}}(\mathbf{x}, s)\cdot p_d(\mathbf{x}\,;s)\,\mathrm{d}\mathbf{x}. \qquad (5)$$

The probability, $p_d(\mathbf{X}\,;s)$, that a marker has a displacement $\mathbf{X}$, after elapsed time s, is assumed to be Gaussian with variance $D(t = s)$. Equation (5) is solved by an iterative procedure where the correlation function, $R_d^{\mathrm{L}}(s)$, is assumed. The variance is calculated from equation (2) and a new estimate of $R_d^{\mathrm{L}}(s)$ is obtained from equation (5). This procedure is repeated until a convergence is reached. A similar iterative method was first introduced by Lundgren and Pointin [6] to relate the Lagrangian to the Eulerian correlation and it was later extended to the case of real particles by Pismen and Nir [7] and further refined by Mei [8]. The chief difference in this work is that the method is formulated in physical space (rather than wavenumber space) with the advantage that the physics emerges more naturally. Moreover, the influence of molecular diffusion is included. The approach is similar to that used by Saffman [9] who pursued Corrsin's suggestion (without considering molecular diffusivity effects) by assuming Gaussian forms for the Eulerian space–time correlation and for the displacement probability density.

The interaction between molecular and turbulent diffusion can be quantified by the difference between the standard Lagrangian autocorrelation for fluid particles and the property autocorrelation, $[R_{\mathrm{f}}^{\mathrm{L}}(s) - R_d^{\mathrm{L}}(s)]$. Saffman [1] found that initially $[R_{\mathrm{f}}^{\mathrm{L}}(s) - R_d^{\mathrm{L}}(s)] = (5\mathcal{D}s)/\lambda^2$, where λ is the Taylor microscale. For longer diffusion times Saffmann [1, 10] made a number of speculative proposals in which the dependence of the property autocorrelation on Prandtl number varies according to the range of Prandtl and Reynolds numbers being considered. For very small Peclet numbers he obtained results in agreement with the intuitive proposal of Hinze [11], although the latter was proposed with no restriction placed on the Peclet number. More recently, Phythian and Curtis [12] developed an iterative technique for calculating the effective long-time eddy diffusivity that uses a self-consistent renormalized perturbation expansion. Drummond [13] calculated the long-time effective turbulent diffusivity of a passive scalar quantity from a path-integral solution of the diffusion equation, assuming Gaussian turbulence. Drummond *et al.* [14] simulated scalar transport subject to molecular diffusion in a model isotropic turbulent field. Sawford and Hunt [15] studied molecular diffusivity effects on scalar fluctuations in homogeneous turbulence by employing a Lagrangian stochastic model of turbulent diffusion, developed from the marked-particle model of Durbin [16].

In this paper the Eulerian correlation in equation (5) is represented as the product of a function of space and a function of time. Two forms are explored: one is Gaussian and the other is exponential in space and time. The use of either of these correlations in equation (5) and the assumption that the displacements are Gaussian yields a ratio of the Lagrangian and Eulerian time correlations that is a function of the mean-square particle displacement, D, made dimensionless with the Eulerian length scale, L.

The most important results obtained from this relation and equation (2) is the definition of the influence of the Peclet number, $Lu/\mathscr{D}$, on the function representing the property autocorrelation, $R_d^L(su/L)$, and on the turbulent diffusivity. These results are interpreted by deriving two asymptotic relations from the expected behavior of D/L^2 for large and small dimensionless times, tu/L. Relations derived in this way are consistent with previous results by Saffman, but are less restrictive.

2. METHOD

2.1. *General description*

The Eulerian space–time velocity correlation is defined as

$$R_{ij}^E(\mathbf{r},s) \equiv \frac{\langle u_i(\mathbf{x},t)\cdot u_j(\mathbf{x}+\mathbf{r},t+s)\rangle}{u^2} \tag{6}$$

where the brackets indicate averaging. Space–time correlations of the following form are assumed:

$$R_{ij}^E(\mathbf{r},s) = R_{ij}^E(\mathbf{r})\cdot R^E(s) \tag{7}$$

where $R^E(s)$ is the one-point Eulerian velocity autocorrelation defined as

$$R^E(s) \equiv \frac{1}{3}\,\frac{\langle u_i(\mathbf{x},t)\cdot u_i(\mathbf{x},t+s)\rangle}{u^2}. \tag{8}$$

For isotropic turbulence the tensor $R_{ij}^E(\mathbf{r})$ can be expressed as

$$R_{ij}^E(\mathbf{r}) = [f(r)-g(r)]\cdot\frac{r_i\cdot r_j}{r^2}+g(r)\delta_{ij} \tag{9}$$

where r is the measure of the separation vector $\mathbf{r}$.

