Conditional scalar mixing statistics in homogeneous isotropic turbulence

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Abstract. We use simple scalar mixing models coupled to a Lagrangian stochastic trajectory model to calculate a range of conditional scalar statistics for three different source configurations, a uniform gradient source, a line plume and a scalar mixing layer. Comparison with appropriate direct numerical simulation results and experimental data shows that the interaction by exchange with the conditional mean mixing model gives good results for statistics conditioned on the scalar concentration (mean velocity, mean scalar diffusion and mean scalar dissipation rate) for the uniform gradient source and the line plume and for the mean velocity conditioned on the concentration in the mixing layer. The simpler interaction by exchange with the mean model does not perform as well and in particular does not capture the non-linearity of the conditional diffusion for the line plume and the mixing layer. Our results suggest that some of the approximations used for these conditional statistics may not be appropriate.
1. Introduction

Scalar mixing in turbulence influences many aspects of environmental and engineering processes and has been studied widely at both a fundamental and applied level. The dispersion and dilution of pollutants, heat and mass transfer, the airborne spread of pests, spores and diseases, the use of chemical plumes by animals to seek food or a mate and chemical reactions in engines and other reactors and in the environment all are strongly influenced by turbulent mixing.

The transport of material, which is at the core of scalar mixing, is most naturally dealt with in a Lagrangian reference frame, i.e. in a frame which moves with the material itself. Lagrangian methods have been used to describe turbulent transport at least since the classic paper of Taylor [1], but have now become widespread in fundamental studies [2], in environmental applications [3, 4] and in combustion and chemical reactions in engineering [5, 6].

In the latter case, so-called mixing models are used to represent the change in scalar concentration along a trajectory through the fluid and so to model the dissipation of scalar fluctuations explicitly. Recently, Sawford [7] and Luhar and Sawford [8] have used the mixing model approach to calculate scalar fluctuation statistics in turbulent plumes in grid turbulence and in a laboratory flow simulating convective boundary layer turbulence in the atmosphere.

These mixing models represent a closure for conditionally averaged scalar statistics, such as the mean scalar dissipation conditioned on the concentration which enters the evolution equations for the probability density function (pdf) for the scalar concentration. The great advantage of these methods is that the non-linear convection term, and in the case of reactive scalars the reaction source term, are represented exactly and do not have to be modelled. The approach is readily generalized to a large number of scalar species and chemical reactions, although then the computational load becomes a significant constraint.

The conditional moment closure (CMC) theory developed by Klimenko [9] and Bilger [10] greatly reduces this computational load by developing a closure for the mean concentration of a reactive scalar conditioned on the concentration of a conserved scalar, thus in a sense partitioning the mixing and chemical reaction into separate steps. The CMC method also carries
an equation for the conserved scalar pdf and unconditional reactive scalar statistics are calculated by averaging over the conserved scalar pdf. The CMC equation itself depends on the conditional scalar dissipation and other conditional statistics such as the mean velocity conditioned on the scalar concentration. In practical applications of the CMC method, it is common to use a presumed form for the conserved scalar pdf, and to make simplifying assumptions about the form of the conditional mean velocity and scalar dissipation, but errors can arise due to inconsistencies in these assumptions. Recently, Klimenko and Pope [11] developed a self-consistent approach by combining CMC with a mixing model closure for the conserved scalar pdf.

In the present paper, we explore the consequences of simple mixing model closures for the form of a range of conditional statistics. We use the two simplest mixing models, the interaction by exchange with the mean (IEM) and the interaction by exchange with the conditional mean (IECM) models to calculate the mean velocity, the mean scalar diffusion and the mean scalar dissipation, all conditioned on the scalar concentration, and the conditional mean diffusion conditioned on the velocity, for a uniform gradient source, a line plume and a scalar mixing layer.

Our main motivation is ultimately the extension of pdf methods to the calculation of both conserved and reactive scalar statistics in turbulent plumes in the atmosphere and other environmental flows. In this context, the line plume case is of primary interest here, and the other cases are included mainly to explore the effect of the source distribution on the structure of these conditional statistics. The IECM model is particularly well suited to the treatment of turbulent plumes because it accounts for the effect of the bulk motion of the plume (known as plume flapping or meandering) near the source. This bulk motion contributes to the scalar variance, but not to the dissipation, and it is important that this partitioning of the scalar fluctuations into bulk and in-plume, or dissipative, components is properly represented.

Where possible we compare our results with direct numerical simulation (DNS) or experimental results. We also use our results to test some of the approximations to these conditional statistics commonly used in practical CMC modelling.

The outline of the paper is as follows. In section 2 we describe the theory underlying the closures. We apply the closures to the three different source configurations in sections 3–5 and summarize our conclusions in section 6.

2. Theory

2.1. Exact velocity-scalar joint pdf

There are several ways in which the evolution equation for the joint velocity-scalar pdf $P(V, \psi; x, t)$ can be derived [5, 12]. For constant density flows it can be written as

$$\frac{\partial P}{\partial t} + V_j \frac{\partial P}{\partial x_j} = - \frac{\partial \langle A_j \rangle}{\partial V_j} P - \frac{\partial \langle \Theta \rangle}{\partial \psi} P,$$

where $A$ and $\Theta$ are given from the conservation equations for momentum and scalar concentration respectively by

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = A_j = - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2}$$

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and
\[
\frac{\partial \phi}{\partial t} + \sum_{j} u_j \frac{\partial \phi}{\partial x_j} = \Theta = \kappa \frac{\partial^2 \phi}{\partial x_i^2}.
\]
(3)

In (1)–(3), \(V\) and \(\psi\) are the sample space variables corresponding to the fluid velocity \(u(x, t)\) and scalar concentration \(\phi(x, t)\), respectively, \(\nu\) and \(\kappa\) the kinematic viscosity and molecular diffusivity, \(\rho\) the fluid density and \(p\) the pressure. We denote the minimum and maximum values of the concentration by \(\psi_{\text{min}}\) and \(\psi_{\text{max}}\), respectively. More generally, (2) might include body forces and (3) might include a source term due to chemical reaction if the scalar is reactive. The terms \(\langle A_j | V, \psi \rangle\) and \(\langle \Theta | V, \psi \rangle\) are averages conditional on the specified values \(u(x, t) = V\) and \(\phi(x, t) = \psi\) and from (2) and (3) can be interpreted as the conditional mean acceleration and the conditional mean diffusion, respectively. Here we are mostly interested in closures for the scalar term \(\langle \Theta | V, \psi \rangle\) and hence will not be concerned with the details of closures for the conditional mean acceleration.

Thus, writing out the conditional mean diffusion explicitly, the evolution equation (1) becomes
\[
\frac{\partial P}{\partial t} + V_j \frac{\partial P}{\partial x_j} = -\frac{\partial \langle A_j | V, \psi \rangle P}{\partial V_j} - \kappa \frac{\partial \langle \partial^2 \phi/\partial x_i^2 | V, \psi \rangle P}{\partial \psi}.
\]
(4)
The evolution equation for the scalar pdf, denoted by \(P_\phi\), can be obtained by integrating (4) over the velocity,
\[
\frac{\partial P_\phi}{\partial t} + \frac{\partial \langle V_j | \psi \rangle P_\phi}{\partial x_j} = -\kappa \frac{\partial \langle \partial^2 \phi/\partial x_i^2 | \psi \rangle P_\phi}{\partial \psi}.
\]
(5)
Using the fine-grained properties of the pdf [12], (5) can also be written in terms of the conditional dissipation
\[
\frac{\partial P_\phi}{\partial t} + \frac{\partial \langle V_j | \psi \rangle P_\phi}{\partial x_j} = -\kappa \frac{\partial^2 \langle \partial \phi/\partial x_i \rangle^2 | \psi \rangle P_\phi}{\partial \psi^2} + \kappa \frac{\partial^2 P_\phi}{\partial x_i^2}.
\]
(6)
Note that (5) and (6) include direct molecular terms which arise from the contribution of the mean concentration in the conditional moments and from the last term on the right-hand side of (6). For example,
\[
\langle \left( \frac{\partial \phi}{\partial x_i} \right)^2 | \psi \rangle = \langle \left( \frac{\partial \phi'}{\partial x_i} \right)^2 | \psi \rangle + \left( \frac{\partial \phi}{\partial x_i} \right)^2,
\]
where we have written the concentration as the sum of fluctuating and mean parts \(\phi'\) and \(\bar{\phi}\). These direct molecular terms are negligible at large Reynolds number (and finite Schmidt number), but are retained here for completeness.

