

On the physical accuracy of scalar transport modeling in inhomogeneous turbulence

Peter S. Bernard

Department of Mechanical Engineering, University of Maryland, College Park, Maryland 20742

Amy L. Rovelstad

Naval Research Laboratory, Washington, DC 20375

(Received 10 August 1993; accepted 2 May 1994)

Direct numerical simulations of scalar fields produced by uniform and line sources in channel flow are used as the basis for examining the accuracy of random flight and closure models in predicting turbulent scalar transport rates. Closure models of gradient form with an anisotropic eddy diffusivity tensor perform well for the uniform source flow and the far field of plumes. In the near field, the plumes are seriously distorted due to the inappropriateness of gradient transport in modeling the streamwise flux rate. Random flight models are most successful in producing a qualitative rendering of the near field of plumes, but are subject to significant quantitative inaccuracies for the low Reynolds and Schmidt number flows considered here. Ensembles of particle paths having common end points are used to explore the physics of the scalar transport correlation. For plume flows, transport in the near field is found to be primarily due to the average effect of the meandering of the turbulent fluid over the source, in which the amount of scalar dispersed by a fluid particle correlates with the local velocity fluctuation. Farther downstream, displacement transport—which may be reasonably modeled via gradient physics—emerges as the principal mechanism behind the scalar flux.

I. INTRODUCTION

Thermal and mass concentration fields diffusing within turbulent shear flows are found in many guises in environmental science and engineering. Current methods for numerically predicting such phenomena are largely confined to solutions of the Reynolds averaged equations for which the turbulent scalar flux rate must be modeled^{1–3} and random flight models which mimic the motion of individual tracers in turbulence through an assumed Markov process.^{4–7} Since the physical processes underlying the turbulent flux of scalar contaminants are only partially understood at the present time, closure models for the scalar transport correlation have tended to adopt the gradient form. Numerous examples of nongradient transport are known to exist in applications,⁸ however, and it has long been recognized^{8–10} that gradient transport models are incapable of representing dispersion near the source of contaminant plumes even under homogeneous conditions. The limitations of gradient models and the success of random flight models in capturing short time diffusion in homogeneous turbulence, have been an impetus for the extension and application of random flight models to inhomogeneous flows. Since gradient transport models are compatible with plume growth in the far field, however, they have remained a desirable choice in such situations.

Random flight algorithms suitable for nonhomogeneous turbulence have seen widespread use in meteorological^{5–7,11–13} and engineering¹⁴ applications. Though the “well-mixed” criterion¹⁵ provides necessary conditions on the moments of the random velocity increments of the tracers, practical considerations require that random flight models be applied under simplifying assumptions. Many tests of the predictions of such models have been made against experimental data, sometimes including direct

comparisons between random flight and closure models. On the whole, however, such studies have not been in controlled settings where accurate information about the turbulence scales and other correlations appearing in the models are available. As a result, it has been difficult to discern what the relative strengths of the two methodologies are, and especially if the substantially greater computational cost of random flight methods in comparison to closure models pays off in the form of greater accuracy in the prediction of the near field of scalar dispersal.

Direct numerical simulations (DNS) of turbulent flows including scalar transport, provide a useful setting from which to carry out objective tests of prediction techniques,^{2,3,16} though admittedly, the attainable Reynolds and Schmidt numbers are lower than optimal for the random flight methodology. From the DNS all of the necessary fluid mechanical correlations—including time and length scales—needed in implementing scalar diffusion algorithms can be computed from the simulated flow. Scalar transport fluxes and the mean scalar field itself can also be known to any desired extent, so the predictions of the various theories can be tested without ambiguity. The wealth of information provided by DNS also supplies a means of establishing relationships between scalar transport and the underlying turbulent fluid motion.^{17–21} Such knowledge may be instrumental in deriving future improvements to prediction techniques.

The interest of the current work is twofold. First, we use a DNS of diffusing scalar fields in a turbulent channel flow to assess the performance and physical integrity of scalar transport models under conditions where the turbulence is inhomogeneous. Second, we examine the relationship between current gradient type closure models and the actual physical mechanisms leading to the scalar flux correlation.

The intent is to develop an understanding of the physics of transport in the near field of plumes to aid in deriving physically accurate closure models. We consider scalar fields in a turbulent channel flow resulting from a constant source distributed uniformly throughout the flow and from a transverse line source. In the case of the former, zero boundary conditions are applied so that the fully developed scalar field is one-dimensional, i.e., losses of scalar by diffusion through the boundary balance its internal production. This flow has been considered in several previous studies.^{2,16-18} The second example consists of plumes developing downstream of spanwise-oriented line sources with zero flux, i.e., insulated, wall boundary conditions. In one case the source is held at $y^+ = 15$ and in the other at $y^+ = 30$. The developing plumes are two-dimensional in the mean and are strongly affected by the shear and anisotropy of the channel flow.

Our exploration of the physics of scalar transport is through application of a formal analysis of ensembles of fluid particle paths computed from a direct numerical simulation of turbulent channel flow. The approach has been applied extensively in previous work to study the rates of momentum²² and vorticity^{23,24} transport. Subsequently, it was extended²⁵ to include the effects of vortical structures in causing Reynolds stress. The methodology finds immediate application in explaining the physical nature of scalar transport. The present study initiates such an investigation in the context of the DNS of the uniform and line source scalar fields. For the plume flow, the properties of transport near the source are considered, including how the physical transport mechanisms change with downstream distance. The degree to which gradient diffusion plays a legitimate role in transport is explained, as are the physical processes which should be taken into account in a physically appropriate model.

The next section considers some of the current trends in modeling scalar fluxes and their relationship to the physics of transport as viewed through the Lagrangian technique. We then consider in turn the uniform and line source flows in which we directly compare the predictions of closure and random flight models. In the last two sections we provide an analysis of the physics of the transport correlation in plumes and then present conclusions.

II. TRANSPORT MODELS

We consider the diffusion of a passive scalar, C , satisfying the convective diffusion equation

$$\frac{\partial C}{\partial t} + U_i \frac{\partial C}{\partial x_i} = \frac{1}{\text{Re Sc}} \frac{\partial^2 C}{\partial x_i^2} + Q \quad (1)$$

where U_i is the turbulent velocity field, Q is a nonrandom source term, Sc is the Schmidt number and Re is the Reynolds number. Alternatively, in the case of the passive diffusion of internal energy, C may be considered to be the temperature in which case Sc is replaced by the Prandtl number, Pr . After averaging, Eq. (1) yields

$$\frac{\partial \bar{C}}{\partial t} + \bar{U}_i \frac{\partial \bar{C}}{\partial x_i} = \frac{1}{\text{Re Sc}} \frac{\partial^2 \bar{C}}{\partial x_i^2} - \frac{\partial \overline{u_i c}}{\partial x_i} + \bar{Q} \quad (2)$$

where $\bar{C}$ and $\bar{U}_i$ are ensemble averaged means, c and u_i are fluctuations, $C = \bar{C} + c$ and $U_i = \bar{U}_i + u_i$. Closure to Eq. (2) depends on modeling the scalar flux rate, $\overline{u_i c}$. Most commonly this is done via a gradient law of the form

$$\overline{u_i c} = -K_{ij} \frac{\partial \bar{C}}{\partial x_j} \quad (3)$$

where K_{ij} is an anisotropic eddy diffusivity tensor. Our intent here is to develop a formal treatment of $\overline{u_i c}$ so that Eq. (3) can be viewed from a perspective in which the proper form for K_{ij} is revealed as well as the relative magnitude that Eq. (3) occupies among all of the physical processes causing transport.

Analysis of $\overline{u_i c}$ proceeds by a Lagrangian technique²²⁻²⁴ generalizing a methodology developed by Taylor.⁹ In this we consider an ensemble of fluid particles traveling over a time interval τ which arrive at a given point a at time zero. Denoting the initial locations of the fluid particles by b —points which vary from one realization to the next—the transport correlation $\overline{u_i c}$ may be expanded via the identity

$$\overline{u_{i_a} c_a} = \overline{u_{i_a} c_b} + \overline{u_{i_a} (\bar{C}_b - \bar{C}_a)} + \overline{u_{i_a} (C_a - C_b)} \quad (4)$$

where $\bar{C}_b$ denotes $\bar{C}$ evaluated at the random point b and so forth. As discussed in related contexts and verified numerically,²²⁻²⁴ the mixing condition $\overline{u_{i_a} c_b} = 0$ is satisfied for τ large enough. We define the mixing time, say τ_m , as the smallest interval at which $\overline{u_{i_a} c_b} \approx 0$; τ_m may be thought of as the time over which events in the flow cause the correlation between u_i and c to develop. Equation (4) thus shows that for times $\tau > \tau_m$, $\overline{u_i c}$ is a result of the processes represented by the last two terms in Eq. (4).

The second term on the right-hand side of Eq. (4) represents transport arising solely from the displacement of fluid particles in the presence of an inhomogeneous mean scalar field. It formally expresses the concept that the correlation between u_{i_a} and c_a arises from fluid particles carrying—unchanged—the local mean scalar field of their starting point, i.e., $\bar{C}_b$, to the point a over a mixing time. This expression is more general than that derived from the classical argument linking the scalar flux to a gradient model. For convenience, we will refer to this expression below as the “displacement transport” term.

Nongradient sources of transport are contained in the last term in Eq. (4) which can be expanded as

$$\overline{u_{i_a} (C_a - C_b)} = \frac{1}{\text{Re Sc}} \int_{-\tau}^0 \overline{u_{i_a} \nabla^2 C(s)} ds + \int_{-\tau}^0 \overline{u_{i_a} Q(s)} ds \quad (5)$$

after integrating Eq. (1) along a particle path from b to a and substituting for $C_a - C_b$. Here, $\nabla^2 C(s)$ and $Q(s)$ denote evaluations of $\nabla^2 C$ and Q , respectively, at positions of fluid particles at time s . The first term on the right-hand side represents the correlation between u_i and the cumulative changes to the scalar field of a fluid particle by molecular diffusion along its path. The second term in Eq. (5) expresses transport resulting from fluid particles acquiring the scalar as they pass through the source. Each of these terms will later be shown to play an important role in the plume flow.

The displacement term in Eq. (4) can be expanded using a Taylor series representation of $\bar{C}_b$ yielding

$$\overline{u_i(\bar{C}_b - \bar{C}_a)} = - \int_{-\tau}^0 \overline{u_i(0)u_j(s)} ds \frac{\partial \bar{C}}{\partial x_j} + \Phi_1 \quad (6)$$

where Φ_1 contains expressions originating in the higher order terms in the $\bar{C}_b$ expansion. In a steady, linearly varying mean scalar field this term is identically zero. It is clear from Eq. (6) that the eddy diffusivity in Eq. (3) will be compatible with the underlying physics of the transport correlation if

$$K_{ij} = \int_{-\tau}^0 \overline{u_i(0)u_j(s)} ds. \quad (7)$$

When $\tau > \tau_m$ is large enough so that $\overline{u_i(0)u_j(s)} = 0$ for $|s| > \tau$, Eq. (7) can be expressed more simply as

$$K_{\alpha\beta} = T_{\alpha\beta} \overline{u_\alpha u_\beta}, \quad (8)$$

where Greek indices are not summed and we have introduced a Lagrangian integral time scale through

$$\overline{u_\alpha u_\beta} T_{\alpha\beta} \equiv \int_{-\infty}^0 \overline{u_\alpha(0)u_\beta(s)} ds. \quad (9)$$

In summary, if $\overline{u_i \bar{C}}$ were entirely due to gradient transport, so that Eq. (3) were exactly true, then K_{ij} would have to be given by Eq. (8). As it stands, however, if Φ_1 in Eq. (6) and the terms given in Eq. (5) are not zero, as they very likely will not be under most circumstances, then by assuming Eq. (3) is true, one is in effect using K_{ij} to account for both gradient and nongradient physical processes. In this case it cannot be expected that Eq. (8) will hold.

Anisotropy of K_{ij} is essential for a reasonable treatment of the wall bounded flows considered here. For example, in the case of a unidirectional flow where $\bar{C} = \bar{C}(y)$ and diffusion is in the wall-normal direction y , it is well recognized²⁶ that the model

$$\overline{v \bar{C}} = -\nu_c \frac{d\bar{C}}{dy}, \quad (10)$$

where ν_c is the scalar eddy viscosity, must have

$$\nu_c = T \overline{v^2} \quad (11)$$

where T is an appropriate time scale, often set equal to $2k/\epsilon$. Recently developed high Reynolds number models for scalar transport^{1,27} which take

$$\nu_c \propto \frac{k^3}{\epsilon^2} \frac{d\bar{U}}{dy} \quad (12)$$

cannot be meaningfully applied near boundaries since in effect they replace $\overline{v^2}$ by k which have wholly different behaviors. Consequently, we limit the models under consideration to those which are consistent with Eq. (11) as a minimum condition.

