Parameterizing Mesoscale Wind Uncertainty for Dispersion Modeling

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(Manuscript received 21 September 2009, in final form 25 March 2010)

ABSTRACT

A parameterization of numerical weather prediction uncertainty is presented for use by atmospheric transport and dispersion models. The theoretical development applies Taylor dispersion concepts to diagnose dispersion metrics from numerical wind field ensembles, where the ensemble variability approximates the wind field uncertainty. This analysis identifies persistent wind direction differences in the wind field ensemble as a leading source of enhanced ''virtual'' dispersion, and thus enhanced uncertainty for the ensemble-mean contaminant plume. This dispersion is characterized by the Lagrangian integral time scale for the grid-resolved, large-scale, ''outer'' flow that is imposed through the initial and boundary conditions and by the ensemble deviation-velocity variance. Excellent agreement is demonstrated between an explicit ensemble-mean contaminant plume generated from a Gaussian plume model applied to the individual wind field ensemble members and the modeled ensemble-mean plume formed from the one Gaussian plume simulation enhanced with the new ensemble dispersion metrics.

1. Introduction

Atmospheric dispersion of an airborne contaminant is a complex physical process involving a three-dimensional wind field complicated by turbulence effects over a wide range of spatial scales. This wind field is affected by the local meteorology and local forcings by terrain, heating, land use, and coastlines as well as the larger-scale atmospheric flow. The nonlinear physics underlying these wind field responses makes the instantaneous, local state of the wind field chaotic and impossible to predict with certainty. Yet dispersion of contaminants in the atmosphere is an important problem that must be addressed. Examples include plumes emitted from industrial complexes, smoke stacks, and traffic sources; chemical plumes from accidental releases; and chemical, biological, radiological, or nuclear (CBRN) clouds from deliberate releases.

Modern atmospheric transport and dispersion models couple a representation of a contaminant source with a meteorological forecast to predict the expected contaminant trajectory and its concentration distribution plus an estimate of the expected hazard area. Because of the sensitivity of this nonlinear dynamical system to its initial and boundary conditions, the uncertainty in the wind field is expected to grow in time. That uncertainty is bounded by the constraints of the underlying attractor, although these bounds are seldom quantitatively known (Lorenz 1963). Thus, both the predicted wind fields and the resulting atmospheric dispersion are inherently uncertain because of this sensitivity to initial conditions.

Note that there are model uncertainties due to a multitude of other causes, including inexact formulations of the physics and dynamics, numerical truncation and approximation errors, and errors in sensor observations that are assimilated into the model. Thus, even an analysis or nowcast, which incorporates observations into the space of the model, includes such error. The mean-squared error between the model estimate and the actual value (observation), or Brier score, is often decomposed into three parts: reliability (conditional bias), resolution (ability to discern correct relative frequencies of

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DOI: 10.1175/2010JAMC2396.1

events), and uncertainty (irreducible error in the observation) (Wilks 2006). Here we are dealing with the uncertainty portion of the error. That uncertainty is due solely to the inherent unpredictability of the atmosphere.

The wind field uncertainty in dispersion prediction has two causes. The first, which we shall call ''inner variability,'' stems from the turbulence in the unresolved flow field. Since turbulence differs from realization to realization, effluent plumes also differ in detail from realization to realization. As a result the ensemble-average plume has a broader, more diffuse form than any ensemble member. This ''virtual'' dispersion exists only as an average over many realizations. To illustrate, imagine a nondeformable, nondiffusive parcel of effluent released into a turbulent flow. The parcel has a unique trajectory in each realization; averaging over an ensemble of realizations yields a broad and diffuse mean concentration field that clearly displays this virtual dispersion.

A second cause of wind field uncertainty, which we shall call ''outer variability,'' is that in the meteorological field at grid-resolved and larger scales. Lamb (1984) referred to this nondeterministic class of flow in regional modeling that blends the concepts of turbulence and mean flow as ''metulence.'' He then developed methods to use an ensemble of states to compare predictions with observations. Lamb and Hati (1987) further developed this concept by constructing a method for generating ensembles of wind fields for use in regional-scale models that predated the availability of multiple simulations of an episode. Lewellen and Sykes (1989) cite this mesoscale meteorological variability as a major source of dispersion uncertainty. Schere and Coats (1992) addressed the data needs for characterizing regional-scale transport in an ensemble and concluded that air quality models should be evaluated in a probabilistic mode. Today this outer variability is seldom parameterized; instead, modern numerical weather prediction (NWP) addresses it by providing ensembles of forecasts differing by variations in initial conditions, boundary conditions, and physics parameterizations (Toth and Kalnay 1993; Hamill et al. 2000; Stensrud et al. 2000; Toth 2001; Deng and Stauffer 2006; Fujita et al. 2007; among others).

Figure 1 summarizes this division into inner and outer variability. At the finest scales the inner variability is a subgrid-scale process and the key to understanding that process can be traced to Taylor (1921). In contrast, the outer variability is resolved by the model but stems from the uncertainty due to the metulence of the mesoscale flow. We attribute recognition of this variability to Lamb (1984). We postulate that the same framework developed by Taylor (1921) for the inner variability

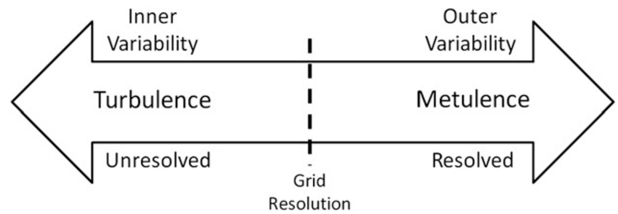

FIG. 1. Schematic of the relationship between inner and outer variability.

problem can be adapted for the outer variability problem: that adaptation is the goal of this current paper.