2.2. Lagrangian stochastic closure with mixing

Lagrangian methods are widely used in modelling turbulent dispersion in engineering and environmental flows [3, 5, 6]. In this approach, the motion of an independent marked particle
along its trajectory is represented as a continuous Markov process and so can be written as the Itô stochastic differential equations (SDEs)

\[
du_i = a_i(\mathbf{u}, \mathbf{x}, t) \, dt + \sqrt{C_0 \varepsilon} \, d\xi_i(t), \quad (8)
\]

\[
dx_i = u_i \, dt + \sqrt{2\kappa} \, d\xi^{(m)}_i(t), \quad (9)
\]

where the drift term \(a_i(\mathbf{u}, \mathbf{x}, t)\) represents a closure for the conditional mean acceleration, \(C_0\) is the Lagrangian structure function constant [13], \(\varepsilon\) the rate of dissipation of turbulence kinetic energy and \(d\xi\) and \(d\xi^{(m)}\) are independent incremental vector Wiener processes [14]. Here \(\mathbf{u}(t)\) and \(\mathbf{x}(t)\) are Lagrangian variables, but to simplify the notation we use the same symbols as for the corresponding Eulerian quantities, emphasizing the time dependence to identify the Lagrangian character when there might be some confusion. Sawford [7] has discussed the different approaches to modelling the drift term in the atmospheric and engineering research communities. Note that we have included the direct effect of molecular diffusion explicitly in (9).

Let us put aside the question of modelling the flow field for a moment and assume that the flow field \(\mathbf{u}(\mathbf{x}, t)\) is given exactly (e.g. from direct numerical simulations). Then the joint displacement statistics of \(N\) marked particles (i.e. molecules) moving according to (9) can be used to calculate the \(N\)th moment of the concentration field exactly for incompressible flow [2, 15]. In this case, the dissipative effect of turbulent and molecular mixing is related to the relative dispersion of pairs of molecules. In the large Reynolds number limit (at finite Schmidt number), the concentration statistics are independent of the molecular diffusivity, but at finite Reynolds number in addition to the direct effect of molecular diffusion there is also an effect due to the interaction between the turbulence and the molecular diffusion [16].

If instead we choose to model the flow field using the SDE (8) then we strictly have a large Reynolds number model for the velocity of the fluid along the trajectory of a single fluid particle (for which \(\kappa = 0\)) and so the pair of equations (8) and (9) neglect the interaction between turbulent dispersion and molecular diffusion. Finite Reynolds number effects can be modelled using a second-order SDE for the acceleration along the trajectory [17]–[19], or more approximately here, by adjusting the value of the constant \(C_0\) in (8) to allow for the effect of Reynolds number on the Lagrangian turbulence time scale [17, 20]. Saffman’s [16] correction to the turbulent dispersion at large time to account for the interaction of turbulence and molecular diffusion can also be accommodated by adjusting \(C_0\) by a factor of \([1 - 0.23\sqrt{15}Sc^{-1}\, Re_\lambda^{-1}]^{-1}\) but for \(Sc\) of order 1 this correction is less than 4% even for values of the Taylor-scale Reynolds number as low as 25. Using DNS for \(Re_\lambda = 92\), Yeung and Borgas [21] confirmed that the correction is only 1% for \(Sc\) of order 1. Thus, the neglect of the interaction between molecular diffusion and turbulent dispersion in (8) and (9) has little influence on the prediction of one-particle scalar statistics such as the mean concentration and the turbulent flux, and for the stationary state where production and dissipation balance, it also has little effect on second-order statistics such as the scalar variance or the dissipation.

The SDEs (8) and (9) can be used only to calculate single-particle statistics. To model higher-order concentration statistics using the marked fluid particle approach, we need to explicitly model the joint motions of \(N\) particles, i.e. for two particles say, we would replace (8) by an appropriate SDE for the joint motion of the particles. This approach has been pursued in the atmospheric research community [22]. An alternative approach widely used in the chemical
engineering community is to retain the independent particle equations (8) and (9) and to model the dissipative effect of mixing explicitly. We follow the second approach here and complete the closure assumptions by adding to (8) and (9) a mixing model to describe the change of the concentration along the particle’s trajectory. We consider only the two simplest such models, known respectively as the IEM model and the IECM model. These models can be written in the form

\[
\frac{d\phi}{dt} = \theta(u, \phi, x, t) = -\frac{\phi - \chi}{t_m},
\]

(10)

where

\[
\chi = \bar{\phi} \quad \text{(IEM)}, \quad \chi = \langle \phi | V \rangle \quad \text{(IECM)}
\]

(11)

and \(t_m\) is the mixing time scale. We noted in the introduction, and we elaborate in section 4, that the IECM model is more appropriate for turbulent plumes because it relates the dissipation of scalar variance to the in-plume fluctuations, rather than to the total variance. The latter includes a contribution from bulk motions of the plume which are not dissipative. Appropriate specification of the mixing time scale is critical to the performance of these mixing models [7].

It is well known [6, 7] that mixing according to the IEM model introduces an extra term in the scalar flux equation which reduces the turbulent flux and in general changes the mean concentration. At first sight, this is precisely what we expect from the interaction of molecular mixing with the turbulent transport. However, we have argued above that the effect of this interaction is small, whereas we will see below that the effect of the extra term arising from the IEM model is far from negligible. Thus, although this is not the full story, the IEM model is generally regarded as unsatisfactory on these grounds. On the other hand, mixing according to the IECM model has no effect on one-particle statistics such as the mean concentration and the scalar turbulent flux, and thus neglects completely the interaction between molecular diffusion and the turbulence, a good approximation except for low Reynolds number and/or low Schmidt number. Thus, most of our attention will focus on the IECM model, although we will also present some results for the IEM model for comparison.

Thus, we have finally a set of SDEs (8)–(10) describing the motion and concentration of a particle along a trajectory through the fluid. The corresponding Fokker–Planck equation is

\[
\frac{\partial P}{\partial t} + V_j \frac{\partial P}{\partial x_j} = - \frac{\partial a_j(V) P}{\partial V_j} - \frac{\partial \theta(V, \psi) P}{\partial \psi} + \frac{1}{2} C_0 \frac{\partial^2 P}{\partial V_i^2} + \kappa \frac{\partial^2 P}{\partial x_i^2},
\]

(12)

where we have suppressed the dependence of \(a\) and \(\theta\) on position and time. Note that the drift term \(a\) does not depend on \(\psi\), reflecting the fact that we assume that the scalar field is passive.

Comparing (12) with the exact equation (4), we see that, as we have already noted, the drift term and the term in \(C_0\) in (8) represent a closure for the conditional mean acceleration, so the mixing model term and the term in \(\kappa\) represents a closure for the conditional mean diffusion

\[
\kappa \frac{\partial \langle \partial^2 \phi / \partial x_i^2 \rangle |V, \psi \rangle P}{\partial \psi} = \frac{\partial \theta(V, \psi) P}{\partial \psi} - \kappa \frac{\partial^2 P}{\partial x_i^2}.
\]

(13)
Integrating (13) using the boundary condition \( \langle \partial^2 \phi / \partial x_i^2 \rangle_{V, \psi_{\min}} P(V, \psi_{\min}) = 0 \) [12] and noting that \( P(V, \psi) = 0 \) for \( \psi < \psi_{\min} \) we obtain an explicit expression for the conditional diffusion:

\[
\kappa \langle \partial^2 \phi / \partial x_i^2 \rangle_{V, \psi} P(V, \psi) = \theta(V, \psi) P(V, \psi) - \kappa \frac{\partial^2}{\partial x_i^2} \int_{\psi_{\min}}^\psi P(V, \psi') d\psi'.
\]

(14)

We are particularly interested in statistics conditioned separately on either the velocity or the concentration for the IEM and IECM models. Substituting for \( \theta \) from (11) and integrating over either \( V \) or \( \psi \) as appropriate, we obtain the conditional diffusion statistics

\[
\kappa \langle \partial^2 \phi / \partial x_i^2 \rangle_{V} = \bar{\phi} - \langle \phi | V \rangle_{tm} + \kappa \frac{\partial^2}{\partial x_i^2} \langle \phi | V \rangle \quad \text{(IEM)}
\]

(15)

and

\[
\kappa \langle \partial^2 \phi / \partial x_i^2 \rangle_{\psi} = -\frac{\psi - \bar{\phi}}{t_m} - \frac{\kappa}{P_\phi(\psi)} \frac{\partial^2}{\partial x_i^2} \int_{\psi_{\min}}^\psi P_\phi(\psi') d\psi' \quad \text{(IEM)}
\]

(16)

where

\[
\bar{\phi}(\psi) = \int \langle \phi | V \rangle P(V | \psi) dV.
\]

(17)

Note that for the diffusion conditioned on the velocity, the contribution from the mixing closure term vanishes for the IECM model, but is non-zero for the IEM model.

