Surface Delays for Gases Dispersing in the Atmosphere

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ABSTRACT

When a particle descends beneath the (nominal) lower boundary of the atmosphere, it may remain there for some time τ before it reemerges into the (resolved) flow. In particle trajectory models, τ is the random duration of unresolved trajectory segments, below the height z_r at which an artificial reflection boundary condition is applied. By computing such paths, for realistic near-ground flows, it was found that the mean delay per reflection is $\overline{\tau} \approx 2.5z_r/\sigma_w$ where σ_w is the standard deviation of the vertical velocity at z_r. The corresponding mean alongwind displacement per reflection, due to the mean horizontal wind $\overline{u}(z)$ below z_r, is $\overline{\delta} \approx \langle \overline{u} \mid z_r \rangle\, \overline{\tau}$, where $\langle \overline{u} \mid z_r \rangle$ is the height average of $\overline{u}$ in the waiting layer. The fluctuating component of the horizontal wind causes no mean drift but upon each reflection contributes a random drift whose root-mean-square value is $\sigma_\delta \approx 2z_r$. From simulations on the continental scale, with a lower boundary placed at $z_r \approx 25$ m, it was found that a typical particle suffered about 15 reflections per day, resulting in a net delay on the order of 30 min per day.

1. Introduction

In atmospheric dispersion models, a lower boundary separates the atmosphere into a resolved upper region and a near-ground region that is ignored, because it is considered to be irrelevant. This paper examines the unresolved delays and displacements that occur while particles are "waiting" in that neglected near-surface layer before reinjection to the flow above—for example, the surface delay τ is the interval between passage of a fluid element (particle) beneath height z_r (with vertical velocity $W < 0$) and its first subsequent passage above z_r, where z_r is the location of the lower boundary. This is a random variable, and its probability distribution $g(\tau)$ embodies physical properties of the "ground" and the near-ground flow, as well as the placing of z_r.

The distribution of particle travel times in turbulent flow has received little attention. Furthermore, where it has been studied (e.g., Wilson and Swaters 1991; Wenzel et al. 1999), only the variability (in travel time) due to the turbulent "interior" of the flow has been considered, not these boundary effects. Surface delays most probably have been left unstudied because in steady-state problems (continuous source in a stationary atmosphere) the mean concentration field is independent of the distribution of travel times; typically theories of dispersion have been tested against such observations, rather than against experiments with transient sources, which demand an ensemble averaging that is never (in the atmosphere) completely satisfactory.

Corresponding to the surface delay τ is a random (vector) displacement $\boldsymbol{\delta}$ in the horizontal which is caused by the action of the horizontal wind during the particle's sojourn below z_r. The customary neglect of delays τ in existing dispersion models *may* partly be compensated by their neglect (also) of the displacements $\boldsymbol{\delta}$, but this depends in detail on (what one assumes to be) the nature of the flow in the unresolved layer. Below we show how to parameterize both τ and $\boldsymbol{\delta}$ so as to eliminate the implicit discontinuities of particle trajectories near the boundary that otherwise exist.

2. Theory for mean surface delay

Consider a passive tracer in an atmosphere bounded by a nonabsorbing surface at $z = 0$ but which is resolved only at $z \geq z_r$. The "waiting layer" spans $0 \leq z \leq z_r$, and we should like to know the mean time $\overline{\tau}$ that a particle remains below z_r, once having been injected there.