One could compute the virtual dispersion due to outer variability by using each meteorological ensemble member to force a dispersion episode and then average the predicted concentration fields, but such an approach may be too time-consuming for emergency response. Here we shall propose potential methods for analyzing existing ensembles of meteorological forecasts to parameterize outer variability. The concept of diagnosing the wind field uncertainty from an appropriately sampled ensemble of wind field predictions underlies this work. It allows us to compute uncertainty fields from NWP ensemble data and extract outer variability uncertainty scales that parameterize the dispersion due to the metulence.

Contemporary research suggests that ensemble approaches to dispersion also provide statistically more reliable dispersion forecasts. Galmarini et al. (2004a) developed statistical measures that summarize the results of multiple dispersion models on a single plot, and Galmarini et al. (2004b) documented their performance in modeling the first release of the European Tracer Experiment (ETEX-1). They assembled their ensemble set of 18 members by using 12 NWP and 16 dispersion models from 12 institutions.

Lewellen and Sykes (1989) developed a framework for computing dispersion uncertainty in the Second Order Closure Integrated Puff (SCIPUFF) dispersion model, which incorporates variances and a length scale discerned from an ensemble of meteorological model runs. Warner et al. (2002) demonstrated the benefits of SCIPUFF's ensemble approach for emergency response using its internal parameterization for ensemble dispersion. SCIPUFF's modeling parameters are the ensemble wind variances that represent outer variability (Sykes et al. 2004). If ensemble members agree, the ensemble approach will contribute no added dispersion to the ensemble-mean plume. Conversely, if the ensemble members differ considerably, the model yields significant additional dispersion. Warner et al. (2002) acknowledged that the appropriate parameterization for this variability is still uncertain. Specifically, the details of how to estimate the appropriate length scale are an open question that we directly address here.

The purpose of this current study is to lay the theoretical groundwork for choosing the parameters that should be used in this ensemble approach. This parameterized approach seeks to estimate the uncertainty in dispersion within a single atmospheric and transport dispersion model run. We then discuss and demonstrate the implications of that theoretical approach in the context of Gaussian plume dispersion. In our companion study (Lee et al. 2009), we demonstrate that parameterization in a case study of an ensemble based on differing physics configurations for the 1983 Cross-Appalachian Tracer Experiment (CAPTEX). That study also uses SCIPUFF as the dispersion model and demonstrates that the plume spread based on its statistical parameterization agrees well with that from an explicit SCIPUFF ensemble. That parameterization is based on the ensemble variance of the wind field and a length scale. In that work that length scale was derived from a Lagrangian integral time scale computed by using a Lagrangian particle model in each of the multiple NWP ensemble members. That derivation is based on the theory derived herein. In complementary work (Kolczynski et al. 2009), the variance statistics discussed here are calibrated using a new linear variance calibration (LVC) technique.

We shall also address how the outer variability, specifically the NWP wind field uncertainty as defined by the ensemble velocity variances, relates to dispersion uncertainty. In section 2 we shall argue that wind direction uncertainty is a leading source of ensemble variability and show, using Taylor dispersion concepts applied to ensemble dispersion, that a modeling length scale can be derived from the ensemble deviation-velocity statistics. We also relate that length scale to the Lagrangian integral time scale for particles dispersing within the NWP ensemble. We consider the appropriate Lagrangian integral time scale in section 3. Using a Gaussian plume model, in section 4 we demonstrate that the modeled ensemble-mean plume from our derived parameterization agrees well with the plume computed directly from a dispersion ensemble. We summarize conclusions and prospects in section 5.

2. Formulation of the ensemble-mean plume dispersion problem

We first show that dispersion from a point source due to the outer variability averaged over an NWP ensemble is a variant of classical ''Taylor dispersion'' (Taylor 1921). We shall also show that it has a new feature—time-persistent differences in wind direction among the ensemble members—that enhances the lateral spread of the mean plume.

Our term ''outer variability'' refers to the inevitable differences between the coarsely resolved meteorological fields used to drive a dispersion model and the wind field (at the same spatial resolution) existing in the specific dispersion episode being modeled (see Fig. 1). These differences occur on spatial scales ranging from the effective grid resolution of the meteorological model to scales even larger than the model domain.

a. A brief review of Taylor dispersion: Inner variability

Since our analysis of outer variability due to metulence is based on Taylor dispersion theory, it is critical that we first briefly review it and introduce the notation to be used in later sections. Remarkably, Taylor (1921) found an analytical solution for dispersion in stationary, homogeneous turbulence, one of the few exact solutions in the entire field of turbulence. We apply it to steady, homogeneous turbulent flow that disperses effluent emitted from a continuous source in a vertically integrated atmosphere.