Alternatively, integrating (12) over the velocity and comparing it with version (6) of the exact equation for the scalar concentration pdf, we obtain a closure for the dissipation conditional on the scalar concentration

\[
\kappa \frac{\partial^2}{\partial \psi^2} \langle (\partial \phi / \partial x_i)^2 \rangle_{\psi} P_\phi(\psi) = -\frac{1}{t_m} \frac{\partial (\psi - \bar{\phi}) P_\phi(\psi)}{\partial \psi} \quad \text{(IEM)}
\]

(18)

Using the boundary conditions

\[
\partial \langle (\partial \phi / \partial x_i)^2 \rangle_{\psi} P_\phi(\psi) / \partial \psi = 0 \quad \text{and} \quad \langle (\partial \phi / \partial x_i)^2 \rangle_{\psi} P_\phi(\psi) = 0 \quad \text{at} \quad \psi = \psi_{\min}
\]

and noting that \( P_\phi(\psi) = 0 \) for \( \psi < \psi_{\min} \), we can integrate (18) twice to give

\[
\kappa \langle (\partial \phi / \partial x_i)^2 \rangle_{\psi} P_\phi = -\frac{1}{t_m} \int_{\psi_{\min}}^\psi (\psi' - \bar{\phi}) P_\phi(\psi') d\psi' \quad \text{(IEM)}
\]

(19)
In the next sections, we apply these results to the temporal evolution of the scalar fields resulting from three specific instantaneous source distributions: a uniform scalar gradient, a localized area source and a mixing layer.

3. Uniform scalar gradient

Here we consider an instantaneous uniform scalar gradient source function \( S(\mathbf{x}, t) = mz \delta(t) \), where, without loss of generality, we have chosen the scalar gradient to be in the \( z \) or \( x_3 \) direction. This case has been studied comprehensively in stationary isotropic turbulence using DNS [23] and theoretically using a generalized mixing model [24]. Almost all our results can be derived analytically, so it is also a useful test case for numerical codes. Since turbulent transport in the \((x, z)\) plane has no effect on the scalar statistics in this case, equations (8) and (9) reduce to one-dimensional forms which, for stationary isotropic turbulence, can be written as [25]

\[
dw = -\frac{C_0 \varepsilon}{2 \sigma_w^2} w \, dt + \sqrt{C_0 \varepsilon} \, d\xi(t),
\]

\[
dz = w \, dt + \sqrt{2 \kappa} \, d\xi^{(m)}(t).
\]

For convenience, we use the Cartesian notation \( \mathbf{V} = (U, V, W), \mathbf{u} = (u, v, w) \) etc for phase space and physical quantities.

The mean concentration is unaltered by turbulent mixing so we have \( \bar{\phi} = mz \). In this case where the scalar source conditions impose no length scale on the scalar field it is usual to take the mixing time scale to be proportional to the turbulence time scale, which is constant. Thus, to be consistent with other work [5, 23, 24] we write

\[
t_m = \frac{2k}{C_\phi \varepsilon} = \frac{3C_0}{2C_\phi} T_L,
\]

where \( k \) is the turbulence kinetic energy, \( T_L (=4k/3C_0 \varepsilon) \) the Lagrangian integral time scale and \( C_\phi \) a constant.

Before proceeding to results for the conditional statistics, we return to a discussion of the role of the explicit representation of molecular diffusion in (9). Let us for the moment consider the calculation of the concentration variance using marked particle displacement statistics. For a uniform gradient source, we have the exact result [22, 26],

\[
\langle \phi'^2(t) \rangle = m^2 (\sigma_z^2(0; t) - \sigma_A^2(0; 0, t)),
\]

where \( \sigma_z^2(0; t) \) is the dispersion in the \( z \)-direction at the time of release \( t = 0 \) of those particles which are at a specified point at time \( t \), i.e. it is the backward dispersion from the measurement point and time to the source time. Similarly, \( 2\sigma_A^2(0; 0, t) = \langle (z^{(1)} - z^{(2)})^2 \rangle \) is the backward relative dispersion of a pair of particles which are together at time \( t \). Since the direct effect of molecular diffusion contributes a term \( 2\kappa t \) to both \( \sigma_z^2 \) and \( \sigma_A^2 \), it cancels in (23). The interaction between molecular diffusion and turbulent dispersion does not cancel, but we have already argued that it is small. Thus, for the case of a uniform gradient source, to first order, the explicit inclusion of
molecular diffusion in equation (9) for the particle’s trajectory does not affect the scalar variance and therefore we set $\kappa = 0$.

Since (20) and (21) are linear, the velocity and displacement are jointly Gaussian so the conditional mean concentration can be calculated analytically following Sawford [7] to give

$$
\langle \phi | V \rangle = \bar{\phi} + \frac{\langle w' \phi' \rangle}{\sigma_w^2} W.
$$

(24)

Thus, the scalar concentration evolution equation (10) is also linear in concentration and velocity and so the velocity component $w$ and the scalar concentration are jointly Gaussian with variances $\sigma_w^2$ and $\sigma_\phi^2$, respectively, and correlation $\rho_{w\phi} = \langle w' \phi' \rangle / (\sigma_w \sigma_\phi)$, where $\langle w' \phi' \rangle$ is the turbulent scalar flux. This joint Gaussianity has been observed in DNS [23], although experimental data [27] and theoretical studies [28] suggest that this is not true in general. As a consequence of joint Gaussianity, the conditional mean velocity is given by

$$
\langle w | \psi \rangle / \sigma_w = \frac{\langle w' \phi' \rangle}{\sigma_w^2 \sigma_\phi} (\psi - \bar{\phi}) = -\rho_{w\phi} (\psi - \bar{\phi}) / \sigma_\phi,
$$

(25)

which is consistent with a Gaussian pdf in (27) of Overholt and Pope [23]. In the stationary state where production and dissipation of scalar variance are in balance the conditional mean velocity can also be written in terms of the unconditional mean scalar dissipation rate $\langle w | \psi \rangle = -(\psi - \bar{\phi}) \varepsilon_\phi / m \sigma_\phi^2$, where $\varepsilon_\phi = \kappa \langle (\partial \phi' / \partial x_i)^2 \rangle$.

Now using (24) we can calculate explicit expressions for the conditional statistics given by (15), (16) and (19), normalized as in [23], giving

$$
\kappa \langle \partial^2 \phi' / \partial x_i^2 | V \rangle \sigma_\phi / \varepsilon_\phi = \frac{W}{\sigma_w} \quad \text{(IEM)}
$$

and

$$
\kappa \langle \partial^2 \phi' / \partial x_i^2 | \psi \rangle \sigma_\phi / \varepsilon_\phi = \frac{\psi - \bar{\phi}}{\sigma_\phi} \quad \text{(IEM and IECM)}
$$

(27)

and

$$
\kappa \langle (\partial \phi' / \partial x_i)^2 | \psi \rangle / \varepsilon_\phi = 1 \quad \text{(IEM and IECM)},
$$

(28)

where, from (17), $\bar{\phi}(\psi) = \bar{\phi} (1 - \rho_{w\phi}^2) + \psi \rho_{w\phi}^2 \bar{\phi}$ and the unconditional dissipation is given by

$$
\varepsilon_\phi = \frac{\langle \phi^2 \rangle}{t_m} \quad \text{(IEM)}
$$

$$
= (1 - \rho_{w\phi}^2) \frac{\langle \phi^2 \rangle}{t_m} \quad \text{(IECM)}.
$$

(29)
We can also calculate the mechanical to scalar time scale ratio \( r = 2k \epsilon_{\phi}/\epsilon \langle \phi'^2 \rangle \) from (22) and (29) to give

\[
    r = C_\phi \quad \text{(IEM)}
\]
\[
    = (1 - \rho_{w\phi}^2)C_\phi \quad \text{(IECM).}
\]

(30)

We have already noted that in the general case according to the IECM model the diffusion conditioned on the velocity vanishes, whereas it is non-zero for the IEM model and, from (26), is linear in the velocity for the uniform gradient case. In the scaled form of (27) and (28), both models give the same result for both the diffusion and the dissipation conditioned on the concentration, but it is clear that this is purely a consequence of the scaling since with the time scale specified by (22) the models give different results for the unconditional dissipation. An alternative interpretation is that the time scale can be chosen to fit the observed unconditional scalar dissipation, in which case different time scales are implied by each model. All these conditional statistics have been expressed in terms of the scalar flux and the scalar variance.