The following relation between $f(r)$ and $g(r)$ is needed to satisfy continuity:

$$g(r) = f(r)+\tfrac{1}{2}r\frac{\partial f}{\partial r}. \tag{10}$$

Substitution of equations (7), (9) and (10) into equation (5) followed by a transformation into spherical coordinates yields the following relation:

$$R_d^L(s) = \sqrt{\left(\frac{2}{9\pi}\right)}\cdot\frac{R^E(s)}{[D(s)]^{3/2}}\int_{r=0}^{\infty} r^2(3f+rf')\cdot\exp\left[-\frac{r^2}{2D(s)}\right]\mathrm{d}r. \tag{11}$$

The term $D(s)$ is given by equation (2) so that equations (2) and (11) are a closed set of equations which can be solved iteratively to evaluate R_d^L. A convenient first iteration is to substitute $R^E(s)$ for R_d^L in equation (2). This procedure was found to converge very quickly especially for high molecular diffusivities. The criterion for terminating the iteration procedure was that

$$\max_s |[R_d^L(s)]_{i+1}-[R_d^L(s)]_i| < \xi$$

where i is the iteration index and ξ is a convergence tolerance.

For arbitrary $f(r)$ the integration in equation (11) can be carried out numerically. For a given time delay, the step size, Δr, for the numerical integration is chosen small enough to resolve the variation of the integrand in equation (11), the scale of which depends on $D(s)$. An appropriate choice, which makes the integration results independent of Δr, is $\Delta r(s) \ll \sqrt{(D(s))}$.

2.2. *Specific forms of $f(r)$—limiting relations for small and large times*

The behavior of $f(r)$ for $r \to 0$ is described by

$$f(r) \approx 1-\frac{r^2}{2\lambda^2}. \tag{12}$$

A macroscale L is defined as

$$L = \int_0^{\infty} f(r)\,\mathrm{d}r. \tag{13}$$

For large Reynolds numbers $\lambda/L \to 0$, and the range of r over which equation (12) is a good approximation becomes quite small.

Two forms of the correlation function $f(r)$ are explored. One of these is a Gaussian function

$$f(r) = \exp\left(-\frac{\pi r^2}{4L^2}\right) \tag{14}$$

for which $L = \lambda\sqrt{(\pi/2)}$. The other

$$f(r) = \exp\left(-\frac{r}{L}\right) \tag{15}$$

does not have the correct shape for $r \to 0$, but is more representative of the behavior at large Reynolds numbers. Similarly, two forms for the time decay of the one-point Eulerian autocorrelation are examined

$$R^E(s) = \exp\left[-\frac{\pi s^2}{4(T^E)^2}\right] \tag{16}$$

and

$$R^E(s) = \exp\left(-\frac{s}{T^E}\right) \tag{17}$$

where T^E is the Eulerian integral time scale.

The ratio $R_d^L(s)/R^E(s)$, according to equation (11), can be viewed as a function of the total dispersion D (for a given $f(r)$). This functionality can be represented for a Gaussian $f(r)$ by the following analytical expression:

$$R_d^{\mathrm{L}}(s) = R^{\mathrm{E}}(s)\left[1+\frac{\pi D(s)}{2L^2}\right]^{-5/2} \tag{18}$$

It is to be noted that Lundgren and Pointin [6] obtained an identical equation with their spectral formulation, limited to the case of fluid particle dispersion. Hinze [17] has also pointed out that Saffman's analysis [9] leads to a $-5/2$ dependence of the Lagrangian autocorrelation on the mean-square displacement. For an exponential correlation function of the form of equation (15) a closed form solution of equation (11) could not be obtained. However, small and long time approximations of R_d^{L} can be easily obtained. By approximating $f(r)$ as $1-r/L$ for $r/L \to 0$, the following series expansion, valid for small D (or equivalently small time), can be derived:

$$R_d^{\mathrm{L}}(s) \approx R^{\mathrm{E}}(s)\left[1-\sqrt{\left(\frac{128}{9\pi}\right)}\left(\frac{D(s)}{L^2}\right)^{1/2}+\frac{D(s)}{L^2}+\cdots\right]. \tag{19a}$$

For large time delays a different approach is followed. It is observed that the term $r^2(3f+rf')$ which appears in equation (11) becomes negligibly small for r larger than some value, say r_M, and consequently the integration has to be carried out only up to $r = r_M$. Therefore, for $D(s)$ values large compared to r_M^2 the Gaussian term in equation (11) is approximated (in the range $0 < r < r_M$) as $1-r^2/2D$ and the integration is carried out analytically to obtain

$$R_d^{\mathrm{L}}(s) \approx \frac{72}{\sqrt{(2\pi)}}R^{\mathrm{E}}(s)\left(\frac{D(s)}{L^2}\right)^{-5/2}. \tag{19b}$$

Equations (18), (19a) and (19b) confirm that $R_d^{\mathrm{L}}(s)/R^{\mathrm{E}}(s) < 1$ (see also Fig. 1).