The ensemble-mean concentration equation is a balance between streamwise (x) mean advection and cross-stream (y) turbulent diffusion,

$$U\frac{\partial C}{\partial x} = -\frac{\partial \overline{\mathrm{cv}}}{\partial y}, \quad (1)$$

where C denotes the mean contaminant concentration, U is the ensemble-mean velocity in the downwind (x) direction, and $\overline{\mathrm{cv}}$ is the covariance of fluctuating concentration and fluctuating cross-stream velocity. The overbar represents an ensemble average. If there exists an eddy diffusivity $K(x)$ such that

$$\overline{\mathrm{cv}} = -K\frac{\partial C}{\partial y}, \quad (2)$$

then the concentration equation has the form

$$U\frac{\partial C}{\partial x} = K\frac{\partial^2 C}{\partial y^2}, \quad (3)$$

which has the Gaussian solution

$$C = \frac{Q}{\sqrt{2\pi}U\sigma}\exp\left(-\frac{y^2}{2\sigma^2}\right), \quad (4)$$

where Q is the emission rate and $\sigma(x)$ is the lateral length scale of the mean plume. Substituting the Gaussian solution (4) into (3) for the mean concentration gives $K(x)$:

$$K(x) = \frac{U}{2}\frac{d\sigma^2}{dx}. \tag{5}$$

Taylor deduced the behavior of the eddy diffusivity $K(x)$ in this problem through the following Lagrangian analysis. The parameter σ^2 in the Gaussian solution is the Lagrangian quantity $\overline{y_p^2}(t)$, the mean-squared value of the instantaneous lateral displacement $y_p(t)$ (relative to the release point) of a diffusing effluent particle. Here $y_p(t)$ is related to the particle lateral velocity $\upsilon_p(t)$ by

$$\frac{dy_p}{dt} = \upsilon_p(t), \tag{6}$$

so the lateral position of the particle at time t relative to its initial position is

$$y_p(t) = \int_0^t \upsilon_p(t')\,dt'. \tag{7}$$

The Eulerian quantity $\upsilon(x, t)$ is $\upsilon_p(t)$ at the location of the particle.

The ensemble-mean plume from a continuous point source in stationary, homogeneous turbulence is described by statistics of these single-particle trajectories. Its width parameter is $\sigma^2 \equiv \overline{y_p^2}$, which is governed by

$$\frac{d\sigma^2}{dt} = 2\overline{y_p\frac{dy_p}{dt}}, \quad \text{so that} \quad \frac{d\sigma^2}{dt} = 2\int_0^t \overline{\upsilon_p(t)\upsilon_p(t')}\,dt'. \tag{8}$$

For a large number of realizations N the Lagrangian velocity autocorrelation function becomes

$$\overline{\upsilon_p(t)\upsilon_p(t')} = \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\upsilon_p(t)\upsilon_p(t'). \tag{9}$$

Taylor (1921) showed that in stationary, homogeneous turbulence the short- and long-time behaviors of Eq. (3) are

$$t \to 0\text{:}\quad \frac{d\sigma^2}{dt} = 2\overline{\upsilon_p^2}t \quad \text{so that} \quad \sigma = (\overline{\upsilon_p^2})^{1/2}t; \tag{10a}$$

$$t \to \infty\text{:}\quad \frac{d\sigma^2}{dt} = 2\int_0^\infty \overline{\upsilon_p(t)\upsilon_p(t')}\,dt' = 2\overline{\upsilon_p^2}\tau_L \quad \text{so that}$$
$$\sigma \sim (\overline{\upsilon_p^2}\tau_L)^{1/2}t^{1/2}, \tag{10b}$$

with τ_L the Lagrangian integral time scale of $\upsilon_p(t)$ defined as $\tau_L = (1/\overline{\upsilon_p^2})\int_0^\infty \overline{\upsilon_p(t)\upsilon_p(t')}\,dt'$. Thus, τ_L measures the length of time that the particle velocity remains correlated with itself.

Lumley (1962) showed that in homogeneous, stationary turbulence the Lagrangian and Eulerian velocity variances are equal; that is,

$$\overline{\upsilon_p^2} = \overline{\upsilon^2}. \tag{11}$$

The short- and long-time behaviors of σ implied by (10) can therefore be written in terms of the Eulerian velocity variance:

$$\sigma = (\overline{\upsilon^2})^{1/2}t, \quad t \ll \tau_L; \tag{12a}$$

$$\sigma \sim (\overline{\upsilon^2}\tau_L)^{1/2}t^{1/2}, \quad t \gg \tau_L. \tag{12b}$$

Taylor dispersion is a "virtual process" created by averaging over an ensemble of realizations of dispersing particles. It is the basis of the "Gaussian plume" solution (4) for ensemble-mean concentration downwind of a continuous source in stationary, homogeneous turbulence (Csanady 1973). This ensemble-mean plume and the instantaneous plume at any time in a realization are very different.

b. *Dispersion on the mesoscale: Outer variability*

Taylor (1921) made his problem tractable by assuming homogeneous turbulence, but the atmospheric boundary layer is at most homogeneous in the horizontal plane. Thus, to use Taylor's result, we will eliminate the vertical coordinate by averaging the wind field over the depth of the atmospheric boundary layer and working in the two horizontal dimensions. We will assume a continuous virtual point source of effluent in the plane and express the mesoscale wind field variability through a number of different realizations of the meteorological fields. We write the total horizontal wind field in realization α as $[\tilde{u}_\alpha(x, y, t), \tilde{\upsilon}_\alpha(x, y, t)]$.