The conservation equations for the scalar flux and scalar variance (see e.g. (41) and (42) in [24]) can be solved analytically for both the IEM and IECM models. The solutions are

\[
    \langle w'\phi' \rangle = -\sigma_w^2 Tm[1 - \exp(-t/T)]
\]

and

\[
    \langle \phi'^2 \rangle = 2\sigma_w^2 Tm m^2 \left\{ \frac{1}{2} \left[ 1 - e^{-2t/t_m} \right] - \frac{T}{2T - T_m} \left[ e^{-t/T} - e^{-2t/t_m} \right] \right\}
\]
\[
    + 2\sigma_w^2 T^2 m^2 \left\{ \frac{1}{2} \left[ 1 - e^{-2t/t_m} \right] - \frac{4T}{2T - T_m} \left[ e^{-t/T} - e^{-2t/t_m} \right] + \frac{2T}{2T - T_m} \left[ e^{-2t/T} - e^{-2t/t_m} \right] \right\},
\]

(32)

where

\[
    T = T_L \left[ \frac{3C_0}{3C_0 + 2C_\phi} \right] \quad \text{(IEM)}
\]
\[
    = T_L \quad \text{(IECM).}
\]

(33)

In the large time limit, both the flux and variance take constant values which can be written in terms of \( C_0 \) and \( C_{\phi} \). Thus, both models can be fitted to the stationary values of the flux and variance and as shown in figure 1, both also give a good representation of the time evolution of these quantities (and of \( \rho_{w\phi} \)) determined by Overholt and Pope [23] in their DNS calculations. Because production balances dissipation in this stationary limit these fitted values of \( C_0 \) and \( C_{\phi} \) also reproduce the stationary value of the unconditional scalar dissipation and of the scalar diffusion and scalar dissipation conditioned on the concentration. However, neither model captures the evolution of the DNS data for the scalar dissipation (as represented by the time scale ratio) at small times. The IEM model overestimates \( r \) and \( \epsilon_{\phi} \) at small times, whereas the IECM model underestimates them both.
Figure 1. Comparison of IECM (——), IEM (----) and VCIEM (– – –) models with DNS results for the normalized scalar variance (♦), normalized scalar flux (■), the correlation between the velocity and scalar concentration (●) and the ratio of the turbulence time scale to the scalar time scale (▲) for (a) $R_{e_{\lambda}} = 28$, (b) $R_{e_{\lambda}} = 52$ and (c) $R_{e_{\lambda}} = 84$. For clarity, the VCIEM results are shown only for the time scale ratio $r$. 

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Table 1. Model parameters which fit the DNS results of Overholt and Pope [23].

| Re_λ | C_0   | C_φ   | ζ   | C_0   | C_φ   | ζ   | C_0   | C_φ   | ζ   |
|------|-------|-------|-----|-------|-------|-----|-------|-------|-----|
| 28   | 1.81  |       | 1   | 1.81  |       | 1   | 2.07  |       | 1   |
| 52   | 2.04  |       | 1   | 2.60  |       | 0.47| 2.04  |       | 1   |
| 84   | 2.08  |       | 1   | 4.74  |       | 0.23| 2.08  |       | 1   |

With these solutions for the scalar flux and variance all the statistics conditional on the concentration (the conditional mean velocity, diffusion and dissipation) are also in good agreement with the DNS of Overholt and Pope [23] for both models. The diffusion conditioned on the velocity is the only quantity which discriminates between the two models in the stationary limit. The DNS results of Overholt and Pope show that this quantity is linear with a positive slope in qualitative agreement with the IEM model, but the slope is only about one-half that predicted by (26). Fox [24] used a linear combination of the IEM and IECM models, which he called the velocity-conditioned IEM (VCIEM) model, to fit the stationary values of $r$, $\rho_w \phi$ and the velocity-gradient-scalar-gradient correlation $\rho \nabla w \nabla \phi$ (which can be calculated from the diffusion conditioned on the velocity). Thus, he effectively fitted three parameters $C_0$, $C_\phi$ and $\zeta$, the weighting of the two models, to the stationary values of the flux, the variance and the diffusion conditioned on the velocity. Of course, this model is also a good representation of the time evolution of the flux, the variance and the correlation, but we see from figure 1 that although it is a closer fit to the time scale ratio for small times than either the IEM or the IECM model, there is still a significant discrepancy there, and a precise fit to the DNS results requires the mixing time scale to be a function of time. Table 1 shows the fitted values of the parameters $C_0$, $C_\phi$ and $\zeta$ for the three models.

Corresponding to (33) we have for the VCIEM model,

$$T = T_L \left[ \frac{3C_0}{3C_0 + 2\zeta C_\phi} \right] \quad \text{(VCIEM)}. \quad (34)$$

The factor in brackets on the right-hand side represents the effect of mixing on the stationary value of the turbulent flux, which we have already noted can only be achieved physically by the interaction of molecular and turbulent diffusion. That is, we should interpret the ratio $T/ T_L$ as the ratio of the Lagrangian integral time scale for the fluid velocity along a molecular trajectory to that along the trajectory of a fluid particle. Thus, the VCIEM model effectively models the Saffman [16] correction to $C_0$ by the factor $1 + \frac{3}{2} \zeta C_\phi / C_0$. Using the fitted values in table 1, we see that this factor ranges from 1.27 at $Re_\lambda = 28$ to 1.09 at $Re_\lambda = 84$. The correction implied by the fitted parameters for the VCIEM model is nearly an order of magnitude larger than the Saffman correction discussed above. Thus, in order to fit the DNS data for the diffusion conditioned on the velocity using the VCIEM model, it is necessary to adopt values for the parameters which strongly overemphasize the effect of mixing on the turbulent flux.

4. Line plume

Conditional scalar statistics such as those discussed in section 2, have been studied recently for a line plume in a turbulent channel flow by Brethouwer and Nieuwstadt [29] using DNS. The source
was located in the centre of the channel of height $H$, and results were presented at distances $x$ up to $14H$ down-stream. For $x$ up to about $8H$, the plume lies completely in the centre region of the channel, where the turbulence is approximately homogeneous. In the far-field, where $x$ is greater than about $12H$, the effects of inhomogeneity due to the walls begin to influence the results. Nevertheless, these results are a useful semi-quantitative test of our model predictions for homogeneous turbulence.