It is common practice in turbulence modeling to introduce a turbulent Schmidt number σ_c so that ν_c can be written as $\nu_c = \nu_t/\sigma_c$ where ν_t is the eddy viscosity appearing in the Reynolds stress model

$$\overline{uv} = -\nu_t \frac{d\bar{U}}{dy}. \quad (13)$$

However, a formal analysis of momentum transport along the same lines leading to Eq. (6) shows that the theoretically correct eddy viscosity for momentum transport²² is identical to Eq. (8). This suggests, in agreement with other analyses,²⁸ that one should have $\nu_t = \nu_c$, i.e., that the physical mechanism underlying gradient transport does not distinguish between scalar and momentum transport. The fact that it is often necessary to assume that $\nu_t \neq \nu_c$ in calculations, is thus an artifice of the use of gradient models in representing physical processes which are not purely gradient in nature.

For the purposes of the present study we take two particular gradient models as representative of closure models for scalar transport. The first is that derived by assuming Eq. (3) and Eq. (8), i.e., the physically correct form of $\overline{u_i \bar{C}}$ if gradient transport were truly the only mechanism causing transport. This is, in effect, a truncation of the exact Lagrangian expansion for the transport correlation. Its use in the subsequent comparisons helps clarify the extent to which transport models need to include the complete set of physical processes causing transport. To implement the use of Eq. (8), the necessary values of $\overline{u_i u_j}$ and the scales T_{ij} are obtained from direct numerical simulations of the flow field.

The second model^{2,16} we consider is derived from an algebraic analysis of the transport equation for $\overline{u_i \bar{C}}$. In this it is assumed that the sum of the scalar flux production terms in its own transport equation are aligned in the direction of the flux vector. From this an algebraic system of equations for $\overline{u_i \bar{C}}$ follows whose solution fits the gradient form Eq. (3) with tensor eddy viscosity given by

$$K_{ij} = \frac{1}{2A} \epsilon_{pki} \epsilon_{lmn} A_{lp} A_{mk} \overline{u_n u_j} \quad (14)$$

where A is the determinant of the matrix $A_{ij} = C_D/T \delta_{ij} + \partial \bar{U}_i / \partial x_j$,

$$C_D \equiv 16.1 \left(1 + \frac{1.17}{Sc} \right)^{0.152} \left(1 + \frac{131}{\sqrt{R_T}} \right)^{-0.535}, \quad (15)$$

and the turbulent Reynolds number, $R_T \equiv 4k^2/\epsilon \nu$. Note that an alternative formula for C_D given in Ref. 2 gives virtually identical results to Eq. (15) in numerical applications and is thus not considered here; T is an appropriate time scale, essentially equivalent to that discussed previously in reference to Eq. (11). There are some important similarities between Eqs. (8) and (14) which will become more evident below when we look at their forms in the particular flows to be considered.

III. UNIFORM SOURCE FLOW FIELD

We now consider the prediction of the mean scalar field due to a steady uniform source in the channel. In this case $\bar{C}(y)$ is one-dimensional and satisfies

$$0 = \frac{1}{Re Sc} \frac{d^2 \bar{C}}{dy^2} - \frac{d\overline{v \bar{C}}}{dy} + \frac{2}{Re Sc}, \quad (16)$$

where we have set $y = x_2$ and $v = u_2$. The arbitrary constant magnitude of the source in Eq. (16) is set to match the value used in previous studies.^{2,16-18} For these conditions Eq. (8) becomes

$$\overline{v\bar{c}} = -T_{22}\overline{v^2} \frac{d\bar{C}}{dy} \quad (17)$$

while the algebraic model Eq. (14) gives

$$\overline{v\bar{c}} = -\frac{2k}{\epsilon} \frac{1}{C_D} \overline{v^2} \frac{d\bar{C}}{dy} \quad (18)$$

showing the close similarity between the two formulations of K_{ij} in this instance. In view of Eq. (17) it is clear that Eq. (18) contains the implicit assumption that

$$T_{22} = \frac{2k}{\epsilon} \frac{1}{C_D}, \quad (19)$$

which is, apart from the additional factor C_D , the standard scaling of the Lagrangian integral scale used in turbulence modeling.

We have performed a direct numerical simulation of the uniform source flow field from which the scalar mean and flux correlations are extracted for comparison with model predictions. This also provides values of $\overline{v^2}$, k , ϵ , and T_{22} appearing in Eqs. (17) and (18). The simulations incorporate a mesh with $64 \times 65 \times 64$ points in the streamwise, wall-normal and spanwise directions, respectively, and the dimensions of the computational box are $1250 \times 250 \times 625$ expressed in wall units. The numerical scheme is equivalent to that used in previous studies and is described in detail by Handler *et al.*²⁹ The Reynolds number $R_\tau = U_\tau h / \nu = 125$, where U_τ is the friction velocity and h is the channel half-width, and $Sc = 0.71$. The $\bar{C}$ and $\bar{U}$ fields, Reynolds stresses, $\overline{u_i u_j}$, and transport correlations, $\overline{u_i \bar{c}}$, agree closely with those found in previous studies.^{2,16-18}

From the simulated velocity field the time scale T_{22} was computed by first generating large ensembles of fluid particles arriving at fixed distances above the wall. To get highly accurate paths, velocities of the fluid particles at off nodal points were found by cubic Hermite interpolation.³⁰ The estimates of T_{22} are limited to the range $0 \leq y^+ \leq 40$, so that it was necessary to extrapolate T_{22} to the centerline to get the complete curve for T_{22} needed in solving Eq. (16) using Eq. (17). Figure 1 shows the computed values of T_{22} , given in wall units, i.e., scaled by ν/U_τ^2 , together with the fitted curve used in Eq. (17). The latter is derived from a least square fit using MATLAB in the region where the data is available, and its smooth extension via a parabola to the "ideal" value of T_{22} at the centerline. By "ideal," we refer to T_{22} computed from (17) using the DNS data. This is the hypothetical magnitude that T_{22} would have at a point if the gradient model were locally exact there. A curve denoting the ideal T_{22} everywhere across the channel is also shown in the figure, together with the time scale given in Eq. (19). Near the wall the ideal form of T_{22} is significantly different from that computed from the DNS, suggesting that other physical effects besides gradient transport influence the $\overline{v\bar{c}}$ correlation in this region. Farther from the wall, the agreement becomes closer

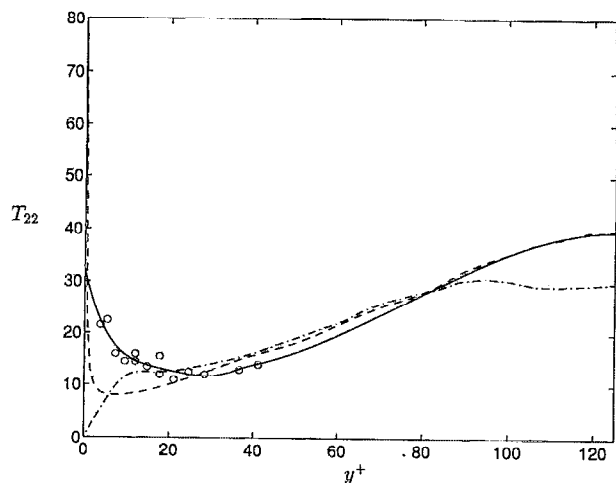


FIG. 1. Lagrangian integral scale T_{22} in channel flow. $\circ$, from DNS; —, fit to DNS; ---, "ideal" values; — · —, computed from Eq. (19).

suggesting that a gradient model may have some legitimacy away from the boundary. It is noteworthy that Eq. (19) agrees closely with the ideal T_{22} for a sizable part of the channel, though they diverge near the centerline and near the wall, where the former goes to zero. The latter difference is largely immaterial to the performance of Eq. (19), however, since the appearance of $\overline{v^2}$ in the eddy viscosity assures that the molecular diffusion coefficient will dominate Eq. (18) near the wall.

Random flight models discussed by Thomson^{5,7} and von Dop *et al.*⁶ were investigated here. For the uniform source channel flow $\bar{C}$ is one-dimensional so that only diffusion in the wall-normal direction need be considered. To implement the models, tracers were released into the flow at each time step $\Delta t^+ = 1$ from 40 uniformly spaced locations spanning the channel. The zero boundary condition was enforced by eliminating particles moving outside the domain. The number of tracers in the calculation grew to a statistically steady state, after which time the instantaneous C field was sampled at every tenth time step over a time period of $t^+ = 5000$. The resulting ensemble of realizations was averaged to obtain a prediction of $\bar{C}$. At equilibrium, approximately 58 000 tracers were contained in the calculation.

We consider two random flight models. In the first, advancement of tracer position, y^n , and velocity, v^n , from time step $n\Delta t$ to $(n+1)\Delta t$ is through the rules

$$y^{n+1} = y^n + v^n \Delta t + \xi \quad (20)$$

and

$$v^{n+1} = v^n \left(1 - \frac{\Delta t}{T_{22}^{n+1}} \right) + \mu^{n+1}, \quad (21)$$

where ξ is a normally distributed random variable with mean 0 and variance $2\Delta t / \text{Re } Sc$, i.e., $\xi = N(0, 2\Delta t / \text{Re } Sc)$. The inclusion of this random change in position is necessary to accommodate molecular diffusion of the scalar; μ is also a random variable, though it is not necessarily Gaussian. For diffusion in nonhomogeneous conditions, necessary values

for its moments have been derived by Thomson.⁵ These show that μ would be Gaussian—to first order in Δt —if both $\bar{v}$ were Gaussian and the condition $T_{22}(d\bar{v}^2/dy)/\bar{v}^2 \ll 1$ were satisfied. In the present case, however, neither of these requirements are met, so it is unlikely that μ should be Gaussian. In generating μ for practical applications it is only possible to force a few of its moments to their correct values, so a degree of arbitrariness in the selection of μ is to be expected.

According to the well-mixed criterion of Thomson,⁵ the mean, $\bar{\mu}$, variance, σ^2 and skewness, S_k , of μ should be, $\bar{\mu} = \Delta t(d\bar{v}^2/dy)$, $\sigma^2 = \Delta t[2\bar{v}^2/T_{22} + (d\bar{v}^3/dy)]$ and $S_k = \Delta t[3\bar{v}^3/T_{22} + (d\bar{v}^4/dy) - \bar{v}^3/\bar{v}^2(d\bar{v}^2/dy)]$. In our implementation of Eq. (21) we took μ to be both Gaussian, in which case the first two moments are specified, or non-Gaussian where a sum of two Gaussian variables⁵ was used to meet the conditions on three moments. We also experimented with simplifications to the exact moment formulas. The most successful of the computations incorporated the non-Gaussian variable with the skewness simplified to $S_k = 3\Delta t\bar{v}^3/T_{22}$. The benefit of taking the skewness into account agrees with the earlier findings of Thomson for a test calculation under highly nonhomogeneous conditions.

A second random flight model consists of replacing Eq. (21) by the relation⁵

$$v^{n+1} = v^n \left(1 - \frac{\Delta t}{T_{22}^{n+1}} \right) \frac{\sqrt{v^2}^{n+1}}{\sqrt{v^2}^n} + \mu^{n+1}. \quad (22)$$

In contrast to the previous algorithm, Gaussianity of v does imply that μ is Gaussian to $O(\Delta t)$, suggesting that there may be somewhat more justification for making μ Gaussian in this case. The computations showed, however, that various choices for μ , both Gaussian and non-Gaussian, give similar results. The best performance, though only marginally, came from specifying the first three moments according to $\bar{\mu} = (\Delta t/2)(d\bar{v}^2/dy)$, $\sigma^2 = \Delta t\{2\bar{v}^2/T_{22} + \bar{v}^2[d(\bar{v}^3/\bar{v}^2)/dy]\}$ and $S_k = 3\Delta t\bar{v}^3/T_{22}$. In this case, the skewness has been abbreviated from its full expression, namely, $S_k = \Delta t\{3\bar{v}^3/T_{22} + \bar{v}^2^{3/2}[d(\bar{v}^4 - 3\bar{v}^2)^2/\bar{v}^2^{3/2}]/dy\}$.