Next we write these velocity components as the sum of mean and fluctuating parts:

$$\tilde{u}_\alpha(x, y, t) = U_\alpha(t) + u_\alpha(x, y, t), \tag{13a}$$

$$\tilde{\upsilon}_\alpha(x, y, t) = V_\alpha(t) + \upsilon_\alpha(x, y, t), \tag{13b}$$

with the mean defined as the average over the dispersion area A:

$$U_\alpha(t) = \langle\tilde{u}_\alpha\rangle = \frac{1}{A}\int\int \widetilde{u_\alpha}(x, y, t)\,dx\,dy, \tag{14a}$$

$$V_\alpha(t) = \langle\tilde{\upsilon}_\alpha\rangle = \frac{1}{A}\int\int \widetilde{\upsilon_\alpha}(x, y, t)\,dx\,dy. \tag{14b}$$

Using this average on (13) and using its property that $U_\alpha = U_\alpha(t)$ shows that $\langle u_\alpha \rangle = 0$, as in traditional Reynolds averaging. In view of (13) and (14), the horizontal spatial scales of the principal motions contributing to both the mean and fluctuating velocities are greater than and smaller than l, respectively, where $l^2 \simeq A$. Thus here the velocity fluctuations include any motions on the scale of the entire length of the regional plume.

Each member of a mesoscale model ensemble incorporates different initial conditions, boundary conditions, or physical parameterizations to produce one realization of the evolving meteorological field. The resulting realization-to-realization differences in these evolving mesoscale fields cause the time-dependent mesoscale mean wind vector (U_α, V_α) to differ somewhat in each realization. This feature, which is not present in the classical Taylor problem, affects the ensemble-mean dispersion.

c. *Mesoscale dispersion as a Taylor problem*

We define *realization coordinates* aligned with the average of U_α over the duration T of the dispersion episode. In general they are different in each realization. Figure 2 diagrams a notional plume in three realization coordinate frames on the left side and shows how they add to form an augmented ensemble-mean plume on the right. In realization coordinates the wind field components in realization α are as indicated in Eq. (13):

$$\text{streamwise velocity: } \tilde{u}_\alpha(x, y, t) = U_\alpha(t) + u_\alpha(x, y, t); \tag{15a}$$

$$\text{lateral velocity: } \tilde{v}_\alpha(x, y, t) = V_\alpha(t) + v_\alpha(x, y, t). \tag{15b}$$

The coordinate alignment imposes the constraint that the area-mean lateral velocity averaged over the episode vanishes:

$$\int_0^T V_\alpha(t)\, dt = 0. \tag{16}$$

The classical Taylor problem is posed in *ensemble-mean* coordinates, in which the mean wind direction is defined through the limit as $N \to \infty$ of the average over N realizations. In our problem we take the mean wind direction as the ensemble average of our time-averaged, area-mean wind vectors. If $\beta(\alpha)$ is the angle between these ensemble-mean coordinates and the realization-α coordinates, then from (15) the velocity field in realization α, expressed in these ensemble-mean coordinates, is

$$\text{streamwise: } \tilde{u}_{\text{em},\alpha}(x, y, t) = [U_\alpha(t) + u_\alpha(x, y, t)]\cos\beta(\alpha) - [V_\alpha(t) + v_\alpha(x, y, t)]\sin\beta(\alpha); \tag{17a}$$

lateral:

$$\tilde{v}_{\text{em},\alpha}(x, y, t) = [U_\alpha(t) + u_\alpha(x, y, t)]\sin\beta(\alpha) + [V_\alpha(t) + v_\alpha(x, y, t)]\cos\beta(\alpha). \tag{17b}$$

Equations (17a) and (17b) show that both the area-mean velocity $[U_\alpha(t), V_\alpha(t)]$ and the submesoscale velocity $[u_\alpha(x, y, t), v_\alpha(x, y, t)]$ contribute to the lateral velocity in ensemble-mean coordinates $\tilde{v}_{\text{em}}(x, y, t)$. Their dependence on the realization index α indicates that they also contribute to mesoscale Taylor dispersion. Without realization-to-realization variability in the area-mean velocity—that is, when $[U_\alpha(t), V_\alpha(t)] = [U_{\text{em},\alpha}(t), V_{\text{em},\alpha}(t)]$—the ensemble-mean and realization coordinates are the same, so that $\beta = 0°$. Thus the lateral velocity reduces to $V_{\text{em},\alpha}(t) + v_{\text{em},\alpha}(x, y, t)$ and only v_{em}, the lateral velocity fluctuation due to submesoscale turbulence, contributes to Taylor dispersion. Thus, the key to enhanced Taylor dispersion for the outer variability is realization-to-realization variability in the area-mean mesoscale velocity.

3. Time scale for a model ensemble

Although every realization of a parcel trajectory in the classical Taylor problem is governed by the same physics, each trajectory is different. We attribute this realization-to-realization variability, or randomness, to the sensitive dependence of turbulence on its initial conditions. This inherent property of turbulence causes us to treat it statistically. The key statistical property in classical Taylor dispersion is the time scale τ_L that emerges from the Lagrangian velocity autocorrelation function in (9) (Wyngaard 2010).

The randomness in a mesoscale model ensemble is artificial: the sensitivity to initial conditions is accommodated by varying initial conditions, boundary conditions, and the physics in the model realizations. So the following question arises: what is τ_L for the Taylor dispersion in such a model ensemble?

We can gain some insight by considering the nature of the realization-to-realization differences in the model ensemble. Say the ensemble members are initialized with slightly different mean wind directions. If those differences persist in time, then the Lagrangian autocorrelation function for the mean wind field will remain significantly different from zero, making τ_L very large. If they evolve in time, however, which is more likely the case, then the time scale of the evolution will determine τ_L.