We consider a particle released at $t = 0$, $z = z_r$, with (negative) velocity w_0. Following the method of Cox

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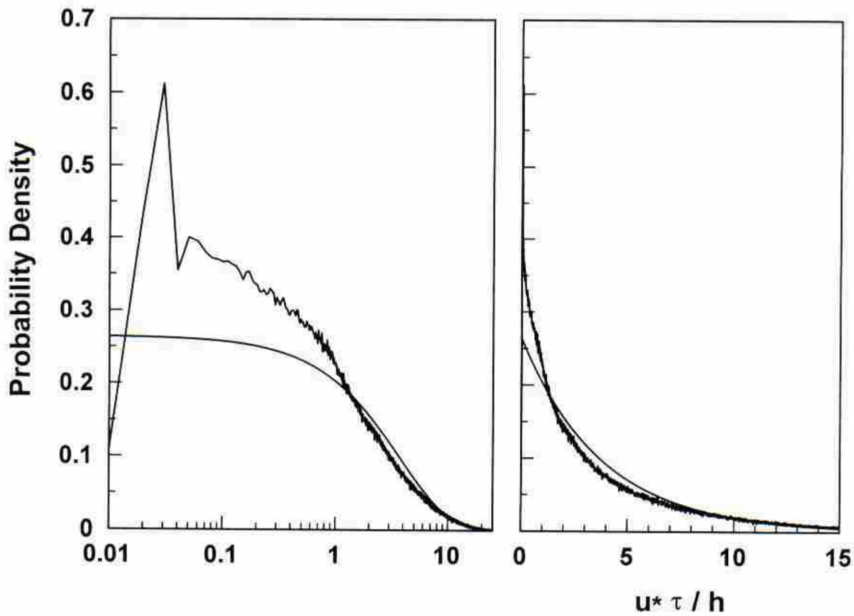

FIG. 1. Empirical probability density function (noisy line) of the normalized delay $u_* \tau/h$ below $z = 2h$, where h is the height of a uniform plant canopy. Constructed from $N = 6 \times 10^6$ consecutive excursions of a single particle below $z = 2h$, as calculated by the Lagrangian stochastic model. The delays were binned with resolution $\Delta(u_* \tau/h) = 0.01$, and the irregularity for small $(u_* \tau/h)$ is due to an inadequate number N of events. The smooth line is an exponential pdf with mean delay equaling that of the calculated pdf.

and Miller (1965, p. 230), let $P(\tau^{w_0} < t)$ be the probability that the time lapsed until first subsequent passage above z_r is less than t. Then $(1 - P)$ is the probability that at time t the particle is *still* resident in the layer $0 \leq z \leq z_r$. It follows that the probability density function (pdf) for the conditional delay $\tau^{(w_0)}$ is

$$g(\tau | w_0) = \frac{\partial P}{\partial t} = \frac{\partial}{\partial t}\left[1 - \int_{z=0}^{z_r} p_a(z, t | z_r, w_0, 0)\, dz\right]. \quad (1)$$

The integrand p_a is the pdf for position, under the condition that the level $z = 0$ is a perfect reflector and the level $z = z_r$ is a perfect sink, that is, p_a vanishes on $z = z_r$ for all $t > 0$. We substitute for $\partial p_a/\partial t$ using the mass conservation law

$$\frac{\partial p_a}{\partial t} = -\frac{\partial F_a}{\partial z}, \quad (2)$$

where the vertical flux F_a may be expressed in terms of the *joint* pdf for position and velocity:

$$F_a(z, t | z_r, w_0, 0) = \int_{w=-\infty}^{\infty} w\, p_a(z, w, t | z_r, w_0, 0)\, dw. \quad (3)$$

Thus, because the flux vanishes at $z = 0$ (because of perfect reflection), we have

$$g(\tau | w_0) = \int_{w=-\infty}^{\infty} w\, p_a(z_r, w, t | z_r, w_0, 0)\, dw, \quad (4)$$

that is, the (conditional) pdf of first passage time is given by the mean flux out of the waiting layer. The conditional mean delay is

$$\overline{\tau}^{(w_0)} = \int_{\tau=0}^{\infty} \tau\, g_a(\tau | w_0)\, d\tau \quad (5)$$

and the unconditional mean delay is

$$\overline{\tau} = \int_{w_0=-\infty}^{0-} \overline{\tau}^{(w_0)} f(w_0)\, dw_0, \quad (6)$$

where $f(w_0)$ is the pdf for w_0.