The time scale in Eqs. (21) and (22) is indicated as T_{22} with the definition given in Eq. (9) since this choice is consistent with the premises upon which the random flight models are based. It should be noted, however, that neither this assumption nor the model itself are rigorously derived, so that it is conceivable that other choices for T_{22} may yield superior performance. Apart from a test calculation with Eq. (19), which did not yield significantly different results, the question was not pursued further except to gauge the sensitivity of $\bar{C}$ to the midchannel values of the DNS predictions of T_{22} which is not precisely known for $y^+ \geq 40$. In this, the previously discussed extrapolation of T_{22} to the centerline was altered by 30%. This had a negligible effect on $\bar{C}$ suggesting that the present conclusions concerning the random flight models would not be significantly different if more complete data for T_{22} were available.

Figure 2 compares $\bar{C}$ predicted from the closure models Eqs. (17) and (18) against the solution determined from the

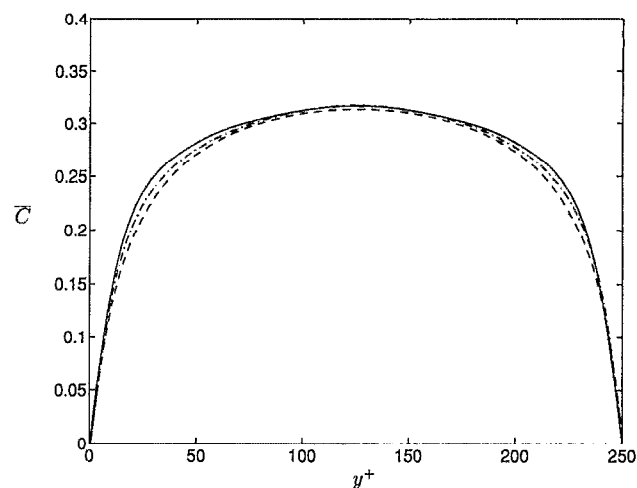


FIG. 2. $\bar{C}$ for uniform source from closure schemes. — : DNS; - - - : from Eq. (17); — · — : from Eq. (18).

direct numerical simulation. A similar comparison, but for the random flight models, is shown in Fig. 3. Evidently, despite whatever limitations there may be in the physical validity of gradient transport models, they are nonetheless quite adequate for predicting this flow. The slightly greater accuracy of the algebraic model over Eq. (17) may be attributed to its time scale being lower than T_{22} in the region out to $y^+ = 20$. This leads to a higher slope in $\bar{C}$ near the wall and thus to a better fit farther from the wall. Figure 3 shows that the scalar fields predicted by random flight models are generally less accurate than the closure models. The model based on Eq. (21) is more quantitatively correct than Eq. (22), though its shape is somewhat unphysical in appearance. The second model does capture the near wall field quite well, but seriously overpredicts $\bar{C}$ near the centerline. The relatively low Schmidt and Reynolds numbers of the calculations may be partly responsible for this outcome since the perceived strength of random flight models is at larger values of these parameters. It may be concluded that under the re-

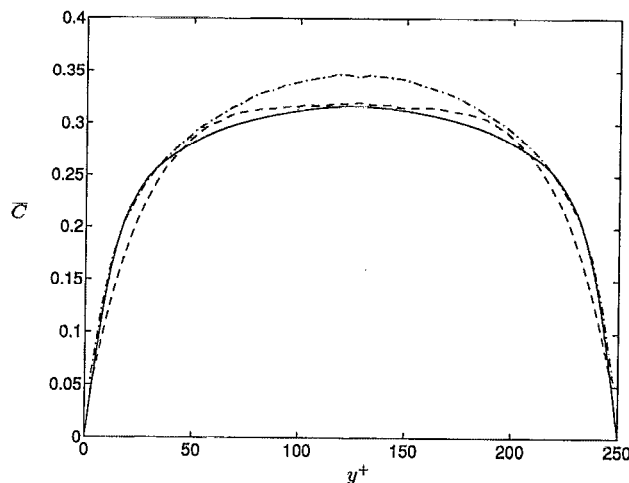


FIG. 3. $\bar{C}$ for uniform source from random flight models. — : DNS; - - - : from Eqs. (20), (21); — · — : from Eqs. (20), (22).

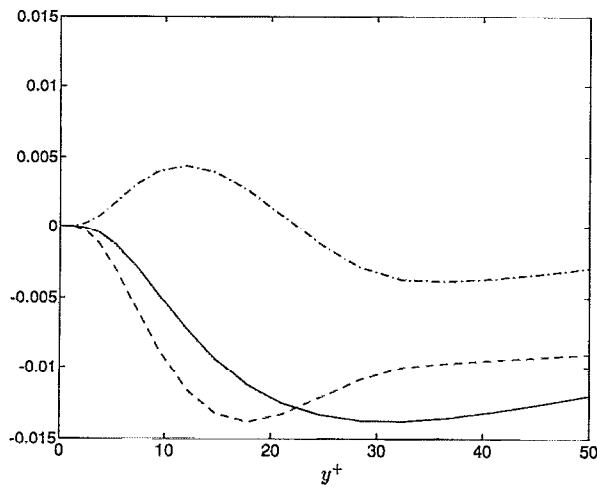


FIG. 4. Lagrangian decomposition of $\overline{v'c'}$ in uniform source flow. — : $\overline{v'c'}$; - - - : gradient contribution from Eq. (17); — · — : nongradient contribution.

striction of low Sc , closure schemes represent a better choice than random flight models for predicting one-dimensional diffusion under highly inhomogeneous conditions.

The total contribution to $\overline{v'c'}$ from nongradient effects may be calculated by taking the difference between $\overline{v'c'}$ and Eq. (17). A plot of the resulting breakdown of $\overline{v'c'}$ is shown in Fig. 4 for the region where T_{22} is known. This has very much the same features²² as a similar decomposition of the Reynolds shear stress $\overline{u'v'}$. In particular, gradient transport overpredicts $\overline{v'c'}$ near the wall and underpredicts it away from the wall. The similarity of the $\tilde{C}$ and $\tilde{U}$ profiles suggests that it is highly likely that this occurs for the same reasons as noted previously for momentum transport. In essence, a linear approximation to $\tilde{C}$ near the wall overestimates the contribution to $v_a(\tilde{C}_b - \tilde{C}_a)$ from particles traveling toward the wall, yet is reasonably accurate for particles traveling away from the wall. The result is an overprediction. Further from the wall the opposite occurs when the linear approximation is acceptable for those particles traveling wallward, yet underestimates the contribution of particles traveling outward, so that $v_a(\tilde{C}_b - \tilde{C}_a)$ is underpredicted. Even though nongradient effects contribute nontrivially to $\overline{v'c'}$, the flux is never countergradient so that the use of Eq. (17) cannot be ruled out *a priori*. Evidently, Eq. (18) is most successful since it beneficially modifies T_{22} to compensate for nongradient physics in the uniform source flow.

Though the streamwise scalar flux $\overline{uc'}$ does not appear explicitly in Eq. (16), it is nevertheless instructive to see how successfully this correlation can be modeled by the algebraic and truncated Lagrangian approaches. Here Eq. (8) gives

$$\overline{uc'} = -\overline{uv}T_{12} \frac{\partial \tilde{C}}{\partial y} \quad (23)$$

while Eq. (14) asserts that

$$\overline{uc'} = -\left(\frac{T}{C_D} \overline{uv} - \frac{ST^2}{C_D^2} \overline{v^2} \right) \frac{\partial \tilde{C}}{\partial y} \quad (24)$$

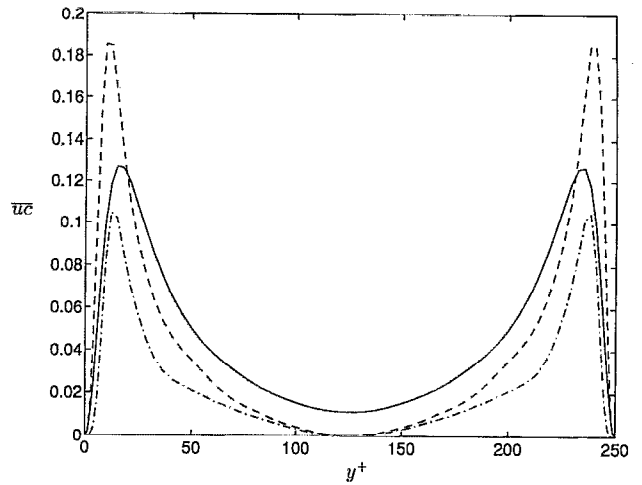


FIG. 5. Comparison of $\overline{uc'}$ predictions in uniform source flow. — : DNS; - - - : from Eq. (23); — · — : from Eq. (24).

where $S = d\tilde{U}/dy$ is the shear rate. Apart from the term depending on S in Eq. (24), one can view the algebraic model as implicitly modeling T_{12} by T/C_D , i.e., identical to the previous model for T_{22} implied by Eq. (18). A comparison of Eqs. (23) and (24) versus the DNS solution is shown in Fig. 5. Values for T_{12} in Eq. (23) were computed from the simulation in very much the same way as T_{22} was calculated. Further discussion of these and other time scales will be presented below in the context of the plume flow field.

Both of the models Eqs. (23) and (24) are in serious disagreement with the simulation results. The error in $\overline{uc'}$ by Eq. (24) is less than it would be if the shear term were not included, though closer agreement still would have been achieved if a larger value of T had been used. Such a choice can be justified, in fact, since T_{12} is much larger than T_{22} as will be seen below. This also helps explain why Eq. (23) very much overpredicts $\overline{uc'}$ in comparison to Eq. (24). The prediction of $\overline{uc'}$ from Eq. (23) follows a similar pattern as for $\overline{v'c'}$ in that it overpredicts near the wall and underpredicts away from it. Presumably this has the same physical explanation. Note that both gradient models are unphysical at the centerline where they predict $\overline{uc'}$ is zero, in contradiction with the simulation which suggests it is not. Evidently, streamwise transport near the centerline owes its presence to physical phenomena distinctly different from gradient transport. This is an interesting point which will be considered in future work.

IV. PLUMES

The simulation of plumes was carried out by equating Q in Eq. (1) to a Gaussian source term of the form

$$Q = \frac{100}{\pi} e^{-100(x^2 + (y - y_o)^2)} \quad (25)$$

where the elevation of the source above the wall, y_o , was set to either $y_o^+ = 15$ or 30. For these calculations $R_\tau = 145$, the mesh contained $96 \times 97 \times 96$ points and the dimensions of the computational region were $1822 \times 290 \times 683$. The

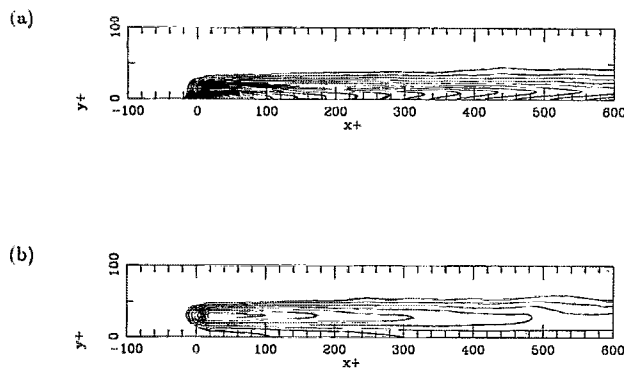


FIG. 6. $\bar{C}$ contours for simulated plume flow. (a) Source at $y^+ = 15$, (b) source at $y^+ = 30$.

source was turned on at $t^+ = 0$ causing the subsequent plume to develop within a fully developed channel flow. Numerical values of $\bar{C}$, $\overline{u\bar{C}}$, and $\overline{v\bar{C}}$ as functions of x and y were obtained by averaging instantaneous realizations across the span. To get smoother statistics, many of the results presented below are the result of averaging over two independent realizations of the flow field.

It is in the nature of the developing plume that its mean properties reach steady state in an ever lengthening region extending downstream from the source. Beyond this domain the average plume properties are time dependent. Our subsequent interpretation of the computed scalar fields considers both steady and nonsteady aspects of the developing plumes. Time accurate numerical schemes were used so that the modeled scalar fields could be meaningfully compared to the DNS field at any time after initiation of the plume. For the present study, comparisons are made generally at $t^+ = 82$.