Sawford [7] has studied concentration statistics for an instantaneous area source in decaying isotropic turbulence using both the IEM and IECM models. Ignoring the effects of streamwise turbulence compared with advection by the mean flow, and invoking the Taylor transformation $x = \bar{u}t$, this instantaneous area source is equivalent to a continuous line source. Sawford showed that good agreement with data from a line source in grid turbulence can be obtained, particularly for the IECM model, if the mixing time scale is based on the time scale of the instantaneous plume. The time scale he used was derived empirically from data for the plume-integrated second moment of the concentration. This empirical time scale is a linear function of time $t_m = 1.2t$ for moderate to large times ($t/t_0 > 0.5$, where $t_0$ is the source release time or equivalently the travel time from the grid to the source), but falls quite strongly below this linear form at smaller times. Sawford ascribed this reduction in the mixing time scale to the effect of molecular diffusion, but in fact it occurs because the correct mixing time scale close to the source is determined by the ratio of the variance of concentration fluctuations internal to the plume, not the total variance, to the scalar dissipation rate. This ratio is represented correctly by the IECM model, for which we have [7]

$$t_m = -2 \left( \int_{-\infty}^{\infty} \phi^2 \, dz - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle \phi | w \rangle^2 P(w) \, dw \, dz \right) / \left( \partial \int_{-\infty}^{\infty} \phi^2 \, dz / \partial t \right).$$

Thus, following Sawford, we take the empirical form

$$t_m / t_0 = 0.6t / t_0 (1 + \tanh((\ln(t/t_0) + 1.5)/0.7)),$$

which represents the mixing time scale for the line source data of Sawford and Tivendale [30]. The precise form of the time scale near the source is dependent on the meandering contribution to the fluctuations, i.e. on factors such as the source size and the molecular diffusivity (for very small sources), and so will be different for different data sets. For example, Sawford found that a slight modification of (36) was needed to fit the data of Warhaft [31].

We evaluated the various conditional statistics numerically using Sawford’s [7] versions of (8)–(11) appropriate to decaying isotropic turbulence to calculate the velocity, position and concentration as functions of time along $N = 6 \times 10^7$ trajectories. The Eulerian turbulence statistics and the molecular diffusivity were specified according to the Sawford and Tivendale [30] data described in table 1 of Sawford [7]. Here we used an instantaneous top-hat source

$$S(x, t) = \Delta_0^{-1}, \quad |z| < \Delta_0/2,$$

$$= 0, \quad |z| > \Delta_0/2$$

of width $\Delta_0 = 4 \times 10^{-4}$ m, instead of the Gaussian source used by Sawford, mainly so that we have a fixed source concentration. The unconditional plume concentration statistics are very close to those described by Sawford.

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The mean concentration profile can be represented analytically as

\[
\bar{\phi}(z, t) = \frac{Q}{2\Delta_0} \left[ \text{erf} \left( \frac{\Delta_0/2 + z}{\sqrt{2}\sigma_z} \right) + \text{erf} \left( \frac{\Delta_0/2 - z}{\sqrt{2}\sigma_z} \right) \right]
\] (38)

and the conditional mean concentration is

\[
\langle \phi | W \rangle = \frac{Q}{2\Delta_0} \left[ \text{erf} \left( \frac{\Delta_0/2 + z - \rho_{wz} W\sigma_z / \sigma_w}{\sqrt{2}\sigma_z (1 - \rho_{wz}^2)^{1/2}} \right) + \text{erf} \left( \frac{\Delta_0/2 - z + \rho_{wz} W\sigma_z / \sigma_w}{\sqrt{2}\sigma_z (1 - \rho_{wz}^2)^{1/2}} \right) \right],
\] (39)

where \(\sigma_z(t)\) is the single-particle dispersion, \(\rho_{wz}(t)\) the correlation between the position and velocity along a trajectory and \(\sigma_w(t)\) the velocity standard deviation. Analytical expressions for these quantities are given by Sawford [7] for decaying grid turbulence. Except for very close to the source, (38) can be approximated by a Gaussian

\[Q\exp\left(-\frac{z^2}{2\sigma_p^2}\right)/\sqrt{2\pi\sigma_p},\]

where \(\sigma_p\) is a measure of the width of the plume. We take the source strength \(Q = 1\).

At specified sampling times, the cross-stream position \(z\), the concentration \(\phi\) and the velocity \(w\) were sorted jointly into bins of width 0.2\(\tilde{\sigma}_p\), 0.0125\(\bar{\phi}_0\) and 0.2\(\sigma_w\), respectively, where \(\tilde{\sigma}_p^2(t) = \Delta_0^2 + \sigma_z^2\) and \(\bar{\phi}_0(t) = \bar{\phi}(0, t)\) is the centreline value of the mean concentration profile. For \(t/t_0 \geq 0.32\), \(\tilde{\sigma}_p\) is essentially the same as the width of the mean plume \(\sigma_p\), but closer to the source the plume is narrower than \(\bar{\phi}_0\).

Before proceeding to the conditional statistics which are the main focus of this paper, we digress to examine the results for the scalar pdf. Figure 2 shows the scalar pdf calculated for the IECM mixing model for a range of cross- and down-stream locations. Very close to the source \((t/t_0 = 0.032)\), the pdf on the centreline shows a strong peak at high concentrations and that on the edge of the plume \((z/\sigma_p \approx 2)\) shows a strong peak at zero concentration. At intermediate locations the pdf shows peaks at both high and low concentrations. With increasing distance down-stream, the high-concentration peak weakens and a peak at zero concentration appears in the centreline pdf as shown in figure 2(b) for \(t/t_0 = 0.32\). Far down-stream, as shown in figure 2(c) at \(t/t_0 = 8.39\), the peak at zero concentration disappears again in the core of the plume \((z/\sigma_p \approx 0, 1)\) and is replaced by a peak at intermediate concentrations. Note that in both figures 2(b) and (c), some of the low- and high-concentration peaks have been truncated to emphasize the structure over intermediate values of the concentration.

The largest possible non-dimensional concentration is the source concentration \(Q/(\Delta_0\bar{\phi}_0)\), which takes the values 28, 46 and 95 at the three down-stream locations, and these values are much larger than the apparent cut-offs in figure 2. We conclude that mixing reduces the concentration of most of the particles in the plume to the levels indicated by the cut-offs in the pdf plots in figure 2, and although the pdfs are in principle non-zero up to the source concentration, the probability of observing such a high concentration is extremely low.

The pattern of behaviour shown in figure 2 has been observed experimentally in line plumes [32] and the near- and mid-field behaviour has been explained in terms of a 1D meandering plume model [33]. The far-field behaviour is similar to that observed in the wake from a heated cylinder [34, 35]. The IECM model thus provides a realistic representation of the scalar pdf, which is not surprising since Sawford [7] has already shown that it is a good model for the first four moments. However, a more detailed comparison with the data of Sawford and Tivendale [30] (not shown...
Figure 2. Probability density for the concentration normalized by the mean value on the centreline for cross-stream locations \( z/\sigma_p = 0 \) (---), 1 (---) and 2 (----) at down-stream locations (a) \( t/t_0 = 0.032 \), (b) \( t/t_0 = 0.32 \) and (c) \( t/t_0 = 8.39 \).
shows that the high-concentration peak in figures 2(a) and (b) is too sharp, suggesting that the IECM model underestimates the impact of the internal structure of the instantaneous plume.

We now turn to conditional scalar statistics. Despite the obvious differences in the turbulence fields and the details of the source conditions, we compare our results with those of Brethouwer and Nieuwstadt [29]. This comparison is at best semi-quantitative. They presented results at down-stream distances $x/H = 2.2, 5$ and $14$, where $H$ is the channel height. Here we have attempted to match our results to theirs in a self-consistent way, i.e. by approximately matching the relative distances from the source. We find that, across the range of conditional statistics we have studied, non-dimensional travel times of $t/t_0 = 0.32, 0.65$ and $2.26$ give a good match to the DNS results. We are able to match the cross-stream locations more precisely since in both cases we locate the sampling point in terms of the width of the mean plume, which is Gaussian at these distances from the source.

4.1. Conditional mean velocity

The conditional mean velocity $\langle w | \psi \rangle$ at a given $z$ and $t$ was calculated simply as the average velocity of all particles in the bins centred on $z$ and $\psi$ at time $t$. To compare our results with those of Brethouwer and Nieuwstadt [29] they are plotted against $\psi/\bar{\phi}_0$ in figure 3(a) for $z = \sigma_p$ using the normalization $\langle w | \psi \rangle (\bar{\phi}^2)/\bar{\phi} (w' \bar{\phi})$. With this scaling there is a good collapse of the model results for all three down-stream locations, and for the DNS results at the first two locations, with the far-field DNS results falling significantly below the other data. The model predictions match the DNS at the first two locations very well both in shape and magnitude, but overestimate the far-field results. This is not surprising considering the differences already noted between the two systems. Notice that the model curves diverge to $-\infty$ as the concentration approaches zero. This is expected on theoretical grounds, since for a location above the centreline the concentration can be zero only for particles which do not come from the source, and which do not mix with source material. Such particles must originate infinitely far above the source and so must have infinite negative velocity to reach the receptor in the finite time $t$. The DNS results seem to be consistent with this limit, although sampling fluctuations tend to obscure it in the far field. Our modelling results extend to larger concentrations than do the DNS, and show a sharp cut-off at nondimensional concentration of about three. We noted earlier that as a result of mixing this cut-off concentration is much lower than the source concentration. The sloping straight line is the so-called linear approximation (25) which is used in CMC modelling [12]. Clearly, both the model and DNS results show significant departures from this approximation.