We can estimate a time scale of that evolution in a few ways. Since in principle the models can mimic the atmosphere well only on scales larger than the grid resolution,

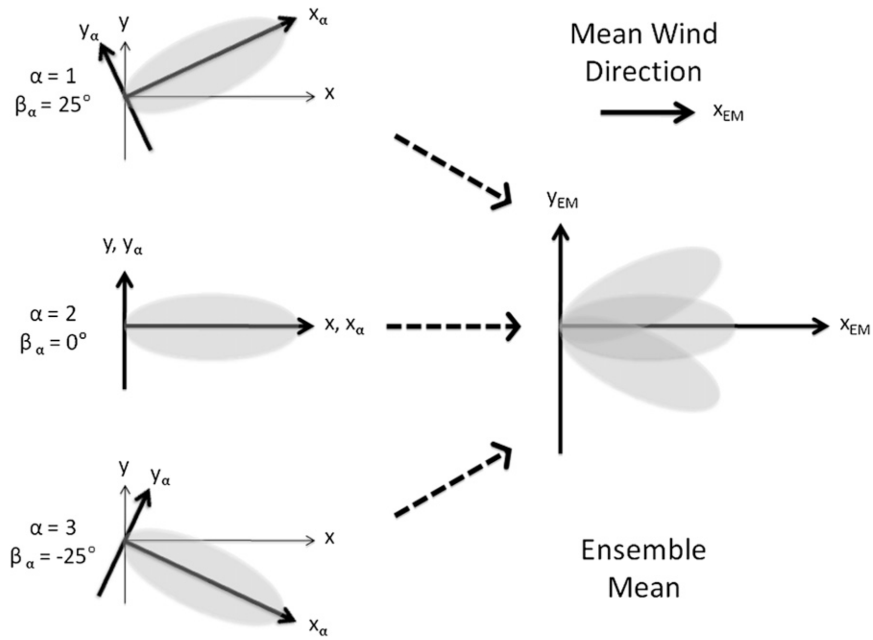

FIG. 2. Notional diagram of plume addition in rotated coordinates.

which is typically on the order of 10 km in operational applications, the Eulerian time scale of the modeled motions on that scale provides one rough lower bound on τ_L. For 1 m s^{-1} motions of 10-km scale that is 10^4 s. Since the Lagrangian integral time scale is typically somewhat larger than this Eulerian time scale, that suggests τ_L here is not less than 10^4–10^5 s.

Another time scale is that of the dynamics that turns the mean wind direction with time. The terms in the evolution equation for mean wind direction are of the order of $1/S$ (where S is the mean wind speed) times those in the equations for the mean wind components. The leading terms in the mean wind equations are of order of the stress divergence term. Thus if we scale terms in the equation for mean wind direction β with a time scale of the realization T_β,

$$\frac{\partial \beta}{\partial t} \sim \frac{\beta}{T_\beta}. \qquad (18)$$

We then conclude that $T_\beta \sim T_U$, the corresponding time scale for the mean streamwise momentum equation:

$$T_U \sim \frac{\text{mean streamwise wind speed}}{\text{stress divergence term}} \sim \frac{\rho U h}{\tau_0}. \qquad (19)$$

Here U is the mean streamwise wind speed, h is the depth of the mixed layer, and τ_0 is the surface stress. For typical values $U \sim 10$ m s^{-1}, $h \sim 10^3$ m, and τ_0/ρ in the range 0.1–1 m^2 s^{-2} this gives $T_\beta \sim 10^4-10^5$ s, in agreement with the estimate above. Similar values are reported by Gifford (1982, 1987), Hanna (1986), and Sørensen (1998). This analysis suggests that initial differences in mean wind direction among the ensemble members could persist for a few hours to a day, giving effective Lagrangian integral time scales of that order. Therefore the linear growth regime of Taylor diffusion could extend to times of that same order. Some atmospheric transport and dispersion models such as SCIPUFF use a length scale rather than the Lagrangian integral time scale to model the outer variability (Sykes et al. 2004). A straightforward method to convert the Lagrangian integral time scale to a length scale Λ would require the variance of the ensemble wind field, which if split into streamwise and cross-stream components translates to a length scale of

$$\Lambda \propto \tau_L \frac{1}{2}\sqrt{\overline{[U_\alpha(t) - \overline{U}]^2[V_\alpha(t) - \overline{V}]^2}}. \qquad (20)$$

This scale is equivalent to the "SLE" studied by Lee et al. (2009).

4. Application to a Gaussian plume model

a. The model

We now demonstrate the effect of the added dispersion from outer mean wind variability. We assume that an ensemble of plume directions can be modeled as drawn from a Gaussian distribution. We also assume