Figure 6 shows the contours of $\bar{C}$ for the simulated plumes at $t^+ = 82$. For these and similar plots, the contour lines are in increments of unity. Contours of Q coming from Eq. (25) are superimposed so that the response of the plumes to source location may be observed. A significant difference between the two figures is the shift in the peak of $\bar{C}$ to a point on the wall surface when the source is brought from $y^+ = 30$ to 15. At $y^+ = 30$, the concentration peak in the near field remains immediately behind the center of the source, very much as it would be if the plume were developing in homogeneous turbulence in a uniform flow. The considerable differences between the plumes is due, in part, to the distributed nature of the source and the very much reduced convection and transport occurring at points close to the wall. The plume at $y^+ = 15$ is consistent with the expectation³¹ that at points sufficiently far downstream, the peak concentration on a given cross section in the steady region of the plume should lie at the wall. The later region may be identified by the presence of contours ending nearly normal to the wall. According to Fig. 6(a) this extends to approximately $x^+ = 250$. For the $y^+ = 30$ plume the point where the maximum $\bar{C}$ at a fixed x is on the surface is much farther downstream, beyond the limit of $x^+ = 600$ shown in the figure.

For a two-dimensional mean scalar field, the truncated Lagrangian expansion Eq. (8) yields

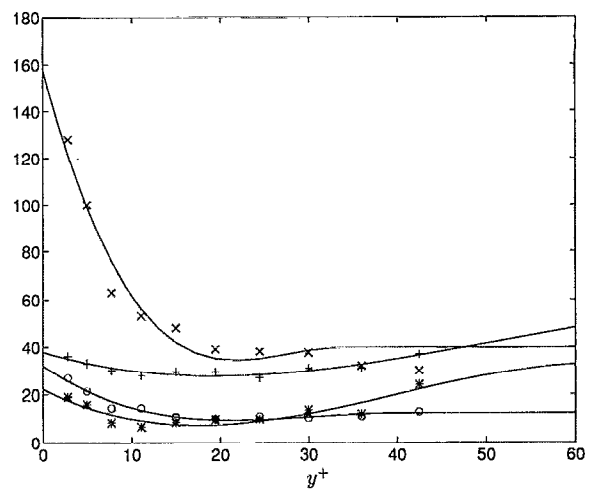


FIG. 7. Lagrangian integral time scales for $R_\tau = 145$ simulation. +: T_{11} ; $\times$: T_{12} ; *: T_{21} ; $\circ$: T_{22} .

$$\overline{u\bar{C}} = -\overline{u^2} T_{11} \frac{\partial \bar{C}}{\partial x} - \overline{uv} T_{12} \frac{\partial \bar{C}}{\partial y}, \quad (26)$$

$$\overline{v\bar{C}} = -\overline{uv} T_{21} \frac{\partial \bar{C}}{\partial x} - \overline{v^2} T_{22} \frac{\partial \bar{C}}{\partial y} \quad (27)$$

in which four distinct Lagrangian integral scales make an appearance. To utilize Eqs. (26) and (27) as a model, the Reynolds stresses and time scales need to be supplied externally. In the present case these were obtained from the channel flow simulation at $R_\tau = 145$. Values of the scales at 10 positions between $y^+ = 0$ and $y^+ = 42$ were obtained from appropriate ensembles of backward particle paths computed over a time interval $t^+ = 43.8$. Least square fits to the scale values were computed for the region encompassing the scale data and these were extrapolated at constant value to cover the lateral extent over which the plumes spread during the time period $t^+ = 82$. Figure 7 shows approximate curves for all four scales together with the data points used in determining them. Note that T_{12} is very large near the wall, as mentioned previously in reference to the evaluation of Eq. (23). For those cases where the scales are of a magnitude close to or greater than 43.8, which applies generally to T_{11} and T_{12} , extrapolation of the partial integrals in Eq. (8) had to be used to estimate the scales, since the correlation functions were not yet zero. The curves in Fig. 7 are fully consistent with similar data acquired for the $R_\tau = 125$ simulation by Rovelstad.²⁴ For example, one may observe the close similarity between the T_{22} data in Figs. 1 and 7.

For two-dimensional mean flows the algebraic model Eq. (14) predicts that

$$\overline{u\bar{C}} = -\left(\frac{T}{C_D} \overline{u^2} - \frac{ST^2}{C_D^2} \overline{uv}\right) \frac{\partial \bar{C}}{\partial x} - \left(\frac{T}{C_D} \overline{uv} - \frac{ST^2}{C_D^2} \overline{v^2}\right) \frac{\partial \bar{C}}{\partial y}, \quad (28)$$

$$\overline{v\bar{C}} = -\left(\frac{T}{C_D} \overline{uv}\right) \frac{\partial \bar{C}}{\partial x} - \left(\frac{T}{C_D} \overline{v^2}\right) \frac{\partial \bar{C}}{\partial y} \quad (29)$$

where, as before, $T \equiv 2k/\epsilon$. When $S=0$ these equations become equivalent to Eqs. (26) and (27) under the assumption that all of the scales are equal to T/C_D . With this restriction, the algebraic approach is equivalent to previously developed models.³²

Numerical solutions to Eq. (2) containing either Eqs. (26) and (27) or Eqs. (28) and (29) were obtained using the ADI algorithm applied to second-order differences of all spatially differentiated terms. The computational domain was taken to be $-200 \leq x^+ \leq 1800$, $0 \leq y^+ \leq 150$. A uniform finite difference mesh was used with dimensions 1000×100 and $\Delta t^+ = 0.1$. Zero flux boundary conditions were imposed on all boundaries. The computed results were found to be independent of time and space discretization as well as domain size.

For the simulation of the plume using the random flight methodology, we used the multidimensional model of Thomson⁷ which generalizes the second of the two one-dimensional models considered previously. In this case tracers are represented by their positions (x^n, y^n) and velocities (U^n, V^n) . The mean and fluctuating velocities at the tracer locations are denoted by $(\bar{U}^n, \bar{V}^n)$ and (u^n, v^n) , respectively. Particle positions are updated by the rules

$$x^{n+1} = x^n + (\bar{U}^n + u^n) \Delta t + \xi_1, \quad (30)$$

$$y^{n+1} = y^n + v^n \Delta t + \xi_2 \quad (31)$$

where (ξ_1, ξ_2) are mutually independent Gaussian random variables with means 0 and variances $2/\text{Re Sc}$. Coupled to Eqs. (30) and (31) are the relations

$$u^{n+1} = \left(u^n - \frac{\Delta t}{T_{11}^{n+1}} u^* - \frac{\Delta t}{T_{12}^{n+1}} v^* \right) + \mu_1^{n+1}, \quad (32)$$

$$v^{n+1} = \left(v^n - \frac{\Delta t}{T_{21}^{n+1}} u^* - \frac{\Delta t}{T_{22}^{n+1}} v^* \right) + \mu_2^{n+1} \quad (33)$$

where (u^*, v^*) are computed on alternate time steps through the relations

$$\begin{pmatrix} u^* \\ v^* \end{pmatrix} = \begin{pmatrix} u^n \\ v^n \end{pmatrix} + \Delta t \begin{pmatrix} (d\bar{u}\bar{v}/dy) \\ (d\bar{v}^2/dy) \end{pmatrix} \quad (34)$$

and

$$\begin{pmatrix} u^* \\ v^* \end{pmatrix} = \begin{pmatrix} \bar{u}^{n+1} & \bar{u}\bar{v}^{n+1} \\ \bar{u}\bar{v}^{n+1} & \bar{v}^{n+1} \end{pmatrix} \begin{pmatrix} \bar{u}^n & \bar{u}\bar{v}^n \\ \bar{u}\bar{v}^n & \bar{v}^n \end{pmatrix}^{-1} \begin{pmatrix} u^n \\ v^n \end{pmatrix}. \quad (35)$$

As discussed by Thomson,⁷ the random vector (μ_1, μ_2) is taken to be Gaussian with zero mean and covariance $\sigma_{ij} \equiv \mu_i \mu_j$ given by

$$\sigma_{11} = 2 \left(\frac{\Delta t}{T_{11}} \bar{u}^2 + \frac{\Delta t}{T_{12}} \bar{u}\bar{v} \right), \quad (36)$$

$$\sigma_{12} = \sigma_{21} = \left(\frac{\Delta t}{T_{11}} + \frac{\Delta t}{T_{22}} \right) \bar{u}\bar{v} + \frac{\Delta t}{T_{12}} \bar{u}^2 + \frac{\Delta t}{T_{21}} \bar{v}^2, \quad (37)$$

$$\sigma_{22} = 2 \left(\frac{\Delta t}{T_{22}} \bar{v}^2 + \frac{\Delta t}{T_{21}} \bar{u}\bar{v} \right). \quad (38)$$

Alternative choices for (μ_1, μ_2) involving conditions on the higher moments can be postulated as in the one-dimensional case, though the advantages of this strategy remains unclear at the present time. In fact, for the high shear environment of the current application, this may be detrimental.¹¹

As in the one-dimensional case considered previously, it is natural to equate the scales in Eqs. (32), (33) and (36)–(38) with the equivalent Lagrangian integral scales. The connection is not rigorous and other choices may be justified. In this regard it was found that for the scale values in Fig. 7, σ_{22} is negative near the wall due to the term containing $\bar{u}\bar{v}$, so some modification of the scales is necessary. Several different strategies for ensuring the positive definiteness of σ_{22} were explored including replacing T_{21} by T_{12} , dropping the $\bar{u}\bar{v}$ terms in Eqs. (36) and (38) and eliminating all terms containing T_{21} and T_{12} from Eqs. (32), (33) and (36)–(38). For the latter case a calculation was also done with $T_{11} = T_{22} = T/C_D$ as used in Eqs. (28) and (29), though this had little effect on the solution. For all these approaches it was verified that the realizability condition $|\sigma_{12}| \leq \sqrt{\sigma_{11} \sigma_{22}}$ was satisfied. The best results were obtained when the terms depending on T_{21} and T_{12} were dropped. This solution, with T_{11} and T_{22} given from Fig. 7, is featured below.

Random variables with the specified covariances Eqs. (36)–(38) were generated by computing two independent random variables $\eta_1 = N(0, (\sigma_{11} + \sigma_{22} + \Sigma)/2)$ and $\eta_2 = N(0, (\sigma_{11} + \sigma_{22} - \Sigma)/2)$ where $\Sigma \equiv \sqrt{(\sigma_{11} - \sigma_{22})^2 + 4\sigma_{12}^2}/2$, and then setting

$$\mu_1 = (\sigma_{12} \eta_1 - \frac{1}{2}(\sigma_{22} - \sigma_{11} + \Sigma) \eta_2)/D, \quad (39)$$

$$\mu_2 = (\frac{1}{2}(\sigma_{22} - \sigma_{11} + \Sigma) \eta_1 + \sigma_{12} \eta_2)/D \quad (40)$$

where $D \equiv \sqrt{(\Sigma^2 + \Sigma(\sigma_{22} - \sigma_{11}))/2}$. To simulate the plume flow, tracer particles were released into the channel at each time step from a grid of locations covering the source: 200 in the case of the $y^+ = 15$ plume and 225 for the $y^+ = 30$ plume. The amount of scalar given to each tracer depended on the amplitude of Q at its initial location. The integration time step was $\Delta t^+ = 0.5$ and the plume was computed for 164 time steps representing an elapsed time of $t^+ = 82$. To get smooth statistics, the calculation was repeated 500 times and averaged. The independence of the algorithm to time step was tested by repeating the calculation with $\Delta t^+ = 0.4$ for 205 time steps. The average statistics from this calculation could not be distinguished from the first.