A specific result for $\overline{\tau}$ demands specification of the turbulence and the pdf (p_a). The simplest case is homogeneous turbulence, for which a suitable Langevin equation for increments dW in particle velocity (over time step dt) is

$$dW = -W\frac{dt}{T_L} + b\, d\xi, \quad (7)$$

where $b = (2\sigma_w^2/T_L)^{1/2}$, σ_w is the Eulerian velocity standard deviation, T_L is the Lagrangian timescale, and $d\xi$ is a standard Gaussian random number with variance dt. The corresponding Fokker–Planck equation satisfied by the joint pdf $p_a(z, w, t \mid z_r, w_0, 0)$ is

$$\frac{\partial p_a}{\partial t} = -\frac{\partial}{\partial z}(wp_a) - \frac{\partial}{\partial w}\left(-\frac{w}{T_L}p_a\right) + \frac{b^2}{2}\frac{\partial^2 p_a}{\partial w^2}, \quad (8)$$

which must be solved subject to $p_a(z, w, 0 \mid z_r, w_0, 0) = \delta(z - z_r)\delta(w - w_0)$, with boundary conditions

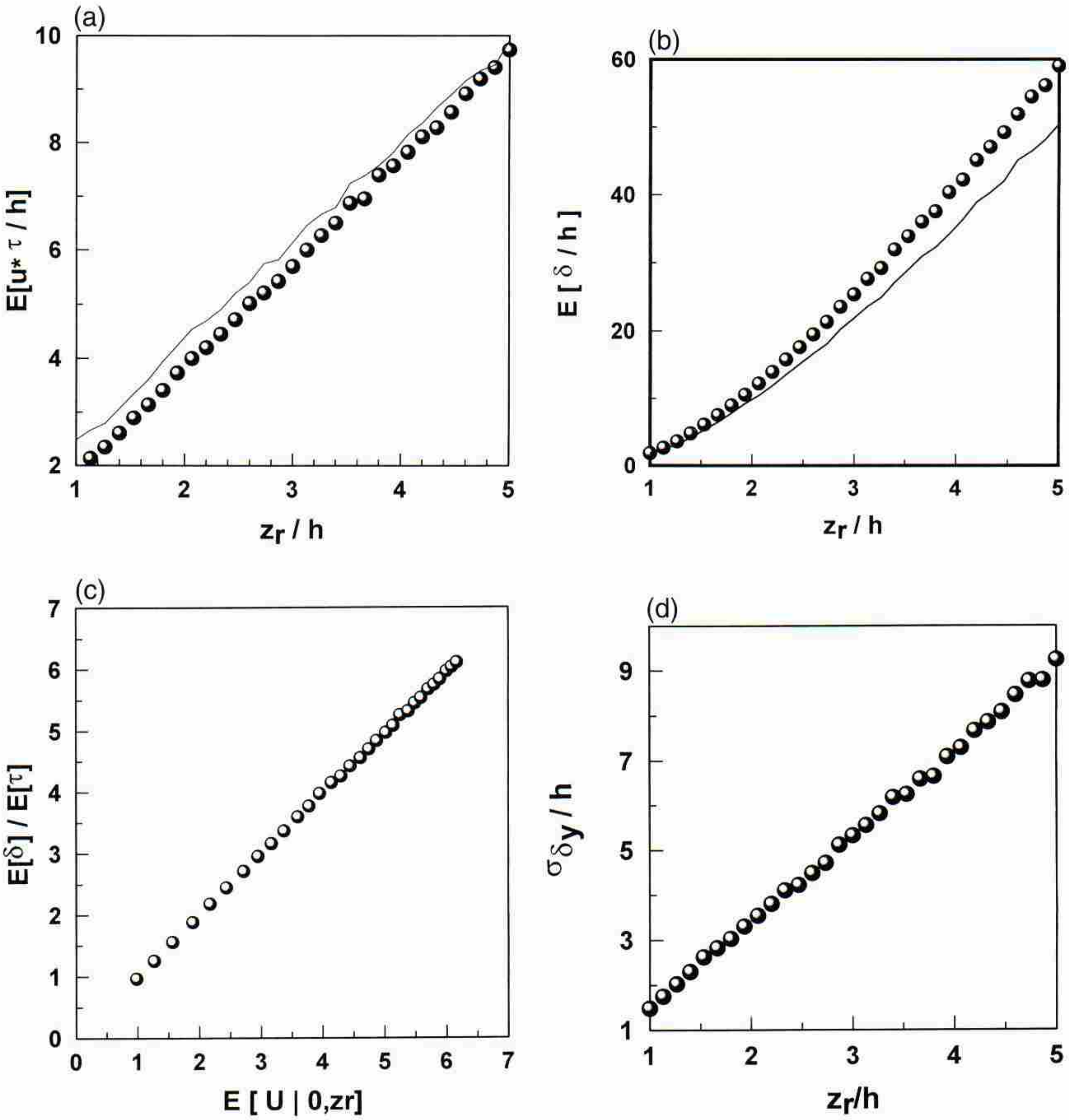

FIG. 2. (a) Mean value (symbols) and std dev (line) of the normalized delay $u_*\tau/h$ below z_r vs reflection height z_r/h (particle released at $z/h = 10$, reflecting upper boundary at $z/h = 40$). (b) Mean value (symbols) and std dev (line) of the normalized waiting *distance* $\overline{\delta}/h$ traveled below z_r during a "reflection event" vs reflection height z_r/h. (c) Plot showing that the ratio $\overline{\delta}/\overline{\tau}$ of the mean drift to the mean delay is equal to the mean horizontal velocity $\langle \overline{u} \mid z_r \rangle$ in the waiting layer. (d) Std dev of the normalized lateral displacement, *per reflection*, from the fluctuating crosswind velocity v' in the waiting layer. All of the above is for trajectories over a uniform plant canopy of height h.

of absorption on $z = z_r$ (at $t > 0$) and reflection on $z = 0$.

We now examine surface delays and displacements numerically, by calculating trajectories in realistic near-ground turbulence in and above a plant/forest canopy and over smooth ground.

3. Calculations of surface delay and drift

Lagrangian stochastic (LS) models mimic atmospheric dispersion by calculating an ensemble of individual, independent particle trajectories. The form of a first-order multidimensional LS model is (Thomson 1987):