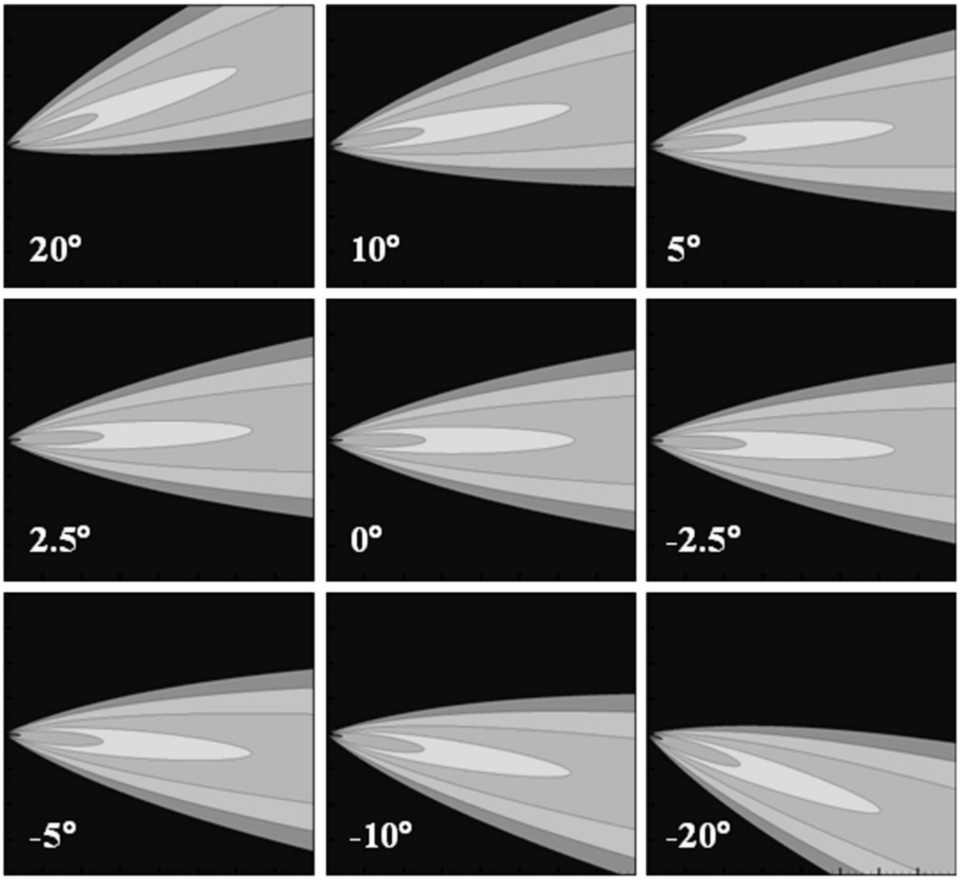

FIG. 3. Example ensemble plume members for β from $-20°$ to $20°$.

isotropy on the mesoscale. Finally we calculate that enhanced mesoscale plume by modeling the Lagrangian autocorrelation function with an exponential separation in time.

We first consider various possible realizations of a plume that differ by wind direction only. A Gaussian plume model represents each of the depth-averaged horizontal plumes represented in Fig. 3. The depth-averaged plume concentration in realization α is given by

$$C_\alpha = \frac{Q}{U\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{y_\alpha}{\sigma}\right)^2\right], \tag{21}$$

where y_α denotes the lateral distance in realization coordinates. We assume that σ remains constant across all realizations.

We assume a steady mean wind field that differs between ensemble members only in its direction. Under this condition, the upper limit of the time scale τ_L^U approaches infinity, which implies that if we were to average these plumes, the ensemble-mean plume would always be in the linear regime for mean wind angle effects; that is, the mean wind field never ''forgets'' its original direction. We consider a model for the Lagrangian velocity autocorrelation $\overline{v_p(t)v_p(t')}$ that has an exponential dependence on the separation time $t - t'$, so that

$$\overline{v_p(t)v_p(t')} = \overline{v_p(t)^2}\, \exp\left(-\frac{|t-t'|}{\tau_L}\right). \tag{22}$$

For the mesoscale Taylor problem, we square (17b) and ensemble average to obtain

$$\begin{aligned}\overline{\tilde{v}_{\rm em}^2} &= \overline{U^2\sin^2\beta(\alpha)} + \overline{2Uu\sin^2\beta(\alpha)} + \overline{u^2\sin^2\beta(\alpha)}\\ &\quad + \overline{2\sin\beta(\alpha)\cos\beta(\alpha)(VU + Uv + Vu + uv)}\\ &\quad + \overline{V^2\cos^2\beta(\alpha)} + \overline{2Vv\cos^2\beta(\alpha)} + \overline{v^2\cos^2\beta(\alpha)}.\end{aligned} \tag{23}$$

Applying the averaging rules results in means of all cross terms with deviations becoming zero. From (16) the V^2 terms are also zero. By isotropy, we have both $\overline{uv} = 0$ and $\overline{u^2} = \overline{v^2}$ leaving

$$\overline{\tilde{v}_{\rm em}^2} = \overline{U^2\sin^2\beta(\alpha)} + \overline{v^2}. \tag{24}$$

Substituting (24) and (22) into (8) gives

$$\frac{d\sigma^2_{\rm meso}}{dt} = 2U^2\,\overline{\sin^2\beta}t + 2\overline{v_p(t)^2}\int_0^t \exp\left(-\frac{\tilde{t}}{\tau_L}\right)d\tilde{t}. \quad (25)$$

After integrating the second term on the right we have

$$\frac{d\sigma^2_{\rm meso}}{dt} = 2U^2\,\overline{\sin^2\beta}t + 2\overline{v_p(t)^2}\,\tau_L\left[1-\exp\left(-\frac{t}{\tau_L}\right)\right]. \quad (26)$$

Integrating the entire expression over time gives

$$\sigma^2_{\rm meso}(t) = U^2(\alpha)\,\overline{\sin^2\beta_\alpha}t^2 - 2\overline{v_p(t)^2}\left\{\tau_L^2\left[1-\exp\left(-\frac{t}{\tau_L}\right)\right]-\tau_L t\right\}. \quad (27)$$

As expected, $\sigma_{\rm meso}$ grows linearly for short times t. At long times the second term grows as the square root of t. Note, however, that the mean mesoscale variability denoted by the first term continues to grow linearly at all times because of the persistent wind direction differences.