Plots of the predicted plumes based on Eqs. (26)–(29) and the random flight model are shown in Figs. 8–10. Comparing these to the direct numerical simulation results in Fig. 6 gives insight into the qualitative performance of the models. It is noteworthy that all of the models successfully predict that the peak of the $y^+ = 15$ plume is at the wall surface and not behind the source, as it is for the $y^+ = 30$ plume. By

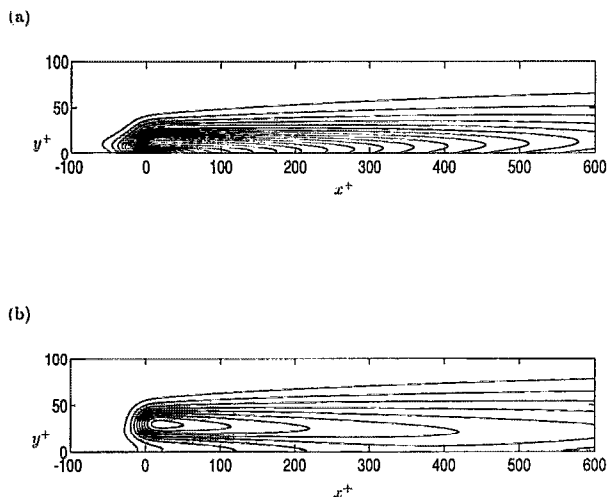


FIG. 8. $\tilde{C}$ contours computed using Eqs. (26) and (27). (a) Source at $y^+ = 15$, (b) source at $y^+ = 30$.

counting the number of contour lines in each figure, it may be concluded that the maximum $\tilde{C}$ tends to be overpredicted by all of the models with the exception of the random flight model at $y^+ = 15$. Here, the accumulation of the scalar on the wall surface near the source is underpredicted. All of the models slightly overpredict the downstream widening of the plumes. Focusing on the downstream extent of the steady regime at $t^+ = 82$, Figs. 8(a)–10(a) show that the closure models are qualitatively correct in this regard while the random flight model at $y^+ = 15$ does not show an adequate response to the presence of the wall, having similar characteristics as the $y^+ = 30$ plume. All of the models are better at predicting the structure of the $y^+ = 30$ plume than the $y^+ = 15$ plume, presumably because the greater homogeneity of the turbulence away from the wall places less of a demand on the modeling.

The expectation that the random flight model should be better at capturing the near field dispersion than gradient

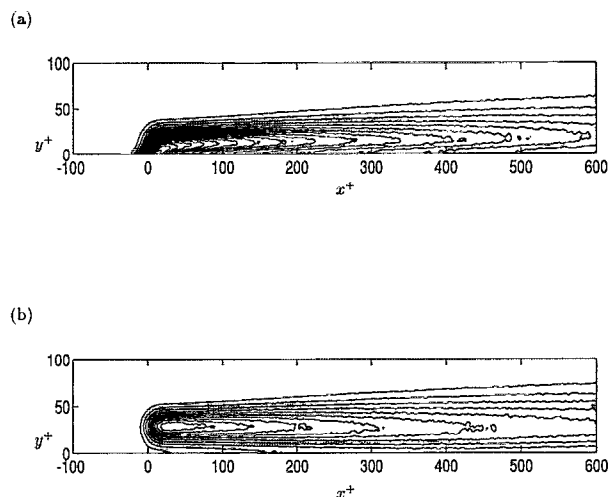


FIG. 10. $\tilde{C}$ contours computed using random flight model Eqs. (30)–(38). (a) Source at $y^+ = 15$, (b) source at $y^+ = 30$.

models is well borne out, at least qualitatively, by the current results. This is especially apparent from comparing the plumes in Figs. 6(a) and 10(a). In contrast, Figs. 8(a) and 9(a) show an unphysical distortion of the plume in which $\tilde{C}$ diffuses too far upstream. A similar exaggeration of the upstream dispersion by the closure models is also visible for the $y^+ = 30$ plume.

The near field errors associated with the closure models may be attributed to a fundamental failure of Eqs. (26) and (28) to accurately represent $\overline{uc}$ near the source. In particular, Fig. 11 is a plot of the DNS prediction of $\overline{uc}$ on a streamwise cut at $y^+ = 15$ through the $y^+ = 15$ plume, together with evaluations of Eqs. (26) and (28) using the $\tilde{C}$ field computed from the DNS solution. The latter are the values $\overline{uc}$ would have if the models were free of error. It is seen that $\overline{uc}$ is negligible upstream of $x^+ = -20$, becomes negative through the source region and then slowly rises into the steady part of the plume. In contrast, Eqs. (26) and (28) predict a large

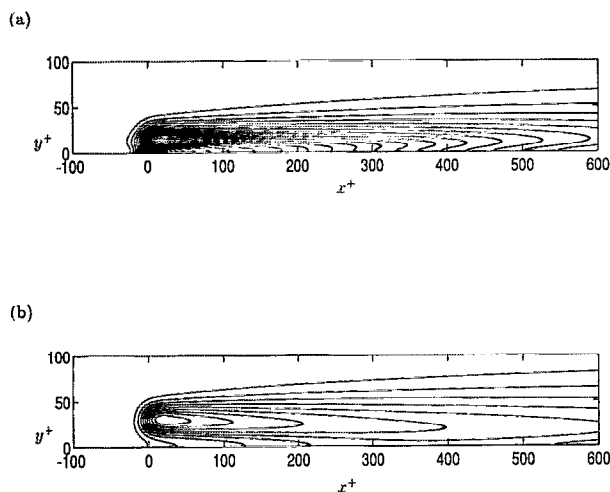


FIG. 9. $\tilde{C}$ contours computed using Eqs. (28) and (29). (a) Source at $y^+ = 15$, (b) source at $y^+ = 30$.

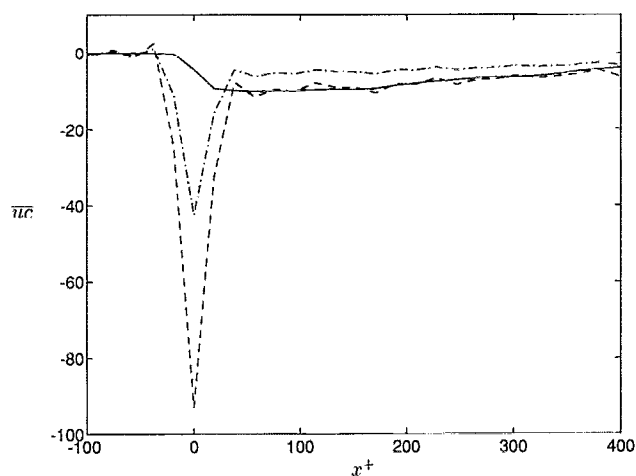


FIG. 11. $\overline{uc}$ for $y^+ = 15$ plume on the line $y^+ = 15$. — : DNS; --- : Eq. (26) using correct $\tilde{C}$; - · - : Eq. (28) using correct $\tilde{C}$.

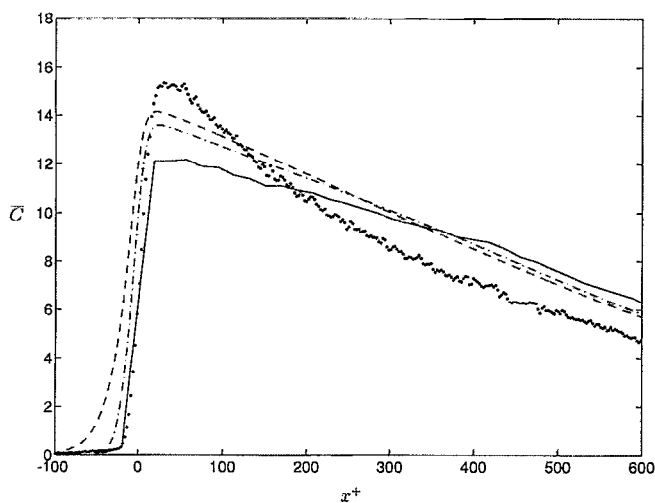


FIG. 12. Comparison of $\bar{C}$ on line $y^+ = 15$ for $y^+ = 15$ plume. —: DNS; ---: from Eqs. (26) and (27); — · —: from Eqs. (28) and (29); ···: random flight model.

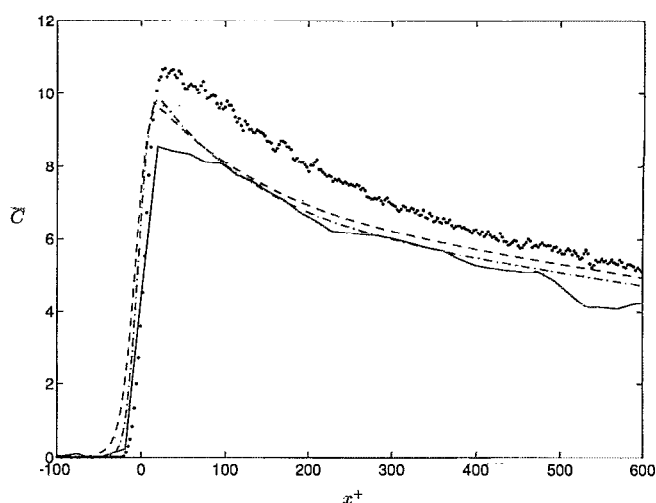


FIG. 13. Comparison of $\bar{C}$ on line $y^+ = 30$ for $y^+ = 30$ plume. —: DNS; ---: from Eqs. (26) and (27); — · —: from Eqs. (28) and (29); ···: random flight model.

negative spike in $\bar{u}\bar{c}$ near the origin of the plume. This behavior is attributable to the dependence of Eqs. (26) and (28) on $\partial\bar{C}/\partial x$, which is large and positive at the upstream end of the plume. Since T_{11} is much larger than T/C_D , Eq. (26) is less accurate than Eq. (28) and the plume in Fig. 8(a) spreads farther upstream than that in Fig. 9(a). Note that in this situation the shear term in Eq. (28) does not act to improve the prediction of $\bar{C}$ as it did in the case of the uniform source. Downstream of the source, Eqs. (26) and (28) quickly relax to slowly varying negative values attributable to their terms depending on $\partial\bar{C}/\partial y$. For the truncated Lagrangian model in Eq. (26) this agrees closely with the correct value, suggesting that $\bar{u}\bar{c}$ may very well be describable by gradient transport far enough downstream of the source. Note that the greater accuracy of Eq. (26) over (28) in this instance must stem from the use of the physical time scales rather than the model T/C_D . In particular, if gradient transport were the only significant process present in the flow, then Eq. (26) would have to be more accurate than Eq. (28).

A quantitative view of the accuracy of the models is given in Figs. 12–15 showing the predicted $\bar{C}$ fields on x and y coordinate lines intersecting the plumes. Figures 12 and 13 are cuts in the streamwise direction at the level of the centers of the sources at $y^+ = 15$ and 30, respectively. The scalar field distribution across the $y^+ = 15$ plume at $x^+ = 100$ and 500 is shown in Figs. 14(a) and 14(b), and a similar plot for the $y^+ = 30$ plume is shown in Figs. 15(a) and 15(b). The line $x^+ = 100$ is relatively close to the source, where the plume has reached steady state, while $x^+ = 500$ is away from the immediate sphere of influence of the source in the region which is still developing at $t^+ = 82$. According to Figs. 12 and 13, the closure models achieve considerable quantitative accuracy downstream of the source, in fact, reproducing the general trends quite well. Only in the near field is their accuracy seriously degraded by overprediction brought on by the unphysical upstream diffusion caused by the gradient models. Evidently, this has little consequence for the down-

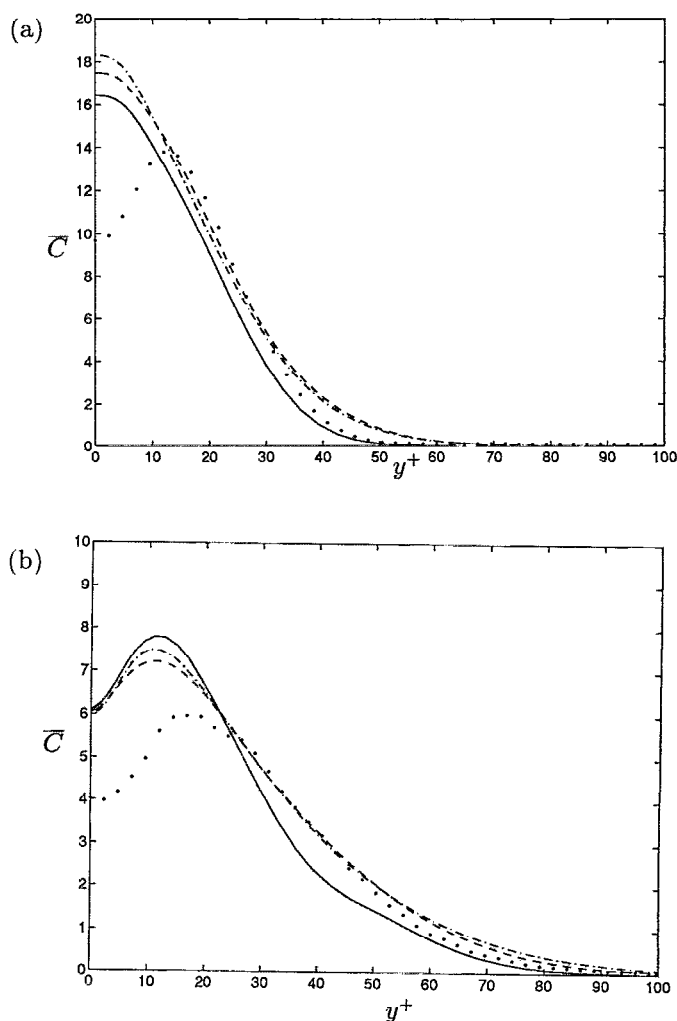


FIG. 14. Comparison of $\bar{C}$ for $y^+ = 15$ plume. —: DNS; ---: from Eqs. (26) and (27); — · —: from Eqs. (28) and (29); ···: random flight model. (a) $x^+ = 100$, (b) $x^+ = 500$.