$$dU_i = a_i(U_i, X_i, t)\,dt + b_{ij}d\xi_j \qquad dX_i = U_i dt \quad (9)$$

(no summation over i), where dt is the time step along the trajectory (limited to be small relative to all pertinent flow timescales), a_i is the conditional mean acceleration, and $d\xi_j$ is a Gaussian random variable (mean zero, variance dt). Kolmogorov similarity determines that the model coefficients $b_{ij} = (C_0\varepsilon)^{1/2}\delta_{ij}$, where ε is the turbulent kinetic energy dissipation rate and C_0 is a universal constant. Thomson's well-mixed condition constrains the a_i by requiring that an LS model for fluid element trajectories should have the property that if it is hypothetically applied to the motion of a set of marked fluid elements that are initially well-mixed in the flow, with respect both to position and velocity, then those marked fluid elements must *remain* well mixed in position–velocity space.

Lagrangian stochastic models of the atmosphere usually resort to reflection of trajectories at boundaries—boundaries that are always in some sense artificial. Although criteria for reflection algorithms have been given (Wilson and Flesch 1993; Thomson and Montgomery 1994; Anfossi et al. 1997), it has not been considered important that the intervention of reflection implies a discontinuity along the trajectory.

a. Well-mixed trajectory model for particles in Gaussian inhomogeneous turbulence

In simulations to follow, particle velocity is $[\overline{u}(Z) + U, V, W]$, where $\overline{u}$ is the local mean Eulerian velocity in the alongwind (x) direction (nonzero shear stress implies that U and W are correlated). Trajectories are generated using Thomson's (1987) well-mixed three-dimensional model for Gaussian inhomogeneous turbulence,[1] that is, turbulence whose Eulerian velocity pdfs are joint Gaussians, with parameters varying only along the vertical. Although velocity statistics in a plant canopy are non-Gaussian, neglect of third and higher statistical moments is not the most important approximation of an LS model for trajectories in a canopy (Flesch and Wilson 1992).