A consideration of the $D(t)$ relation for a fluid particle (i.e. equation (2) with $\mathscr{D} = 0$) suggests two limiting behaviors: for times small with respect to the eddy circulation time scale (i.e. $tu/L \ll 1$)

$$\frac{D(t)}{L^2} \approx \frac{u^2t^2}{L^2} \tag{20}$$

and for large tu/L

$$\frac{D(t)}{L^2} \approx 2\frac{\varepsilon_{\mathrm{f}}(\infty)}{Lu}\left(\frac{tu}{L}-\tau_{\mathrm{f}}^*\right). \tag{21}$$

Here $\varepsilon_{\mathrm{f}}(\infty)$ is the Lagrangian turbulent diffusivity of a fluid particle at large times and constant τ_{f}^* equals

$$\tau_{\mathrm{f}}^* = \frac{u}{L}\left(\frac{S_{\mathrm{f}}^{\mathrm{L}}}{T_{\mathrm{f}}^{\mathrm{L}}}\right) \tag{21a}$$

where

$$S_{\mathrm{f}}^{\mathrm{L}} = \int_0^\infty sR_{\mathrm{f}}^{\mathrm{L}}(s)\,\mathrm{d}s \tag{21b}$$

and

$$T_{\mathrm{f}}^{\mathrm{L}} = \int_0^\infty R_{\mathrm{f}}^{\mathrm{L}}(s)\,\mathrm{d}s. \tag{21c}$$

Substitution of equation (20) into equations (18) and (19a) will produce a small time approximation for $R_{\mathrm{f}}^{\mathrm{L}}/R^{\mathrm{E}}$ for Gaussian and exponential $f(r)$, respectively. Similarly, substitution of equation (21) into equations (18) and (19b) will produce a large time approximation for $R_{\mathrm{f}}^{\mathrm{L}}/R^{\mathrm{E}}$.

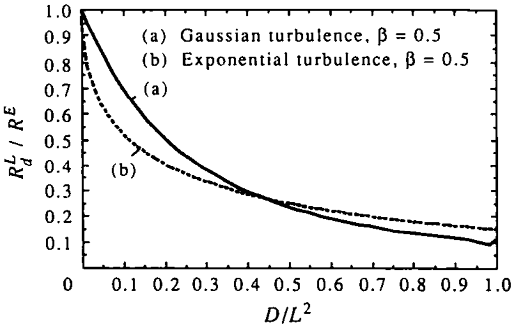

FIG. 1. Influence of dispersion on the ratio of the Lagrangian and Eulerian time correlations.

The above discussion can be extended to the case of *non-zero molecular diffusivity*. In this case two time scales in addition to the time scale of the large eddies, L/u, can be defined. The initial rate of spread of material by turbulent velocities is zero, so molecular diffusion is controlling the diffusion process. Scale $\mathscr{D}/u^2$ represents the time required for the spread due to turbulence to equal the spread due to molecular diffusion. Scale $\lambda^2/\mathscr{D}$ represents the time required for molecular diffusion to cause a spread of material that equals the microscale of the turbulence. For small tu/L, the approximation

$$\frac{D(t)}{L^2} \approx \frac{u^2t^2}{L^2}+\frac{2\mathscr{D}t}{L^2} \tag{22}$$

can be made. From equations (22) and (18) the following relation is obtained:

$$R_d^{\mathrm{L}}(s) \approx R^{\mathrm{E}}(s)\left[1+\frac{\pi u^2s^2}{2L^2}+\frac{\pi\mathscr{D}s}{L^2}\right]^{-5/2}. \tag{23}$$

For small $su^2/\mathscr{D}$ equation (23) simplifies to

$$R_d^{\mathrm{L}}(s) \approx R^{\mathrm{E}}(s)\left[1+\frac{\pi\mathscr{D}s}{L^2}\right]^{-5/2} \tag{24a}$$

or

$$R_d^{\mathrm{L}}(s) \approx R^{\mathrm{E}}(s)\left[1+\frac{2\mathscr{D}s}{\lambda^2}\right]^{-5/2} \tag{24b}$$

if the Taylor microscale λ is used instead of the integral scale L. With the assumption of small $s\mathscr{D}/\lambda^2$, equation (24b) gives

$$R_d^{\mathrm{L}}(s) \approx R^{\mathrm{E}}(s)\left(1-\frac{5\mathscr{D}s}{\lambda^2}\right). \tag{25}$$

With the observation that $R^{\mathrm{E}}(s \to 0) \approx 1$, the limiting relation developed by Saffman [1] for $s \to 0$ is recovered from equation (25). The same result is obtained for any form of $f(r)$ which complies with equation (12) at its vertex.

Similar approximations can be derived for the case of an exponential $f(r)$. From equation (19a) it is seen that the approximation for small tu/L, equation (22), gives

$$R_d^{\mathrm{L}}(s) \approx R^{\mathrm{E}}(s)\left[1-\sqrt{\left(\frac{128}{9\pi}\right)}\left(\frac{u^2s^2}{L^2}+\frac{2\mathscr{D}s}{L^2}\right)^{1/2} + \left(\frac{u^2s^2}{L^2}+\frac{2\mathscr{D}s}{L^2}\right)+\cdots\right]. \quad (26)$$

For $(su^2/\mathscr{D}) \to 0$ this simplifies to

$$R_d^{\mathrm{L}}(s) \approx R^{\mathrm{E}}(s)\left[1-\sqrt{\left(\frac{256}{9\pi}\right)}\left(\frac{\mathscr{D}s}{L^2}\right)^{1/2}+2\left(\frac{\mathscr{D}s}{L^2}\right)+\cdots\right]. \quad (27)$$

As expected, this does not reduce to Saffman's result because the assumed correlation function does not have the correct behavior for small r.