The scaling in figure 3(a) does not collapse results at different cross-stream locations very well, and indeed the strong $z$ dependence of the concentration mean, flux and variance masks any dependence of the conditional velocity on $z$. In figure 3(b) therefore we have scaled the conditional mean velocity by the velocity standard deviation for different cross- and down-stream locations. We see that the magnitude is smaller in this scaling (by a factor of about 10 for $z/\sigma_p = 1$) and that the conditional mean velocity increases in magnitude with distance from the centreline.

Now, the velocity required for a particle to move directly in a straight line from the source location $z = 0$ at time $t = 0$ to the measurement location $z$ at time $t$ is just $z/t$ and is plotted as the horizontal lines in figure 3(b) for $t/t_0 = 0.32$ and $2.26$ at the two cross-stream locations. We see that for mid-range concentrations the conditional mean velocity is close to this straight-line velocity, i.e. particles arriving at the receptor with these concentrations have trajectories...
Figure 3. (a) Comparison of IECM model conditional mean velocity with DNS results of Brethouwer and Nieuwstadt [29] for $z/\sigma_p = 1$. Lines are model results for $t/t_0 = 0.32$ (— — —), 0.65 (– – –) and 2.26 (- - - -) and the linear approximation (——). Symbols are DNS results for $x/H = 2.2$ (●), 5 (♦) and 14 (■). (b) IECM model conditional mean velocity for different locations within the plume. Lines as in (a) with the lower pair for $z/\sigma_p = 1$ and the upper pair for $z/\sigma_p = 2$. The horizontal lines represent the velocity $w = z/t$ for straight-line trajectories from the source to the receptor. Note the different non-dimensionalization in the two panels.

distributed evenly about the straight-line path and have undergone an ‘average’ amount of mixing with the ambient. Particles arriving at the receptor with concentrations near the high concentration cut-off have undergone less mixing with the ambient. For this to be so they must spend more time in the centre of the plume (i.e. near $z = 0$) and so, on average, must have a higher velocity when they arrive at the receptor. The converse is true for particles which have low concentrations and, as we noted above, in the limit of zero concentration, particles arrive at the receptor with an infinite negative velocity. It can be seen from figure 3(b) that the correspondence between the conditional mean velocity and the direct-flight velocity is closer and covers a
wider range of concentrations as the receptor point moves closer to the centreline and further down-stream.

4.2. Mean diffusion conditioned on concentration

The mean diffusion conditioned on the concentration was calculated for the IECM model from the second of (16). The mixing closure term $-(\psi - \bar{\phi})/\tau_m$ dominates over the second term which arises from the direct molecular diffusion term in (9) and (12). We calculated the quantity $\bar{\phi}$, defined in (17), as the average of $\langle \phi|W \rangle$ over those particles in the bins centred on $z$ and $\psi$ at time $t$. Figures 4(a) and (b) compare centreline and off-axis (at $z/\sigma_p = 1$) results, respectively, with the DNS again at approximately matching down-stream locations. The normalization again is that

\[ \frac{\langle (\nabla^2 \phi) \psi \rangle}{\omega \phi \phi} \]
used by Brethouwer and Nieuwstadt [29]. Note that, as defined by Brethouwer and Nieuwstadt, for the IECM model the factor $\omega \phi = 2 \varepsilon \phi / \langle \phi'^2 \rangle$ is not equal to $2 / t_m$ (see (35)). The model captures the shape and magnitude of the DNS very well, and also reproduces the relative magnitudes at the different down- and cross-stream locations, including the crossover of the near- and far-field results with increasing concentration. It also correctly predicts that the conditional diffusion vanishes for zero concentration. As noted by Brethouwer and Nieuwstadt, the IEM model, which we see from (16) is linear in $\phi$, is not a good representation of the DNS results. The shape of the curves in figure 4 is similar to that observed in the wake of a cylinder by Kailasnath et al [35].

4.3. Mean dissipation conditioned on concentration

The mean dissipation conditioned on the concentration was calculated from (19). Care is needed with the integration, especially near the concentration limits where the pdf has sharp gradients. The integral over all concentrations vanishes (i.e. $\kappa \langle (\partial \phi / \partial x)^2 \mid \psi_{\text{max}} \rangle P_{\phi}(\psi_{\text{max}})$ vanishes), and residual integration errors for $\psi$ near $\psi_{\text{max}}$ are amplified when divided by a pdf which is close to zero. We therefore evaluated the dissipation by integrating in both directions (i.e. from $\psi_{\text{min}}$ to $\psi$ and from $\psi_{\text{max}}$ to $\psi$) and merging the two results. The term involving the mean square gradient (see (7)) is negligible, so that the results calculated from (19) essentially represent the conditional dissipation and we refer to them as such.

Figure 5 shows the conditional dissipation non-dimensionalized by the centreline mean concentration and the mixing time scale for various cross- and down-stream locations, and figure 6 shows contour plots at two down-stream locations. Near the source (figures 5(a) and 6(a)), the conditional dissipation is uni-modal with an approximately symmetrical peak near $\psi / \phi_0 \approx 1.2$ and the cross-stream variation is weak with the peak value increasing by only about 25% from the centreline to the edge of the plume. With increasing distance down-stream the dissipation becomes increasing asymmetrical and more strongly dependent on the cross-stream location. Far down-stream there is a tendency similar to, but not as strong as, the case of a wake from a cylinder [35], for a bi-modal shape to appear. At the high concentration end, the results tend to collapse for different cross-stream locations, but there is a stronger dependence on $z$ at mid-to-low-concentrations, although even at those concentrations there is only a difference of about a factor of 2 from the centreline to $z / \sigma_p = 2$. With increasing $z$ the peak moves to lower concentration.

The conditional scalar dissipation and the scalar pdf are connected through the pdf evolution equation (6) and, in principle, if the pdf is known then the conditional dissipation can be calculated [12]. This connection is clearly not simple, but Sardi et al [36] suggest that a qualitative description of the conditional scalar dissipation can be obtained in terms of the reciprocal of the pdf. Comparing figures 2(b) and 5(a) for $t / t_0 = 0.32$ we can see that this is the case up to about $\psi / \phi_0 \approx 2$, with the larger values for the pdf on the centreline corresponding to lower values of the conditional dissipation. Furthermore, although the other cases presented in figures 2 and 5 do not match fully, with increasing distance down-stream the dependence on cross-stream location becomes stronger in a reciprocal way, i.e. the conditional dissipation increases more strongly with distance from the centreline while the pdf decreases more strongly. The reciprocal relation is not complete however, since both the pdf and the conditional dissipation vanish for large values of $\psi / \phi_0$ for $t / t_0 \geq 0.32$.