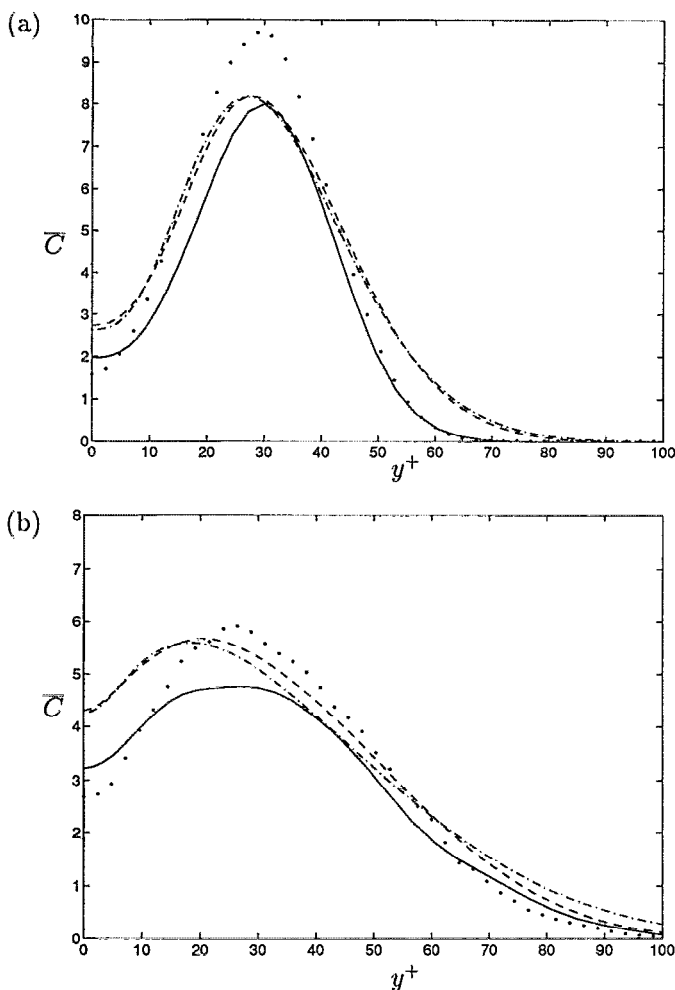


FIG. 15. Comparison of $\bar{C}$ for $y^+ = 30$ plume. —: DNS; ---: from Eqs. (26) and (27); — · —: from Eqs. (28) and (29); ···: random flight model. (a) $x^+ = 100$, (b) $x^+ = 500$.

stream solution. The near field errors are noticeably less for the $y^+ = 30$ plume presumably because the greater convection velocity of the flow counteracts the errors in $\overline{uc}$.

The figures call into question the quantitative accuracy of the random flight model for treating two-dimensional plumes in low Reynolds number turbulence. It substantially overpredicts the plume magnitude near the source in both cases, while in the far field it underpredicts the $y^+ = 15$ plume yet overpredicts the $y^+ = 30$ plume. The principal strength of the method is in capturing the distribution of $\bar{C}$ at the upstream end of the plumes, a property which is clearly superior for the random flight model than the closure schemes.

The mean scalar profiles for the cross-stream slice shown in Fig. 14(a) reveal that the closure models are relatively successful in capturing the complete trend of the plume in the steady region. The accuracy is fairly well maintained into the nonsteady region as well, as seen in Fig. 14(b). For the $y^+ = 30$ plume in Fig. 15(a), similar results are obtained, though there is a slight overprediction in the lateral spreading and the errors near the wall become fairly pronounced downstream, as seen in Fig. 15(b). The plots of

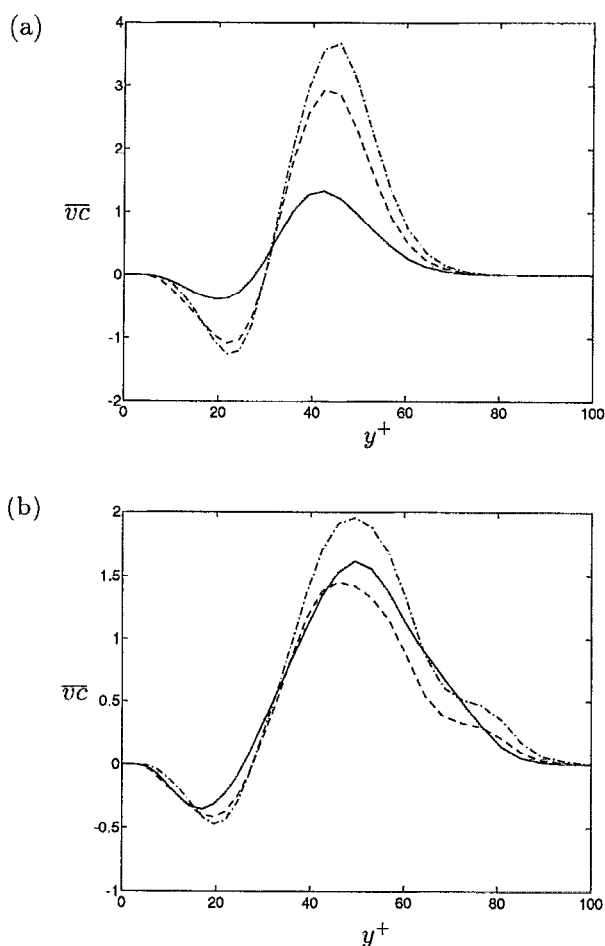


FIG. 16. $\overline{uc}$ for $y^+ = 30$ plume. —: DNS; ---: Eq. (27) using correct $\bar{C}$; — · —: Eq. (29) using correct $\bar{C}$. (a) $x^+ = 100$, (b) $x^+ = 300$.

$\bar{C}$ for the random flight model bring into sharper focus the difficulty faced by this method in correctly perceiving the influence of the boundary. As seen in Fig. 14(a), reasonable accuracy is achieved only for $y^+ > 20$, while the behavior adjacent to the wall is clearly unsatisfactory. For the $y^+ = 30$ plume, the difficulty in resolving the wall influence becomes quite noticeable in Fig. 15(b) at $x^+ = 500$ where the plume is now in contact with the wall. At $x^+ = 100$, before the wall effect is significant, the trend of $\bar{C}$ is well represented, apart from the peak which is too high.

We have previously considered the suitability of gradient modeling of $\overline{uc}$ in the near and far field of the plume, and we now consider the same question for the lateral transport correlation $\overline{uc}$. Figure 16 compares $\overline{uc}$ from the DNS with Eqs. (27) and (29) evaluated using the correct $\bar{C}$ field, at cuts across the $y^+ = 30$ plume at 100 and 300. Significant errors in the gradient models are evident at $x^+ = 100$ in Fig. 16(a) but not in Fig. 16(b) at $x^+ = 300$. At the first of these locations fluid particles are within an integral time scale of the origin, so the gradient model should be of questionable validity, as first predicted by the classical analysis of Taylor.⁹ The second position belongs to the approximately steady region downstream of the near field where gradient transport

has a greater likelihood of being legitimate. Evidently, Fig. 16(b) does not contradict this supposition. In the next section we will discuss in greater detail the physical mechanisms behind these properties of $\overline{v'c}$.

The quantitative differences between the scalar fields and fluxes predicted by the two closure models are almost entirely due to the different values used for the scales. In particular, applying Eqs. (28) and (29) with $S=0$ was found to cause less than a one percent change in the computed mean scalar. This appears to be a consequence of the fact that beyond the source region, $\overline{v'c}$ is the dominant turbulent influence on the plume and its modeling via Eq. (29) has no dependence on shear. In summary, gradient models may have some success in predicting the far field of plumes in nonhomogeneous turbulence, so long as they include the basic dependence on Reynolds stress exhibited by Eqs. (26) and (27) or Eqs. (28) and (29). The use of physically accurate scales improves the predictions of the far field fluxes at the expense of greater errors in the near field, while the opposite happens if the modeled scales are used. Both strategies give comparable predictions of the mean scalar field.

V. TRANSPORT PHYSICS

Our previous results suggest that improvements to the modeling of the turbulent flux rate in the near field of plumes are essential if progress is to be made in predicting contaminant dispersal through the Reynolds averaged formulation. Errors associated with gradient models near sources may not only affect the near field, but may also contribute to inaccuracies downstream, even where they do have a degree of legitimacy. The Lagrangian methodology presented earlier provides a systematic means for exploring the physics of the flux correlation. In the following we adopt this approach toward illuminating the physical processes responsible for transport, including an analysis of how and where the changeover to gradient physics takes place along the plume. The results given here cover only some of the principal aspects of the $\overline{v'c}$ correlation. We leave a more comprehensive treatment to a subsequent study in which the influence of coherent vortical structures is also taken into account.

The physics of the scalar flux in the near field of a turbulent plume was first considered by Taylor⁹ who showed that the lateral growth rate near the source is incompatible with the $\sqrt{t}$ growth implied by a diffusion equation. In particular, for flight times less than the local Lagrangian integral scale, the random positions of fluid particles initially at the source cannot be accurately described as having undergone a sum of independent random steps. Instead, their initial motion persists over a time on the order of the integral time scale, leading to a lateral growth rate in the plume proportional to t . Through various devices^{31,33} it has been argued that a gradient law modified to admit space or time dependent eddy diffusivities may account for the near field flux rate. These theories lack rigorous justification, however, and are subject to a number of conceptual difficulties, including the assumption that the eddy diffusivity is a property of the plume and not exclusively of the underlying turbulent flow. For plumes with countergradient transport in the near field,¹¹

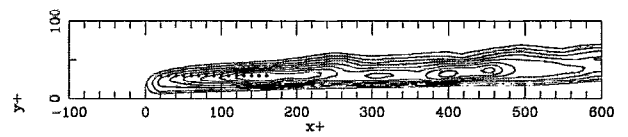


FIG. 17. Contours of $\overline{v'c}$ for $y^+=15$ plume. Points represent locations where Eqs. (4) and (41) were evaluated.

such models may be *a priori* disqualified. After we formally apply our transport analysis, it will become still more evident that the physics of the near field must have little to do with the gradient transport mechanism, even if modified to have a variable eddy diffusivity.

Our analysis of $\overline{v'c}$ proceeds by evaluating the terms in the Lagrangian decomposition Eqs. (4) and (5) applied to the plume flow. We specifically consider the $y^+=15$ plume at a series of points arrayed along the line $y^+=30$. These intersect the region of peak $\overline{v'c}$ as may be seen in Fig. 17 where the positive contours of $\overline{v'c}$ are plotted together with the points where the Lagrangian decomposition is evaluated. Note that $\overline{v'c}$ is positive on the side of the plume facing away from the wall in accordance with the expected direction of the turbulent flux. To evaluate Eqs. (4) and (5), ensembles of 200 particle paths each were computed with termination points distributed uniformly across the span at each of the points in Fig. 17. A second ensemble at each point was obtained using a later realization of the flow field so as to enhance the smoothness of the statistics.

It is a property of the plume flow that fluid particles upstream of the source must necessarily have $C=0$. Since we have defined the mixing time as the earliest time at which $\overline{v_a c_b} \approx 0$, τ_m must always be less than or equal to the minimum time needed for the fluid particles in an ensemble to have traveled from positions b upstream of the plume origin to the point a . In particular, for such a time interval, $C_b = \bar{C}_b = c_b = 0$ so certainly $\overline{v_a c_b} = 0$. When point a is just downstream of the source, the fluid particles arriving at a were upstream of the plume a short time earlier, and it can be expected that $\overline{v_a c_b}$ will be zero for relatively small τ . It is thus evident that the mixing time must be small for points near the source, and progressively increase downstream. For distances far enough downstream, it is likely that the natural decorrelation caused by random motion would cause $\overline{v_a c_b}$ to be zero for a time interval τ well before all the fluid particles in an ensemble are located upstream of the source. This implies that τ_m will approach an equilibrium value as x^+ increases.