For large tu/L the dispersion can be approximated as

$$\frac{D(t)}{L^2} \approx 2\left(\frac{\varepsilon_d(\infty)}{\varepsilon_{\mathrm{f}}(\infty)}\right)\left(\frac{\varepsilon_{\mathrm{f}}(\infty)}{Lu}\right)\left(\frac{tu}{L}-\tau_d^*\right)+2\left(\frac{\mathscr{D}}{Lu}\right)\left(\frac{tu}{L}\right). \quad (28)$$

Here, $\varepsilon_d(\infty)/\varepsilon_{\mathrm{f}}(\infty)$ is the ratio of the long time diffusivities of the substance (or heat) and of fluid particles; it is a function of the Peclet number. Constant τ_d^* is defined similarly to τ_{f}^* and its dependence of Pe is weaker than that of $\varepsilon_d(\infty)$.

Equation (28) can be substituted into equation (18) or equation (19b) to obtain an approximation of $R_d^{\mathrm{L}}(s)$ for large times. In both cases this reduces to

$$\frac{R_{\mathrm{f}}^{\mathrm{L}}(s)-R_d^{\mathrm{L}}(s)}{R_{\mathrm{f}}^{\mathrm{L}}(s)} \approx 1-\left[\frac{\varepsilon_{\mathrm{f}}(\infty)/uL}{\varepsilon_d(\infty)/uL+1/Pe}\right]^{5/2} = fct(Pe) \quad (29)$$

for $su/L \to \infty$, where $R_{\mathrm{f}}^{\mathrm{L}}(s)$ is the Lagrangian correlation for a fluid particle, $\varepsilon_{\mathrm{f}}(\infty)/uL$ is a constant, and $\varepsilon_d(\infty)/uL$ is a function of Pe. This seems consistent with the hypothesis explored by Saffman [1, 10] that the ratio represented by the left side of equation (29) should become independent of time at long times. From equation (29) it is noted that for $Pe \to 0$

$$\frac{R_{\mathrm{f}}^{\mathrm{L}}(s)-R_d^{\mathrm{L}}(s)}{R_{\mathrm{f}}^{\mathrm{L}}(s)} = 1 \quad (30)$$

in agreement again with the predictions of Saffman [10].

3. RESULTS

3.1. *Parametrization*

When all the equations presented in the previous section are nondimensionalized with scales constructed using u and L, only the following three independent dimensionless variables appear in the resulting set of equations: a dimensionless time, tu/L, a dimensionless molecular diffusivity (or inverse Peclet number), $\mathscr{D}/uL$, and a dimensionless Eulerian integral time scale defined as

$$\beta = \frac{T^{\mathrm{E}}u}{L}. \quad (31)$$

On dimensional grounds, the integral time scale of the Eulerian space–time correlation, T^{E}, is related to the eddy circulation time, L/u, and β is expected to be a function of the Reynolds number.

Two flow cases are examined: (a) Gaussian turbulence (equations (14) and (16)); and (b) exponential turbulence (equations (15) and (17)). The choice of a Gaussian $f(r)$ is consistent with one of the spectral energy function prescriptions of Kraichnan [18]. Most of the results of this paper were obtained with $\beta = 0.5$. It is noted that this choice of β (in conjunction with a Gaussian $R^{\mathrm{E}}(s)$) is again consistent with one of the choices of Kraichnan [18]. For an error tolerance of $\xi = 0.001$, convergence is achieved in no more than five iterations depending on the value of Pe and β.

3.2. *Lagrangian autocorrelations*

The dependence of $R_d^{\mathrm{L}}/R^{\mathrm{E}}$ on the total dispersion D/L^2, calculated from equation (11), is examined in Fig. 1. Since D is an increasing function of time this ratio is found to decrease monotonically with time.

Calculated Lagrangian correlations for *fluid particles* are compared with the Eulerian time correlations in Fig. 2. It is observed that the Lagrangian correlation is approximately equal to the Eulerian correlation for small time (small D) and significantly less for larger times. The ratio of the Lagrangian, $T_{\mathrm{f}}^{\mathrm{L}}$, to the Eulerian integral time scale, T^{E}, is calculated to be 0.728 for a Gaussian and 0.567 for an exponential correlation. The dashed curves in Fig. 2 represent the small and large time limiting approximations discussion in Section 2.2. Figure 2 indicates that the small time approximation is acceptable for $su/L < 0.4$ or $s/T_{\mathrm{f}}^{\mathrm{L}} < 1.09$ for Gaussian $f(r)$ and $su/L < 0.15$ or $s/T_{\mathrm{f}}^{\mathrm{L}} < 0.53$ for exponential $f(r)$. The relatively narrower range of validity in exponential turbulence is a consequence of the series approximation of $f(r)$ involved in the derivation of equation (19a); in contrast, equation (18) is derived from equation (11) by exact analytical integration. The large time approximation is acceptable for $su/L > 0.4$ or $s/T_{\mathrm{f}}^{\mathrm{L}} < 1.09$ for the case of Gaussian turbulence; for exponential turbulence, equation (19b) becomes valid only in the range of very long times (not shown in Fig. 2) where $R_{\mathrm{f}}^{\mathrm{L}}$ is negligible.