The results in figures 5 and 6 can be viewed in the light of the commonly used approximations, e.g. in CMC calculations [10, 12] of neglecting the $z$ dependence of the
Figure 5. IECM model predictions for the mean scalar dissipation conditioned on the concentration at cross-stream locations $z/\sigma_p = 0$ (——), $z/\sigma_p = 1$ (—–) and $z/\sigma_p = 2$ (----) and down-stream locations (a) $t/t_0 = 0.32$, (b) $t/t_0 = 0.65$ and (c) $t/t_0 = 2.26$. 
conditional mean concentration, or replacing the conditional dissipation by the unconditional dissipation. By integrating (19) over the concentration we obtain the unconditional dissipation

\[ \kappa \langle (\partial \phi / \partial x_i)^2 \rangle \approx \varepsilon_\phi = \frac{1}{t_m} \left( \langle \phi^2 \rangle - \int_{-\infty}^{\infty} \langle \phi | w \rangle^2 P(w) \, dw \right) , \]

where the term in braces on the right represents the scalar variance due to concentration fluctuations internal to the plume, i.e. the difference between the total variance and the variance due to plume meandering [7]. Figure 7 shows the unconditional dissipation, non-dimensionalized in the same way as the conditional dissipation in figures 5 and 6, as a function of cross-stream position within the plume at different down-stream positions. The unconditional dissipation is a strong function of \( z \), varying by about an order of magnitude from the centreline to \( z / \sigma_p = 2 \), because the in-plume concentration variance decreases strongly with distance from the centreline. In contrast, we noted that the conditional dissipation is only a weak function of cross-stream position. This strong difference between the \( z \) dependence of the conditional and unconditional dissipation arises because in averaging the conditional dissipation over the distribution of concentrations, at the edge of the plume there is a much stronger weighting towards low concentrations, where the conditional dissipation is small. Our results thus suggest that the approximations described above, particularly that of replacing the conditional dissipation by the unconditional value, may not be justified, but a full assessment of their impact through explicit solutions of the CMC equations for a plume in homogeneous turbulence is required.
The unconditional dissipation itself is sometimes modelled in terms of the scalar variance, assuming that the turbulence to scalar time scale ratio is independent of cross-stream location. However, we see from figure 7(b) that this is not a good assumption close to the source, although it improves with increasing distance down-stream. The reason for the strong dependence of the time scale ratio on cross-stream position close to the source is again the presence of scalar fluctuations due to bulk motions. Since the dissipation is related to in-plume fluctuations, the time scale ratio defined in terms of the total fluctuations behaves like the ratio of the in-plume scalar variance to the total variance.

4.4. Mean diffusion conditioned on velocity

Finally, we calculate the mean diffusion conditioned on the velocity from (15). We can do this analytically since we have analytical expressions for $\bar{\phi}$ and $\langle \phi | W \rangle$ via (38) and (39). As we noted earlier, only the molecular contribution is non-zero for the IECM model, whereas the
Figure 8. Comparison of model mean diffusion conditioned on velocity for a line plume with DNS results at (a) $t/t_0 = 0.32$ (model) and $x/H = 2.2$ (DNS) and (b) $t/t_0 = 2.26$ (model) and $x/H = 14$ (DNS). Symbols are DNS results at $z/\sigma_p = 0$ (▲) and $z/\sigma_p = 1$ (■). Lines are for IECM model on the centreline $z/\sigma_p = 0$ (−−−−) and at $z/\sigma_p = 1$ (——) and for the mixing closure part of the IEM model on the centreline (−−−) and at $z/\sigma_p = 1$ (– – –). Note that the magnitude of the IECM results has been arbitrarily rescaled.

IEM model has a term $\left(\bar{\phi} - \langle \phi | W \rangle \right)/t_m$ from the mixing closure. We compare the results of our model calculations with the DNS of Brethouwer and Nieuwstadt in figure 8. The dashed lines represent the turbulent contribution for the IEM model and are essentially inverted Gaussian functions offset by the mean concentration. They have a minimum value at $W/\sigma_w = z/(\rho_w \sigma_z)$ and approach a maximum at $W = \pm \infty$. On the centreline and for $|W|/\sigma_w < 1$, the model results agree well with the DNS, but the off-axis results are somewhat larger than the DNS. Perhaps, more importantly, the IEM model results are the wrong shape. For example, at $x = 2.2H$ and $z = \sigma_p$, the DNS results peak only slightly on the negative side of zero velocity (at $W/\sigma_w \approx -0.25$) and then decrease towards a lower constant value with increasingly negative velocity. There are similar, but less obvious, symmetrical peaks at $W/\sigma_w \approx \pm 1.5$ in the DNS results on the centreline.
which are also absent in the IEM model. Similarly, at the far down-stream location \( x = 14H \), the off-axis DNS results have a maximum at \( W/\sigma_w \approx -1.25 \), whereas the model monotonically approaches a constant value at large negative velocities.

It is more difficult to compare the magnitude of the molecular contribution, which we recall is the sole contribution for the IECM model, with the DNS results since we do not have an estimate for the molecular diffusivity for the DNS. Thus, we have focused on the shape of the curves and simply rescaled the model predictions (by factors of 5 and 4 at \( x = 2.2H \) and \( 14H \), respectively) to approximately match the magnitude of the DNS results. We see that the molecular term matches the shape of the DNS results very well. In particular, for the near-field runs it shows the peaks at \( W/\sigma_w \approx \pm 1.5 \) for the centreline data and the peak at \( W/\sigma_w \approx -0.25 \) for \( z/\sigma_p = 1 \). With increasing distance down-stream, these peaks move to larger velocities and for \( t/t_0 = 2.26 \) the results at \( z/\sigma_p = 1 \) peak at \( W/\sigma_w \approx -1.25 \), in agreement with the DNS.

Since these shape effects in the data are strong, we conclude that the direct molecular contribution to the conditional diffusion is significant and perhaps dominant. Indeed, it is possible that in accord with the IECM model, the molecular contribution accounts completely for the observed DNS results. Such a conclusion would be in contrast to the uniform gradient case, where we saw that at low \( Re \) some contribution from the IEM model was needed to fit the DNS data. Perhaps the effective \( Re \) in the data of Brethouwer and Nieuwstadt [29] is large enough that the IEM contribution is negligible.

5. Scalar mixing layer

The scalar mixing layer in grid turbulence has been used to study unconditional passive and reactive concentration statistics in both the laboratory [34, 37] and numerically [38]. Li and Bilger [39] describe laboratory results for the conditional mean velocity in a scalar mixing but we are unaware of laboratory or numerical results for the other conditional statistics considered here.

The source configuration for a scalar mixing layer is illustrated in figure 1 of Bilger et al [40]. In their experiments, as in those of La Rue and Libby [34] and the toaster experiments of Ma and Warhaft [37], the grid is the origin for mixing of the two streams, whereas for the mandoline experiments of Ma and Warhaft the mixing layer was set up using a source down-stream of the grid. For our model calculations, it is convenient to locate the source at a distance \( x_0 \) (actually, a travel time \( t_0 = x_0/U \)) down-stream of the grid. Experiments in which the grid is the origin of the two streams correspond to the limit \( t/t_0 \rightarrow \infty \) in our calculations. The characteristics of the turbulence, mixing time scale and molecular diffusivity are the same as those for the line source calculations reported in section 4.

We represent the source as an instantaneous step function at time \( t_0 \) as

\[
S(x, t) = (1 - H(z))\delta(t - t_0),
\]

where \( H(z) \) is the Heaviside function and we have taken the source concentration in the lower stream to be unity. Then as for the line source case, we have analytical results for the mean concentration and conditional mean concentration profiles given respectively by

\[
\bar{\phi}(z, t) = \frac{1}{\sqrt{2\pi}}[1 - \text{erf}(z/\sqrt{2}\sigma_z)]
\]

\[
\tilde{\phi}(z, t) = \frac{1}{\sqrt{2\pi}}[1 - \text{erf}(z/\sqrt{2}\sigma_z)]
\]
and

\[
\langle \phi | w \rangle = \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{z - \rho w z w z / \sigma_w}{\sqrt{2} \sigma_z (1 - \rho w z / \rho w z)^{1/2}} \right) \right].
\] (43)

Conditional statistics were calculated in the same manner as for the line source using (42) and (43) in place of (38) and (39). In all the results which follow, the concentration scale is taken to be the source concentration in the lower stream, i.e. unity.

Figures 9(a) and (b) show the conditional mean velocity on the centreline at three downstream locations, \( t/t_0 = 0.32, 2.26 \) and 8.39, and as a function of cross-stream location at \( t/t_0 = 8.39 \), respectively. The conditional mean velocity on the centreline shown in figure 9(a) is antisymmetric about the centreline mean concentration of 0.5. It is positive for concentrations larger than the centreline mean concentration, and vice versa for concentrations less than the centreline mean value. For concentrations of 0 and 1, the conditional mean velocity diverges to \(-\infty\) and \(+\infty\), respectively. Li and Bilger [39] obtained good agreement with their data using a model in which the shape of the conditional mean velocity is given by a function which is the inverse to the mean concentration profile, i.e. on the centreline, \( \langle w | \psi \rangle / \sigma_w = z_\psi / \sigma_z \), with \( z_\psi \) being the location where the mean concentration is equal to \( \psi \). This function is shown as the short-dashed line in figure 9(a). It becomes a better approximation to our model results with increasing distance down-stream. This is consistent with the mixing-length basis for the Li and Bilger theory since the Lagrangian transport model we use approaches a diffusion limit far down-stream. The Li and Bilger model breaks down closer to the source.