Now we wish to consider the shape of this broadened plume defined by averaging over the realizations. Defining the reference length $\ell \equiv U\tau_L$, the dimensionless plume can be written

$$C(\hat{x},\hat{y}) \equiv C(x,y)\frac{U^2\tau_L}{Q} = \frac{1}{\hat{\sigma}_{\rm meso}\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(\frac{\hat{y}}{\hat{\sigma}_{\rm meso}}\right)^2\right], \quad (28)$$

where $\hat{x} \equiv x/U\tau_L$ and $\hat{y} \equiv y/U\tau_L$. Thus the virtual plume remains Gaussian in the mapped mesoscale coordinates with

$$\hat{\sigma}^2_{\rm meso}(t) \equiv \left[\frac{\sigma_{\rm meso}(t)}{U\tau_L}\right]^2 = \overline{\sin^2\beta}\left(\frac{t}{\tau_L}\right)^2 + 2I^2\left\{\left[\exp\left(-\frac{t}{\tau_L}\right)+1\right]-\frac{t}{\tau_L}\right\}, \quad (29)$$

where the squared turbulence intensity is

$$I^2 = \overline{v_p(t)^2}\Big/U^2. \quad (30)$$

b. The ensemble members

We construct a set of plume ensemble members by varying the angle from the ensemble mean β. Example members for β between $\pm 20°$ and $I = 0.15$ are shown in Fig. 3. We wish to compute ensemble average plumes. We assume that the angle distribution of the ensemble-mean wind field is drawn from a Gaussian distribution in β with standard deviation σ_β:

$$\psi(\beta) = \frac{1}{\sigma_\beta 2\sqrt{\pi}}\exp\left[-\frac{1}{2}\left(\frac{\beta}{\sigma_\beta}\right)^2\right]. \quad (31)$$

Ensemble averaging then is accomplished in two ways and compared in Fig. 4 for $\sigma_\beta = 10°$ and $\sigma_\beta = 20°$. The average concentrations in the top row (Figs. 4a and 4b) are computed by explicitly averaging ensemble members drawn from the Gaussian distribution (31), such as those represented in Fig. 3. These explicitly averaged ensemble-mean plumes (Figs. 4a and 4b) are broader than any of the individual ensemble members, as expected. The ensemble-averaged plumes in the bottom row (Figs. 4c and 4d) are computed using the Taylor theory-derived σ from (29). These modeled mean plumes using the Taylor dispersion-based width parameter are a very good representation of the explicit mean plume; that is, Fig. 4c matches Fig. 4a quite well and the same is true when comparing Fig. 4d with Fig. 4b.

c. Limiting cases

Finally we quantitatively compare how well the Taylor-modeled plume agrees with an explicit average over the ensemble of realizations. The thin solid line in Fig. 5 plots the correlation between the explicitly averaged ensemble-mean plumes with those computed using our Taylor theory as a function of σ_β. Although the correlation is quite high for small values of σ_β, it decreases as σ_β becomes larger, dropping below 0.9 when $\sigma_\beta = 90°$, which represents a highly variable wind direction. Can we derive a scaling coefficient C_f to optimally scale the Taylor dispersion coefficient given in (27) to best match the ensemble mean computed by explicitly averaging over all ensemble members as depicted in Figs. 4a and 4b? For each wind field standard deviation σ_β such a match was empirically computed and the coefficient C_f that produces the best match was tabulated for each σ_β. That scaling coefficient that optimizes the match is plotted as the dashed line in Fig. 5: it increases with σ_β. The thick solid line shows the modified correlation when the Taylor dispersion coefficient is scaled by C_f. Note, however, that the scaled dispersion coefficients are always within 10% of the Taylor coefficients, indicating that only small corrections are necessary.

5. Conclusions

We have examined wind direction variability as a source of uncertainty in atmospheric transport and