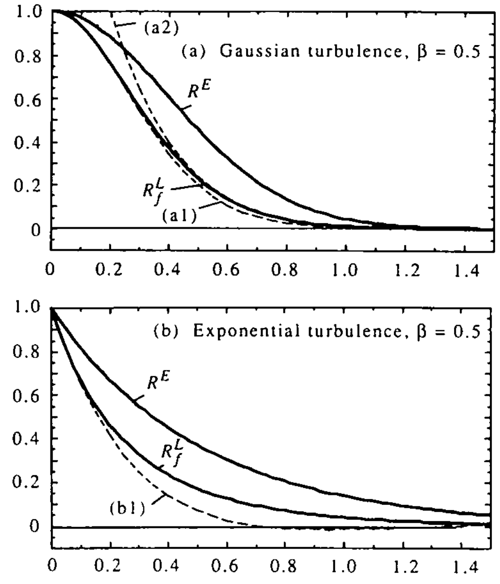

FIG. 2. Comparison of the Lagrangian correlation R_f^L to the Eulerian correlation R^E for (a) Gaussian turbulence with $\beta = 0.5$ and (b) exponential turbulence with $\beta = 0.5$. Curve (a1): small time approximation from equations (18) and (20) (or equation (23) with $\mathscr{D} = 0$). Curve (a2): long time approximation from equations (18) and (21) with $\varepsilon_f(\infty) = 0.3639\, uL$ and $\tau_f^* = 0.2430$. Curve (b1): from equations (19a) and (20) (or equation (26) with $\mathscr{D} = 0$).

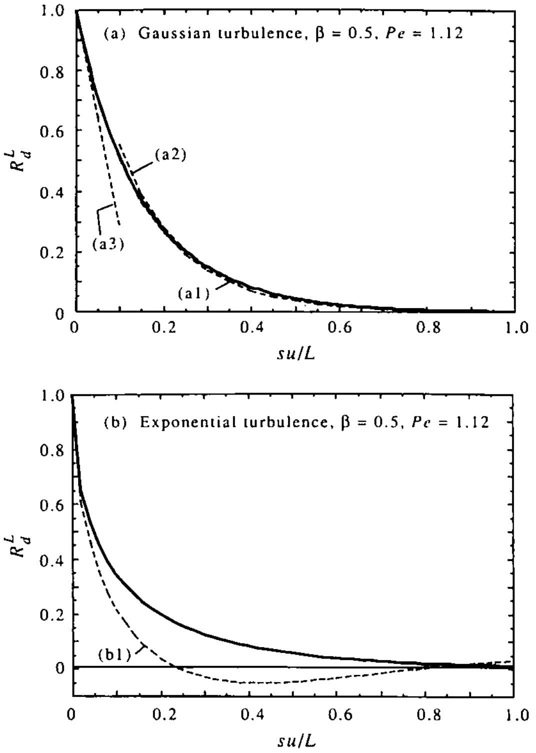

FIG. 4. Limiting approximations of property correlations for $Pe = 1.12$. (a) Gaussian turbulence with $\beta = 0.5$ and (b) exponential turbulence with $\beta = 0.5$. Curve (a1): small time approximation from equations (18) and (22) (or equation (23)). Curve (a2): long time approximation from equations (18) and (28) with $\varepsilon_f(\infty) = 0.3639\, uL$, $\varepsilon_d(\infty)/\varepsilon_f(\infty) = 0.424$, and $\tau_d^* = 0.1577$. Curve (a3): Saffman's small time approximation from equation (25). Curve (b1): small time approximation from equations (19a) and (22) (or equation (26)).

The influence of $Pe = uL/\mathscr{D}$ on the property autocorrelation is shown in Fig. 3. The curves for $Pe = 22.57$, 11.29 are very close to the correlation for a fluid particle, $Pe = \infty$. However, for $Pe = 2.25$, 1.12 molecular diffusion is found to have a strong effect on the property autocorrelation. In Fig. 4 the property correlations for $Pe = 1.12$ are compared to the limiting approximations of Section 2.2. A consideration of the results shown in Fig. 4 indicates that the small time approximation, equation (23), for the Gaussian case is valid for $su/L < 0.25$ or $s/T_d^L < 1.63$. For an exponential correlation, equation (26) is valid for $su/L < 0.05$ or $s/T_d^L < 0.4$. It is noted that equation (22) should be valid for increasingly larger tu/L as the Peclet number decreases and the molecular contribution to dispersion dominates. As a result, equation (23) describes the entire correlation curve in the limit of $Pe \to 0$. This is not true, however, for the analogous equation (26) for exponential turbulence, because the range of validity of equation (19a) diminishes with decreasing Pe (or increasing total dispersion D). Saffman's small time expression equation (25) is also included in Fig. 4(a) for comparison. It is seen that it is far more restrictive than equation (23) for a Gaussian correlation; it would not be applicable for an exponential correlation. A comparison of the results presented in Fig. 3 with the long time asymptotic predictions equation (29) of $[(R_f^L - R_d^L)/R_f^L]$ for two Peclet numbers is shown in Fig. 5.