Figure 18 shows the dependence of mixing time, computed here as the time where $\overline{v_a c_b}$ is within 5% of zero, on the distance downstream of the source. As anticipated, τ_m is small for x^+ near the source, rising linearly until $x^+ \approx 120$, beyond which it shows a tendency toward leveling off to a value near $\tau_m^+ \approx 18$. This is in the same range as τ_m^+ at $y^+=30$ for the uniform source flow, a result which is not unexpected, since the mixing process—when it takes place entirely within the plume—should be similar to that occurring in the uniform source flow.

Insight into the physical processes underlying the scalar

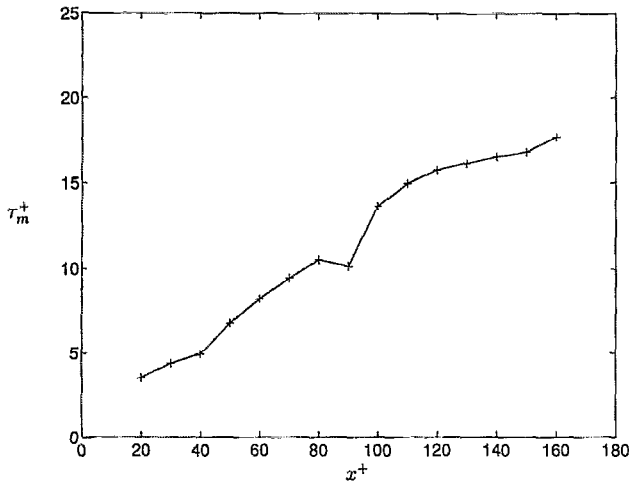


FIG. 18. Mixing time at points in Fig. 17.

flux will now be obtained from evaluating the decomposition in Eq. (4) at $x^+=20$ and 160, the first and last points indicated in Fig. 17. Figure 19 shows the τ dependence of each of the terms in Eq. (4)—scaled by $\overline{v_a c_a}$ —at these two locations. As suggested by Fig. 18, $\overline{v_a c_b}$ is zero after a shorter time interval at $x^+=20$ than at $x^+=160$. In either case the usefulness of Eq. (4) in revealing the transport physics is manifest only after $\tau > \tau_m$.

Contrasting the displacement transport term between Figs. 19(a) and 19(b), it is clear that in the former case it is zero when $\overline{v_a c_b}$ first approaches zero, while in the latter case it is at a peak with intimations of a plateau. Quite the opposite occurs in regards to the correlation $\overline{v_a(C_a - C_b)}$, which equals $\overline{v_a c_a}$ as the mixing time is reached at $x^+=20$ in Fig. 19(a), yet is only a relatively minor effect for the point $x^+=160$. The pattern in Fig. 19(a) rapidly appears in Fig. 19(b) once τ is large enough for the fluid particles in the ensemble to be upstream of the source. In this case the displacement term must be identically zero since $\bar{C}_b = 0$ if b is upstream of the plume.

While the decomposition of $\overline{v c}$ in Eq. (4) is potentially useful for any $\tau > \tau_m$, Fig. 19(b) suggests that the most physically beneficial interpretation occurs when $\tau \approx \tau_m$. From this perspective, it is evident that displacement transport represents a dominant effect in the creation of the $\overline{v c}$ correlation at $x^+=160$, while it has little role at $x^+=20$. Previous analyses^{22,25} have shown that the most significant source of displacement transport lies in motions induced by large quasistreamwise vortical structures. The time scale of these events, which is on the order of the eddy turnover time, is much greater than the short mixing time near the plume origin. Consequently, it is not surprising that displacement transport only becomes a factor in the scalar flux farther downstream, where the mixing time is larger.

Figure 19(a) does show that some of the physics of displacement transport are active in the flow near the source, since this term rises to a positive peak before dropping to zero just when mixing occurs. To gain an idea of when the displacement physics begins to dominate the scalar flux, Fig.

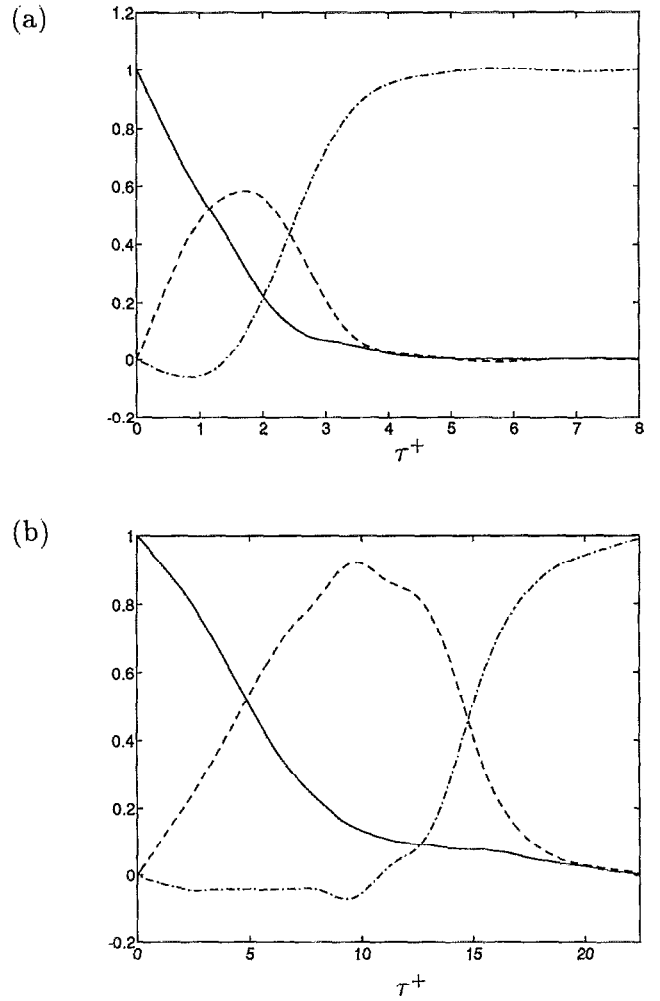


FIG. 19. Evaluation of Eq. (4) normalized by $\overline{v_a c_a}$ for $y^+=15$ plume. — : $\overline{v_a c_b}$; --- : $\overline{v_a(\bar{C}_b - \bar{C}_a)}$; - · - : $\overline{v_a(C_a - C_b)}$. (a) $x^+=20$, $y^+=30$; (b) $x^+=160$, $y^+=30$.

20 gives a plot of the displacement transport terms for several stations between $x^+=20$ and 160. An increasingly broad peak is observed after $x^+ > 130$ indicating the ascendancy of the displacement process at this distance from the source. At points farther downstream than were considered here, it is anticipated that a definite plateau in each of the terms of Eq. (4) will become evident.

Despite the dominant role of displacement physics commencing near $x^+=150$, it is unlikely that the gradient transport mechanism is an accurate model for this process until further downstream. In fact, fluid particles arriving near $x^+=150$ after the mixing time travel through a region of rapid variation in $\bar{C}$ which is poorly modeled by the linear representation required for gradient laws. Only farther downstream is it likely that fluid particles will travel through a relatively uniform part of the plume so that the gradient relation may be more approximately valid.

If the physics of $\overline{v_a c_a}$ in the near field is dominated by the process $\overline{v_a(C_a - C_b)}$, as was concluded from Fig. 19(a), then it is of some interest to explore the relative importance of the terms in the decomposition Eq. (5), viz.

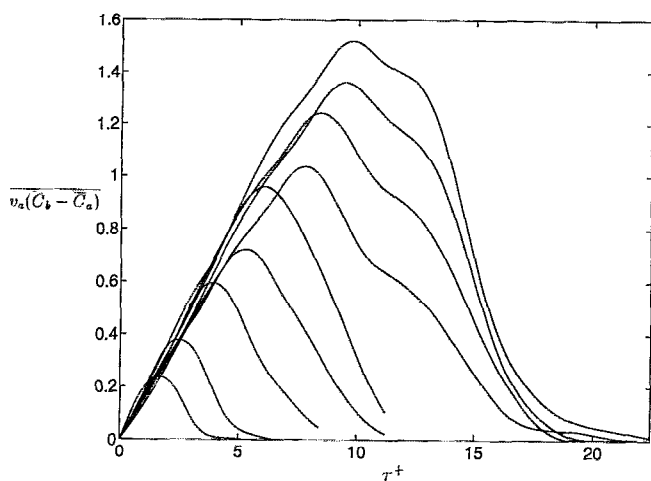


FIG. 20. Displacement transport terms for points in Fig. 17. The curves from smallest to largest peak are for $x^+ = 20, 40, 60, 80, 90, 130, 140, 150, 160$, respectively.

$$\overline{v_a(C_a - C_b)} = \frac{1}{\text{Re Sc}} \int_{-\tau}^0 \overline{v_a \nabla^2 C(s)} ds + \int_{-\tau}^0 \overline{v_a Q(s)} ds \quad (41)$$

in this region. For this purpose Fig. 21 shows the result of an evaluation of Eq. (41) at the representative point $x^+ = 20$, $y^+ = 30$. It is seen that $\overline{v_c}$ chiefly arises from the second term in Eq. (41) accounting for the cumulative scalar acquired by fluid particles as they meander through the source. The overprediction of $\overline{v_c}$ by this term is balanced by a negative contribution from the first term in Eq. (41). Since the latter is nonzero, there must be a correlation between v and the gain or loss of scalar by molecular diffusion.

To better understand the result in Fig. 21, we show the individual contributions to the integral terms in Eq. (41) made by the 400 particles in the ensemble. In Fig. 22 is

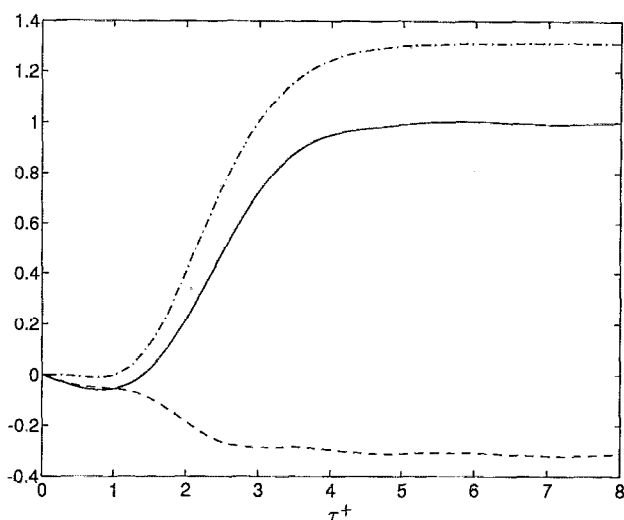


FIG. 21. Evaluation of Eq. (41) normalized by $\overline{v_a c_a}$ for point $x^+ = 20, y^+ = 30$ in $y^+ = 15$ plume. — : $v_a(C_a - C_b)$; --- : molecular diffusion term; - · - : source term.

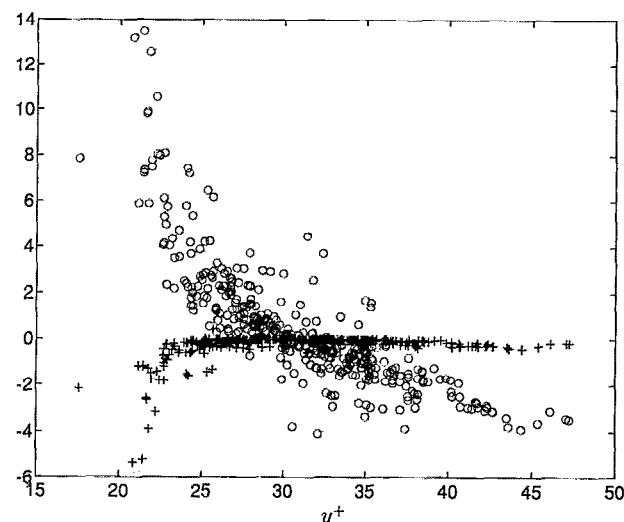


FIG. 22. Individual contributions to $\overline{v_a(C_a - C_b)}$ from paths in ensemble. $(1/\text{Re Sc}) \int_{-\tau}^0 v_a \nabla^2 C(s) ds$: +; $\int_{-\tau}^0 v_a Q(s) ds$: O.

plotted, for each particle, the magnitude of $(1/\text{Re Sc}) \int_{-\tau}^0 v_a \nabla^2 C(s) ds$ (+ symbol) and $\int_{-\tau}^0 v_a Q(s) ds$ (O symbol) versus initial y^+ location. Since the end points of the fluid particles are at $y^+ = 30$, those beginning at $y^+ < 30$ generally have $v_a > 0$, while those starting at $y^+ > 30$ have $v_a < 0$. Evidently, very few particles gain or lose significant amounts of scalar by molecular diffusion, and those that do are traveling from below $y^+ = 30$ contributing negatively to $(1/\text{Re Sc}) \int_{-\tau}^0 v_a \nabla^2 C(s) ds$. This suggests that $\nabla^2 C(s) < 0$ for these particles so that they are losing the scalar which they recently acquired while passing through the source. This phenomenon is responsible for the negative contribution of the molecular diffusion term to $\overline{v_a(C_a - C_b)}$ shown in Fig. 21. For $\tau^+ < 1$, $\overline{v_a(C_a - C_b)} < 0$ while $\int_{-\tau}^0 v_a Q(s) ds = 0$. In this case, fluid particles which no longer are in the source region are losing scalar by molecular diffusion.