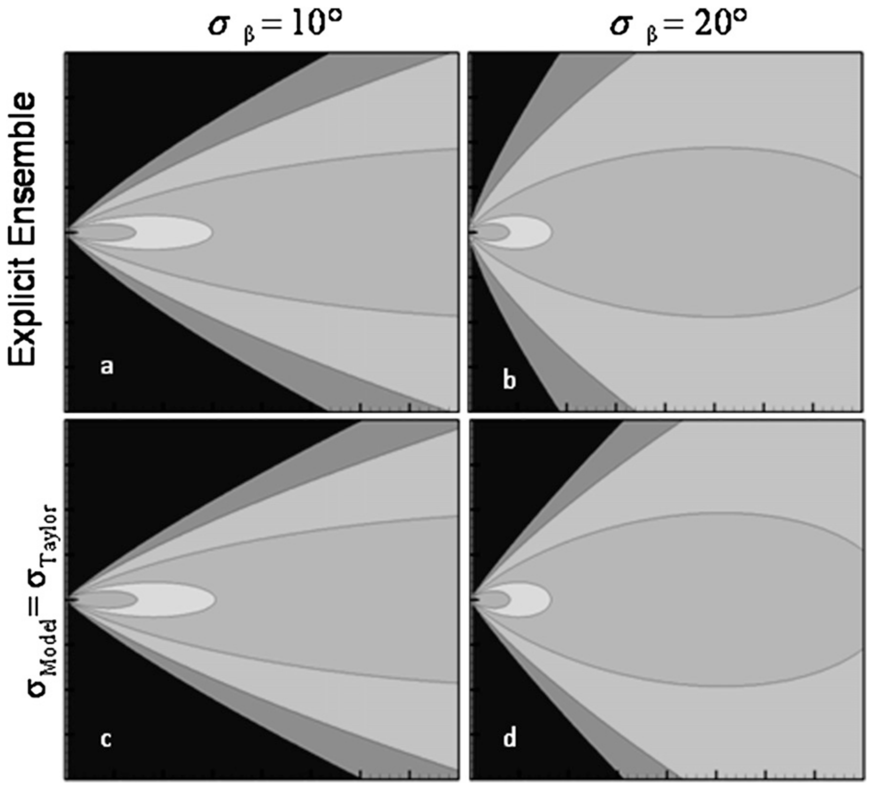

FIG. 4. Ensemble-mean plume (a),(b) computed explicitly from the ensemble set and (c),(d) modeled using the Taylor dispersion-based plume width parameter. This is shown for σ_β (a),(c) = 10° and (b),(d) 20°.

dispersion modeling. We distinguish between the ''inner variability'' that represents the subgrid-scale turbulence causing the dispersion and the ''outer variability'' that represents realization-to-realization resolved-scale differences in the meteorology forcing the transport and dispersion. Outer variability in the form of large-scale inhomogeneity impressed on the turbulent atmospheric boundary layer causes uncertainty in the mean wind direction. By casting different realizations of this outer flow as different ensemble members and by applying Taylor dispersion concepts, we derived statistics for modeling ensemble dispersion in a single run. In effect this allows ensemble techniques to be used in emergency response situations. By comparing the modeled ensemble-mean plume for a persistent wind direction difference to an explicit calculation of the ensemble-mean plume we showed that that our Taylor-based approach can represent the explicit averaging of an ensemble of dispersion plumes. We also showed that an angle-dependent scaling coefficient can improve that match.

The enhancement of dispersion due to the metulence-induced outer variability is important to quantifying uncertainty in regional-scale atmospheric transport and dispersion. The analysis here suggests that uncertainty can be quantified directly from existing NWP ensemble model runs. Thus, a single atmospheric transport and dispersion model run based on a mean or median NWP member plus the ensemble variance statistics can be

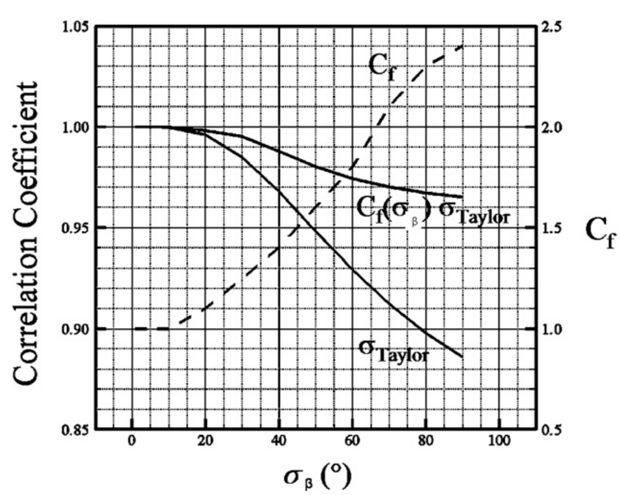

FIG. 5. Spatial correlation between the explicit ensemble-mean plume and the modeled ensemble-mean plume.

used to produce dispersion uncertainty estimates using the framework of Lewellen and Sykes (1989) plus the definition of scales derived herein. This approach could provide uncertainty estimates for emergency response by a computational savings of a factor of $1/N$ where N is the number of ensemble members. For example, if an agency was running a dispersion model based on an NWP ensemble with 15 members, they would only need to produce a single meteorological forcing file based on the mean,[1] augmented with variance and length-scale statistics as calculated. Then a single atmospheric transport and dispersion model run (rather than 15 separate runs) could produce a best estimate of the plume plus an estimate of uncertainty.

This demonstration has considered a basic Gaussian plume with persistent wind direction differences among realizations. In the real atmosphere, one would expect temporal evolution of the wind field rather than persistent differences. A more realistic case study (Lee et al. 2009) confirms the results reported herein with an NWP ensemble and a computed Lagrangian integral time scale of about two hours, which is within the limits estimated here. Other case studies (not shown) have indicated similar time scales. All of our analyses of NWP simulations to date have been constructed with ensembles of opportunity that are not ideally representative of actual mesoscale uncertainty, however. In fact, we believe that these ensembles are underdispersive and thus underrepresent the uncertainty. Although one can derive calibration coefficients (Kolczynski et al. 2009), those also depend on the specific ensemble considered. Our most recent work (Kolczynski et al. 2010) also addresses the issue of ensembles that are too small and shows that correction coefficients can also be derived to calibrate such ensembles.

We expect that an appropriately dispersive ensemble would exhibit a longer Lagrangian integral time scale than we have computed. To assess this issue more accurately would require both case studies of such an appropriately dispersive ensemble and ideally, a long-term statistical analysis of many simulations. We expect to progress in this direction in future work.

Acknowledgments. The authors thank Ian Sykes, Doug Henn, Steve Hanna, and Walter Kolczynski for helpful suggestions during the course of the research. This work was supported by the Defense Threat Reduction Agency under Contracts DTRA01-03-D-0010-004 and DTRA01-03-D-0010-0012 with project managers Stephanie Hamilton and John Hannan, assisted by Patrick Hayes and Christopher Kiley. We also thank three anonymous reviewers whose thoughtful comments helped us to improve the manuscript.

[1] It may be more appropriate to define a ''best member'' and compute the variance statistics around that member.

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