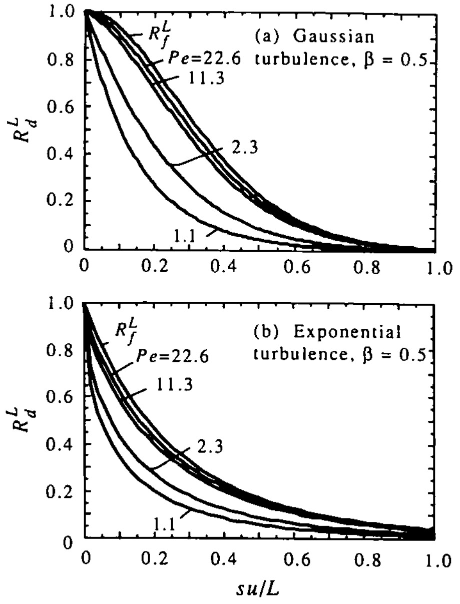

FIG. 3. Influence of molecular diffusion on the property autocorrelation for (a) a Gaussian $f(r)$ and (b) an exponential $f(r)$.

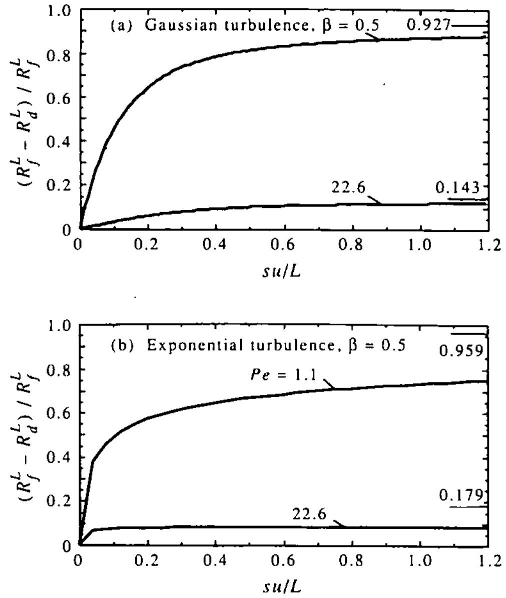

FIG. 5. Long time behavior of property autocorrelation for (a) Gaussian turbulence with $\beta = 0.5$ and (b) exponential turbulence with $\beta = 0.5$.

3.3. *Dispersion and diffusion coefficients*

Turbulent contributions to the dispersions, calculated from equation (2), are presented in Fig. 6. The decrease in the turbulent dispersion with decreasing Pe is clearly shown. For small times, where $R^L_d \approx 1$, the turbulent dispersion is expected to depend primarily on the intensity of turbulent velocity fluctuations. This is illustrated by the approximate independence of the dispersion from Peclet number that is observed for small times.

A turbulent diffusivity can be calculated from equation (3) and the computed property autocorrelation functions. The results of this calculation are shown in Fig. 7. Here the ratio of the property diffusivity and the fluid particle diffusivity at infinite time is plotted against the reciprocal of the Peclet number. As mentioned earlier, an exponential correlation is representative of large Reynolds numbers, whereas a Gaussian correlation would be more representative of low Reynolds numbers. The results appear to be sensitive to the choice of a form for the correlation only at large values of $\mathscr{D}/uL$.

The fluid diffusivity at infinite time is calculated (for $\beta = 0.5$) as

$$\varepsilon_f(\infty) = 0.3639uL \tag{32}$$

for a Gaussian correlation and as

$$\varepsilon_f(\infty) = 0.2834uL \tag{33}$$

for an exponential correlation. Figure 7 indicates that the property eddy diffusivity drops significantly from its value for fluid particles for molecular diffusivities $\mathscr{D}/uL > 0.3$. Thus, molecular diffusion starts having a strong effect on turbulent diffusivity when $\mathscr{D}/uL \approx \varepsilon_f(\infty)/uL$.

Figures 6 and 7 indicate that the turbulent contribution to the total dispersion of an admixture (e.g. heat or mass) from the location of the source, decreases with increasing molecular diffusivity (or decreasing Peclet number). This is because molecular diffusivity causes the admixture to escape from the turbulent motions which attempt to disperse it away from the source.

A time varying turbulent diffusivity can be calculated from equation (3) and the correlation curves presented in Fig. 3. The results for two Peclet numbers ($Pe = 2.25$ and 22.57) and Gaussian turbulence are shown in Fig. 8. It is seen that at small times $\varepsilon_d(t)/uL$ can be represented with a linear function which is not dependent on molecular diffusivity. At large times it reaches a constant value which, as just shown,

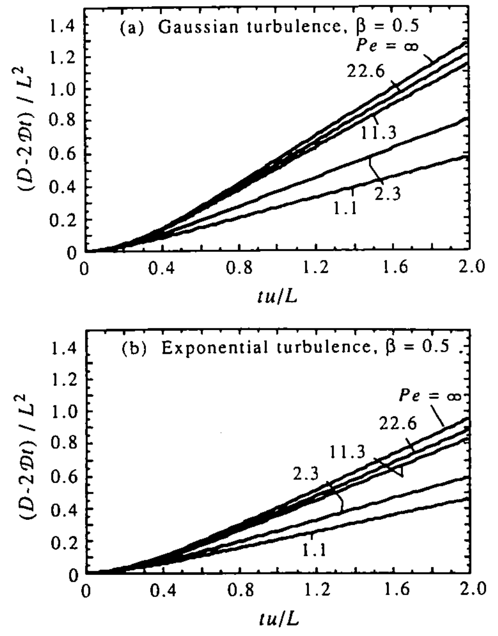

FIG. 6. Turbulence contribution to the dispersion for (a) Gaussian turbulence with $\beta = 0.5$ and (b) exponential turbulence with $\beta = 0.5$.