For negative off-centreline locations the conditional mean velocity profile is offset towards more negative values as can be seen in figure 9(b) and vice versa for positive off-centreline locations. Here we have used results for a far down-stream location \( t/t_0 = 8.39 \) to test the more general Li and Bilger theory which for arbitrary cross-stream locations can be written as

\[
\langle w | \psi \rangle / \sigma_w = \langle w | \psi = \bar{\phi} \rangle / \sigma_w + (z - z_\psi) / \sigma_z.
\] (44)

Clearly at this distance down-stream the theory is in excellent agreement with our model. Although we do not show it here, again the Li and Bilger theory breaks down close to the source.

Figure 9(c) shows results for the conditional mean velocity at a location \( t/t_0 = 0.32 \) much closer to the source for three different cross-stream locations. In this plot, the curves have been displaced by a velocity equal to \( z \sigma_w / \sigma_z \). This simple empirical offset apparently compensates very closely for the change with distance from the centreline at \( \psi = 0.5 \) and to a reasonable approximation for other values of the concentration. It breaks down far from the source.

Figure 10 shows the mean diffusion conditioned on the scalar concentration at various downstream locations (a) on the centreline and (b) at \( z / \sigma_z = -1 \). The non-dimensionalization is the same as that used for the line source case in figure 4 and by Brethouwer and Nieuwstadt [29]. Although in detail the mean diffusion for the mixing layer is clearly different from that for the line source, there are some common features. In both cases, the conditional mean diffusion on the centreline is positive for concentrations less than the centreline mean concentration. Both have a maximum at a concentration less than one-half of the centreline mean concentration, which decreases in magnitude and moves closer to zero concentration with increasing distance.
Figure 9. The conditional mean velocity for a scalar mixing layer according to the IECM model (a) on the centreline \( z/\sigma_z = 0 \) at down-stream locations \( t/t_0 = 0.32 \) (---), 2.26 (-- --) and 8.39 (-- - -). The line (- - - -) is the theory of Li and Bilger [39], (b) at the down-stream location \( t/t_0 = 8.39 \) and cross-stream locations \( z/\sigma_z = 0 \) (●), \( z/\sigma_z = -1 \) (■) and \( z/\sigma_z = -2 \) (♦). The corresponding lines are for the Li and Bilger theory at \( z/\sigma_z = 0 \) (---), \( z/\sigma_z = -1 \) (-- --) and \( z/\sigma_z = -2 \) (-- - -), and (c) at the down-stream location \( t/t_0 = 0.32 \) and cross-stream locations \( z/\sigma_z = 0 \) (-----), \( z/\sigma_z = -1 \) (-- --) and \( z/\sigma_z = -2 \) (-----), with the off-axis curves offset by a velocity \( = \sigma_w z/\sigma_z \).
Figure 10. The mean diffusion conditional on the concentration in a scalar mixing layer for the IECM model at down-stream locations $t/t_0 = 0.32$ (---), 0.65 (---) and 2.26 (---) (a) on the centreline $z/\sigma_z = 0$, (b) at $z/\sigma_z = -1$. The sloping straight line (—) is for the IEM model.

down-stream. The main difference between the two cases arises from the greater symmetry of the mixing layer, where these features are reflected (with a change of sign) for concentrations greater than the centreline mean. Similarly, the mixing layer results show the same sort of relationship between the off-axis and centreline results as do the line source results, namely increased magnitude (in this non-dimensionalization) and increased asymmetry about the centreline mean concentration.

The conditional dissipation non-dimensionalized by the lower side source concentration and the mixing time scale is shown in figures 11(a) and (b) for different down-stream locations on the centreline and for different cross-stream locations, respectively. Again the results are qualitatively similar to those for the line source, but for points on the centreline the symmetry of the mixing layer maintains a symmetrical uni-modal shape in the conditional dissipation at all down-stream locations. This symmetry is destroyed for off-axis locations, where the dissipation is enhanced at low concentrations and diminished at high concentrations for points in the upper...
Figure 11. The mean scalar dissipation conditional on the concentration in a scalar mixing layer (a) on the centreline \( z/\sigma_z = 0 \) at down-stream locations \( t/t_0 = 0.32 \) (——), 0.97 (– – –) and 2.26 (---) and (b) at \( t/t_0 = 0.32 \) and cross-stream locations \( z/\sigma_z = 0 \) (——), \( z/\sigma_z = 1 \) (–––) and \( z/\sigma_z = 2 \) (----).

stream and vice versa for points in the lower stream (not shown). Again, the symmetry is different from the line source case for which the dissipation is the same for locations on either side of the centreline.

6. Conclusions

We have calculated a range of conditional scalar and flow statistics for a uniform gradient source, a line plume and a scalar mixing layer in isotropic turbulence using a Lagrangian dispersion model coupled to two simple scalar mixing models.

The IECM mixing model gives predictions for the statistics conditional on the scalar concentration (the velocity, diffusion and scalar dissipation) in good agreement with DNS results for the uniform gradient and line plume sources. For the uniform gradient source, the simpler IEM mixing model also gives excellent results for these statistics, although with different values for the constants \( C_0 \) and \( C_\phi \), which control the magnitude of the turbulence and mixing time.
scales. However, the IECM model is clearly a better representation of these conditional statistics for the line plume, capturing the non-linearity in the conditional mean diffusion for example.

For the mean diffusion conditioned on the velocity the model predictions are less satisfactory and somewhat ambiguous. For the uniform gradient source, DNS results clearly show that the conditional diffusion is non-zero. The IECM model predicts it to be zero, whereas the IEM model predicts it to be larger than the DNS results by a factor of about 2. Thus, a quantitative fit to the DNS results requires a linear combination of the IECM and IEM models. However, the inclusion of a contribution from the IEM model is not consistent with the requirement that the turbulent flux be at most weakly affected by mixing. We have shown that the effect of the interaction between turbulent and molecular diffusion, the only mechanism which can modify the turbulent flux, is much weaker than the effect due to the IEM model. In the case of a line plume, the contribution to the conditional diffusion that arises from the mixing model, is non-zero for the IEM model but is zero for the IECM model. The term \( \frac{\langle \hat{\phi} - \langle \phi | W \rangle \rangle}{t_m} \) in the IEM model is about the same magnitude as the DNS results of Brethouwer and Nieuwstadt [29] for the conditional diffusion, but is the wrong shape. On the other hand, the contribution which arises from the direct effects of molecular diffusion is a good representation of the shape of the DNS results. Although we could not quantify the magnitude of this term precisely, it seems from the shape of the DNS results that the molecular contribution may be significant in these data.

We also calculated conditional statistics for a scalar mixing layer, showing that far downstream our results for the IECM model are in good agreement with the mixing-length theory of Li and Bilger [39] (and by implication with their experimental data). However, we have no numerical or experimental results for other conditional statistics with which to compare our results for this case. While these statistics are in detail different from those for a line plume, these differences are easily understood in terms of the different symmetries of the mean concentration field (and the conditional mean concentration) for the two cases. These differences are mainly manifested for concentrations larger than the mean concentration on the centreline, where for the line plume the upper concentration limit is effectively determined by the mixing, whereas for the mixing layer it is determined by the initial conditions. It is clear from the success of the mixing models studied here in predicting these conditional statistics that the shape of these statistics is controlled largely by the shape of the mean concentration (or conditional mean concentration) profile and that the main role of the mixing models is to control the magnitude of the scalar fluctuations.

We have also tested various approximations for conditional scalar statistics, particularly those conditional on the scalar concentration. Our results show that for a line plume and a mixing layer, the conditional mean velocity shows significant departures from the so-called linear approximation (25). While the dependence of the conditional mean dissipation (conditioned on the concentration) on the cross-stream location is not as strong as that for the unconditional dissipation, it is not negligible. The significance of this dependence on the cross-stream location remains to be tested, but the approximations of neglecting it, or of replacing the conditional dissipation by the unconditional dissipation, may not be adequate.

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