The proximity of $x^+ = 20$, $y^+ = 30$ to the source accounts for the many significant contributions to $\int_{-\tau}^0 v_a Q(s) ds$ evident in Fig. 22. Since fluid particles traveling away from the wall ($v_a > 0$) are likely to pass through a greater portion of the source than fluid particles heading toward the wall, positive contributions dominate over negative ones, and the net flux is positive. The largest positive contributions to $\int_{-\tau}^0 v_a Q(s) ds$ come from the relatively small number of particles which have traveled from points closest to the wall and thus have had occasion to pass through a greater portion of the source centered at $y^+ = 15$. The relatively large vertical travel of these particles away from the wall suggest that they are associated with ejections of low speed fluid—a major factor in the dynamics of the flow in the vicinity of $y^+ = 30$.

We see from these considerations that scalar transport at a given point near the source depends on its position relative to the source and to the dynamical events associated with the underlying vortical structure of the boundary region. This process has little connection to the mechanisms ordinarily

associated with gradient transport and it is difficult to see how allowing the eddy diffusivity to have plume dependent properties comes closer to modeling the correct physics. The outlook for gradient models improves considerably with distance downstream from the plume origin when displacement transport becomes the dominant mechanism behind the turbulent scalar flux.

VI. CONCLUSIONS

The performance of random flight and closure models in predicting scalar transport under low Reynolds and Schmidt number conditions has been examined within the controlled setting offered by a direct numerical simulation of turbulent channel flow with uniform and line sources. It is evident that under the highly anisotropic and inhomogeneous conditions of the channel, closure models provide substantially better overall quantitative accuracy than random flight models at a reduced computational cost. The range of applications of closure models in the gradient form is limited, however, by their failure to accommodate the near field of plumes. Though random flight models provide greater realism in modeling near the plume source, they are prone to substantial errors in the mean scalar field and do not appear to accommodate well the presence of solid boundaries in multidimensional flow.

The anisotropic gradient models given in Eqs. (26) and (27) or Eqs. (28) and (29) proved to be adequate for modeling the steady far field of plumes. Since the shear terms in Eq. (28) had very little effect on predictions, the most important issue in the development of gradient models is the choice of time scales. The use of the theoretically derived Lagrangian integral scales has the advantage of being more accurate in the far field of the plume, though this is gained only at the expense of a significant distortion in the near field. Through its use of simplified scales, the algebraic model reduces the errors in the near field, but is then somewhat less accurate in representing transport in the far field. For the predicted scalar fields, however, both alternatives are found to have comparable accuracy. Implementation of Eqs. (28) and (29) in applications may be easier than Eqs. (26) and (27) since it may be problematical to obtain values of the four Lagrangian integral scales under general flow conditions. In both cases, the Reynolds stresses need to be available, and for the algebraic model, k and ϵ , as well. Such quantities must generally be acquired from closure schemes which are prone to considerable errors themselves. Consequently, the practical implementation of scalar flux models will often be subject to additional errors which are unrelated to their form.

A high priority in improving the accuracy of predictions based on turbulent scalar transport models must lie in increasing their range of applicability to include the near field of plumes. As a step toward this end, we have made a limited application of the Lagrangian methodology to the lateral transport correlation at various points where it is at a local peak. This showed in some detail why gradient transport is unlikely to be a significant factor in the near field of plumes. In particular, the mixing time is too small for displacement transport to fully create a correlation between u and c . Farther downstream, where fluid particles spend much longer

times within the plume, the physical mechanisms behind the scalar flux shifts to that of displacement transport which may be reasonably well modeled via a gradient term. In the near field, the scalar is dispersed as the turbulent flow meanders over the source. To the extent that organized vortical structures dominate the convection of fluid particles in the wall region, they may be an important factor in near field scalar diffusion. This process is slightly offset by an effective transport caused by fluid particles systematically losing scalar by molecular diffusion after leaving the source. The prediction of scalar fields in inhomogeneous turbulence should be considerably advanced once models of these fundamental processes are developed.

ACKNOWLEDGMENTS

This research was supported in part by the Office of Basic Energy Sciences, U.S. Department of Energy Grant No. DE-FG05-88ER13838 and in part by the Applied Mathematical Sciences Subprogram of the Office of Energy Research, U.S. Department of Energy under Contract No. DE-AC03-76SF00098 while the first author was a visiting professor at Lawrence Berkeley Laboratory and the Department of Mathematics, University of California, Berkeley. ALR acknowledges support through a NRC Postdoctoral Fellowship. Computer time was supplied in part by the Pittsburgh Supercomputing Center.

- ¹A. Yoshizawa, "Statistical modeling of passive scalar diffusion in turbulent shear flows," *J. Fluid Mech.* **195**, 541 (1988).
- ²M. M. Rogers, N. N. Mansour, and W. C. Reynolds, "An algebraic model for the turbulent flux of a passive scalar," *J. Fluid Mech.* **203**, 77 (1989).
- ³K. Horiuti, "Assessment of two-equation models of turbulent passive scalar diffusion in channel flow," *J. Fluid Mech.* **238**, 405 (1992).
- ⁴P. Durbin and J. C. R. Hunt, "Dispersion from elevated sources in turbulent boundary layers," *J. Mec.* **19**, 679 (1980).
- ⁵D. J. Thomson, "Random walk modeling of diffusion in inhomogeneous turbulence," *Q. J. R. Meteorol. Soc.* **110**, 1107 (1984).
- ⁶H. van Dop, F. T. M. Nieuwstadt, and J. C. R. Hunt, "Random walk models for particle displacements in inhomogeneous unsteady turbulent flows," *Phys. Fluids* **28**, 1639 (1985).
- ⁷D. J. Thomson, "A random walk model of dispersion in turbulent flows and its application to dispersion in a valley," *Q. J. R. Meteorol. Soc.* **112**, 511 (1986).
- ⁸M. R. Raupach, "A practical Lagrangian method for relating scalar concentrations to source distributions in vegetation canopies," *Q. J. R. Meteorol. Soc.* **115**, 609 (1989).
- ⁹G. I. Taylor, "Diffusion by continuous movements," *Proc. London Math. Soc.* **XX**, 196 (1921).
- ¹⁰C. A. Degrazia and O. L. L. Moraes, "A model for eddy diffusivity in a stable boundary layer," *Boundary Layer Meteorol.* **58**, 205 (1991).
- ¹¹T. K. Flesch and J. D. Wilson, "A two-dimensional trajectory-simulation model for non-Gaussian, inhomogeneous turbulence within plant canopies," *Boundary Layer Meteorol.* **61**, 349 (1992).
- ¹²H. Van Dop, "Buoyant plume rise in a Lagrangian framework," *Atmos. Env.* **26**, 1335 (1992).
- ¹³Y. Shao, "Turbulent dispersion in coastal atmospheric boundary layers: an application of a Lagrangian model," *Boundary Layer Meteorol.* **59**, 363 (1992).
- ¹⁴J. M. Macinnes and F. V. Bracco, "Stochastic particle dispersion modeling and the tracer-particle limit," *Phys. Fluids A* **4**, 2809 (1992).
- ¹⁵D. J. Thomson, "Criteria for the selection of stochastic models of particle trajectories in turbulent flows," *J. Fluid Mech.* **180**, 529 (1987).
- ¹⁶W. C. Reynolds, M. M. Rogers, and N. D. Sandham, "Advances in turbulent transport modeling based on direct simulations of turbulence," *Transport Phenomena in Turbulent Flows: Theory, Experiment, and Numerical Simulation*, edited by M. Hirata and N. Kasagi (Hemisphere, New York, 1988), pp. 701-713.

- ¹⁷J. Kim and P. Moin, "Transport of passive scalars in a turbulent channel flow," in *Turbulent Shear Flows 6*, edited by J.-C. Andre, J. Cousteix, F. Durst, B. E. Launder, F. W. Schmidt, and J. H. Whitelaw (Springer, New York, 1987), pp. 5-2-1-5-2-8.
- ¹⁸J. Kim, "Investigation of heat and momentum transport in turbulent flows via numerical simulations," in Ref. 16, pp. 715-729.
- ¹⁹N. Kasagi and Y. Ohtsubo, "Direct numerical simulation of passive scalar field in a turbulent channel flow," *ASME J. Fluids Eng.* **114**, 598 (1992).
- ²⁰P. K. Yeung, J. G. Brasseur, and D. M. Bell, "Evolution of passive scalar sources in a numerically simulated boundary layer," in *Near Wall Turbulent Flows*, edited by R. M. C. So, C. G. Speziale, and B. E. Launder (Elsevier, Amsterdam, 1993), pp. 307-316.
- ²¹D. M. Bell and J. H. Ferziger, "Turbulent boundary layer DNS with passive scalars," in Ref. 20, pp. 327-336.
- ²²P. S. Bernard and R. A. Handler, "Reynolds stress and the physics of turbulent momentum transport," *J. Fluid Mech.* **220**, 99 (1990).
- ²³P. S. Bernard, "Turbulent vorticity transport in three dimensions," *Theor. Comput. Fluid Dyn.* **2**, 165 (1990).
- ²⁴A. Rovelstad, "Lagrangian analysis of vorticity transport in a numerically simulated turbulent channel flow," Ph.D. thesis, University of Maryland, College Park, 1991.
- ²⁵P. S. Bernard, J. M. Thomas, and R. A. Handler, "Vortex dynamics and the production of Reynolds stress," *J. Fluid Mech.* **253**, 385 (1993).
- ²⁶P. A. Durbin, "Near-wall turbulence closure modeling without 'damping functions,'" *Theor. Comput. Fluid Dyn.* **3**, 1 (1991).
- ²⁷R. Rubinstein and J. M. Barton, "Renormalization group analysis of anisotropic diffusion in turbulent shear flows," *Phys. Fluids A* **3**, 415 (1991).
- ²⁸J. C. R. Hunt and A. H. Weber, "A Lagrangian statistical analysis of diffusion from a ground-level source in a turbulent boundary layer," *Q. J. R. Meteorol. Soc.* **105**, 423 (1979).
- ²⁹R. A. Handler, E. W. Hendricks, and R. I. Leighton, "Low Reynolds number calculation of turbulent channel flow: a general discussion," Memorandum Report 6410, Naval Research Laboratory, 1989.
- ³⁰A. L. Rovelstad, R. A. Handler, and P. S. Bernard, "The effect of interpolation errors on the Lagrangian analysis of simulated turbulent channel flow," *J. Comput. Phys.* **110**, 190 (1994).
- ³¹G. T. Csanady, *Turbulent Diffusion in the Environment* (Reidel, Dordrecht, 1973).
- ³²O. Zeman and J. L. Lumley, "Modeling buoyancy-driven mixed layers," *J. Atmos. Sci.* **33**, 1974 (1976).
- ³³J. O. Hinze, *Turbulence* (McGraw-Hill, New York, 1976).

Physics of Fluids is copyrighted by the American Institute of Physics (AIP).
Redistribution of journal material is subject to the AIP online journal license and/or AIP
copyright. For more information, see <http://ojps.aip.org/phf/phfcr.jsp>
Copyright of Physics of Fluids is the property of American Institute of Physics and its
content may not be copied or emailed to multiple sites or posted to a listserv without
the copyright holder's express written permission. However, users may print,
download, or email articles for individual use.