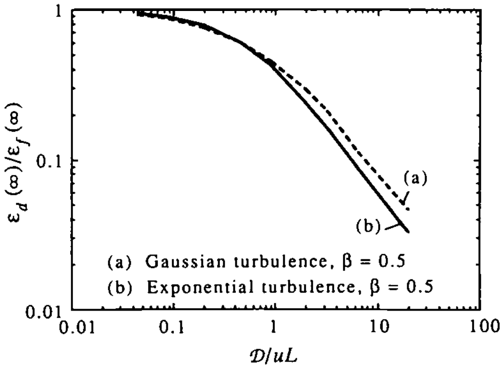

FIG. 7. Influence of molecular diffusion on the long time turbulent diffusivity.

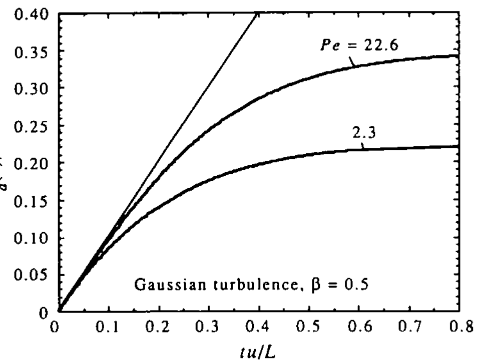

Fig. 8. Time dependency of the eddy diffusivity for (a) $Pe = 2.25$ ($\varepsilon_d(\infty) = 0.221$) and (b) $Pe = 22.57$ ($\varepsilon_d(\infty) = 0.343$).

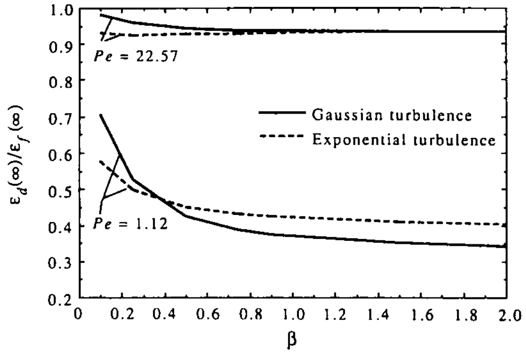

Fig. 10. Effect of the Eulerian integral time scale $\beta = T^{\mathrm{E}}u/L$ on the calculated property eddy diffusivity for $Pe = 1.12$ and $Pe = 22.57$.

decreases with decreasing Peclet number. The time required for $\varepsilon_d(t)$ to reach $\varepsilon_d(\infty)$ decreases with decreasing Peclet number.

One of the more important results in this paper is contained in Fig. 7. Its use in engineering problems will require a determination of the sensitivity of the calculations to the choice of β defined in equation (31). Figure 9 shows the dependence of fluid particle diffusivity on β. Figure 10 gives the dependence of the calculated $\varepsilon_d(\infty)/\varepsilon_f(\infty)$ on the choice of β. It is observed that for large values of β, $\varepsilon_d(\infty)/\varepsilon_f(\infty)$ is almost independent of β. Therefore, in the range of large β, an exact determination of $\beta = T^{\mathrm{E}}u/L$ is not necessary in order to determine the turbulent diffusivity for a given Peclet number.

4. DISCUSSION AND CONCLUSIONS

Diffusion of a heat marker or a molecular species from a point source in isotropic turbulence is considered. The independence approximation of Corrsin and the assumption of a Gaussian displacement distribution give the result that the ratio of the Lagrangian property autocorrelation to the Eulerian autocorrelation is a decreasing function of D/L^2, where D is the mean-squared displacement and L the Eulerian length scale. Since the mean-squared displacement is defined by equation (2) an iterative procedure can be used to calculate the Lagrangian property autocorrelation if the Eulerian turbulence properties are known.

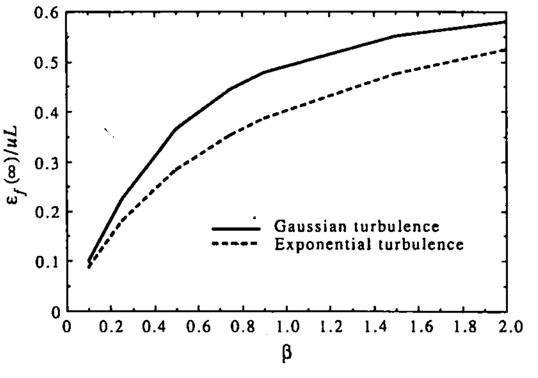

Fig. 9. Effect of the Eulerian integral time scale $\beta = T^{\mathrm{E}}u/L$ on the calculated eddy diffusivity of fluid particles.

For $s = 0$ equation (11) becomes indeterminate. However, the value of $R_d^{\mathrm{L}}(s = 0)$ is known to be unity and equation (11) is applied only for $s > 0$. In any case, equation (11) behaves well for s values in the neighborhood of $s = 0$. As $s \to 0$ (implying also very small dispersion $D(s)$) the Gaussian factor of the integrand in equation (11) decays very quickly to zero with increasing r. Therefore, the integration in equation (11) has to be carried out only up to a small value r^* (on the order of $\sqrt{(D(s))}$), since contributions from values of $r > r^*$ will be negligible. For small r values, however, $f(r)$ approaches unity and $f'(r)$ approaches zero; therefore $r^2(3f + rf') \approx 3r^2$. With these approximations the integration in equation (11) can be carried out analytically to yield $R_d^{\mathrm{L}}(s) \approx R^{\mathrm{E}}(s)$ for $s \to 0$.

The use of Corrsin's hypothesis could be of some concern since Corrsin argued that a relation such as equation (5) is valid only for diffusion times long enough so that the Lagrangian position and velocity of the particle become uncorrelated. Since the integration in equation (2) is to be carried out from $s = 0$, equation (5) has to be employed in the range of small diffusion times. However, a study by Lundgren and Pointin [6] provides encouraging results. Their numerical experiments for fluid particle diffusion using Kraichnan's representation of isotropic turbulence [18] gave the same results as calculations based on Corrsin's hypothesis for all diffusion times. Even for unrealistic random fields, agreement was found for small times. Lundgren and Pointin suggest that in Gaussian fields Corrsin's approximation is acceptable when the displacement of a fluid point is only weakly coupled to any one Fourier mode of the field. The added decorrelating effect of molecular diffusion on the motion of a marker, included in this paper, should be expected to make the use of equation (5) more justifiable.

The accuracy of Corrsin's approximation has been discussed in a number of places. Weinstock [19] concludes that both the approximation of Corrsin and the assumption of a Gaussian distribution for particle displacement are valid for homogeneous isotropic fields and that their use leads to a Lagrangian autocorrelation lower than the Eulerian time correlation for all time delays. Reeks [20] points out that Corrsin's hypothesis is, clearly, less crude than previously thought.

The correct form for the Eulerian velocity correlation is not known. The Gaussian relation, used in this and previous papers (Reeks [20], Lundgren and Pointin [6], Kraichnan [18], Saffman [9], Pismen and Nir [7]) does not represent large scales of turbulence accurately. The exponential form may not represent the inertial range correctly. Furthermore, a space–time correlation of the form of equation (7) has its maximum at $r = 0$ for all time. It is quite possible that qualitatively different results could be obtained for the ratio $R^{\mathrm{L}}_{d}(s)/R^{\mathrm{E}}(s)$ with correlation functions that have maxima at finite values of r for non-zero times. The ramifications of using a separate form for the Eulerian autocorrelation (equation (7)) have not been adequately addressed in the literature; further research in this direction is warranted.

The mathematical technique outlined in this paper allows for the use of any form for the Eulerian correlation; therefore, correlations described by more than one length scale could be explored. Several such forms have recently been used by Mei [8] in an analysis of the dispersion of solid particles. These show that the behaviors at low and high Reynolds numbers are, respectively, represented by the Gaussian and exponential functions.

Because of uncertainties about both the correct form of the Eulerian correlation and the more complicated form of the results when more than one length scale is used, we chose to explore two Eulerian space–time correlations with single length scales that are representative of turbulence at low and high Reynolds numbers. The Lagrangian property autocorrelation, the dimensionless turbulent contribution to the mean-squared displacement and the dimensionless turbulent diffusivity are calculated as a function of a dimensionless time. The influence of molecular diffusivity is represented by a Peclet number, $uL/\mathscr{D}$. A decrease in the Peclet number (or an increase in the molecular diffusivity) causes a decrease in all three of these quantities at any fixed time. However, for time approaching zero the turbulent diffusivity and the turbulence contribution to the mean-squared displacement becomes less sensitive to changes in Pe. Of particular interest is the calculated ratio, for large time, of the Lagrangian turbulent diffusivity for a given Pe to the Lagrangian turbulent diffusivity of fluid particles. For large Peclet numbers this ratio is relatively insensitive to the form of the Eulerian correlation. The turbulent diffusivity is decreased by 10% when the ratio of the molecular diffusivity to the long time turbulent diffusivity of fluid particles equals 0.2, by 30% when the same ratio is unity and by about 50% for a ratio of 2.

Asymptotic relations can be obtained for small and large times by using Taylor's small and large time results for the turbulent contribution to the mean-squared displacement. The small time approximation agrees with Saffman's result but is less restrictive. It requires only that su/L be small, whereas the Saffman approximation has the additional requirement of small $s\mathscr{D}/\lambda^2$. The long time approximation agrees at infinite time with Saffman's suggestion that $[(R^{\mathrm{L}}_{\mathrm{f}} - R^{\mathrm{L}}_{d})/R^{\mathrm{L}}_{\mathrm{f}}]$ is a constant for a given Peclet number, but is applicable over a larger range of times. This can be seen from the comparison of the dashed curve (a2) with the calculations in Fig. 4(a).

Despite the necessary simplifying assumptions, the method described in this paper offers a quantitative approach to engineering heat and mass transfer calculations. The validity of the assumptions and the overall accuracy of the method could be assessed by comparisons with results obtained by a direct numerical simulation of a practical flow. Such results on the effect of molecular diffusivity on the Lagrangian property autocorrelation in the center of a numerically simulated turbulent channel are reported in a recent thesis by Kontomaris [3].

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