The trajectories are calculated according to

$$dX = [\overline{u}(Z) + U]dt, \qquad dY = Vdt, \qquad dZ = Wdt, \quad (10)$$

where increments in particle velocity are given by the generalized Langevin equations. Expressions for the components of the conditional mean acceleration a_i are cumbersome and are given in appendix A. If one wished only to calculate surface delays (but not the corresponding displacements), one could drop the horizontal fluctuations, U and V, in which case the conditional mean vertical acceleration reduces to (Thomson 1987)

$$a_w = -\frac{C_0\varepsilon(Z)}{2\sigma_w^2(Z)}W + \frac{1}{2}\frac{\partial\sigma_w^2}{\partial z}\left(\frac{W^2}{\sigma_w^2} + 1\right), \quad (11)$$

where σ_w^2 is the variance of the Eulerian vertical velocity.

In the "diffusion limit," Thomson's model implies an eddy diffusivity,

$$K = \frac{2(\sigma_w^4 + u_*^4)}{C_0\varepsilon}, \quad (12)$$

where u_* is the friction velocity, for vertical diffusion in the neutral surface layer (Sawford and Guest 1988). This diffusivity may be related to an *effective* Lagrangian decorrelation timescale T_L, by defining $K = \sigma_w^2 T_L$. Thus, for a neutral surface layer, one may relate the model coefficient $b = (C_0\varepsilon)^{1/2}$ to a Lagrangian timescale

$$b = \sqrt{\frac{2\sigma_w^2}{T_L}\left[1 + \left(\frac{u_*}{\sigma_w}\right)^4\right]}. \quad (13)$$

We carried over this identification for a canopy layer. The formulas we used for T_L (given later) imply that for 1D simulations [for which the term in u_* vanishes from Eqs. (12), (13)] $C_0 \approx 3.2$; for the present (3D) calculations, $C_0 \approx 4.5$.

Unless otherwise stated, we set the time step dt/T_L equal to 0.05. Trajectories were reflected at the base of the domain, that is, at $z = z_0$ (roughness length), or, in the case of a resolved canopy, at $z = 0$; they were also reflected (downward) off an upper boundary (whose placing had no influence on statistics of τ). Statistics of the delays and displacement were calculated from N (=16 000) consecutive reflections of a *single* trajectory.

b. Surface delays over a uniform plant canopy

Applied models of dispersion usually neglect to represent properly the flow within a canopy—and may even neglect (omit, or improperly represent) the entire surface layer—by applying a zero-flux boundary condition (or trajectory reflection) some arbitrary distance above ground. To study the consequence of that neglect, for trajectory segments below this artificial computational boundary[2] at z_r, we here *resolve* such trajectory segments in neutrally stratified, horizontally uniform flow through and above a generic plant canopy of height h; that is, we track the particles as they cross below the (arbitrarily chosen) reflection height, possibly (though not necessarily) into the canopy, and finally back into the "outer" flow (recrossing z_r with a positive vertical velocity W). Appendix B gives the vertical profiles of

[1] This model is not unique, that is, it belongs to a *class* of well-mixed LS models for Gaussian inhomogeneous turbulence. However, several studies have shown that it agrees well with observations, and Sawford (1999) confirms it is the best choice, pending development of further criteria.

[2] We do not account for any additional contribution to τ due to residence in the inevitable "unresolved basal layer" (Wilson and Flesch 1993) at the foot of the canopy—in practice, a subcanopy layer, or leaf-litter layer, itself bounded by the soil. The results of this paper, however, suggest any "compounding" of the delay (as the ground is resolved on ever finer scales) should be negligible.

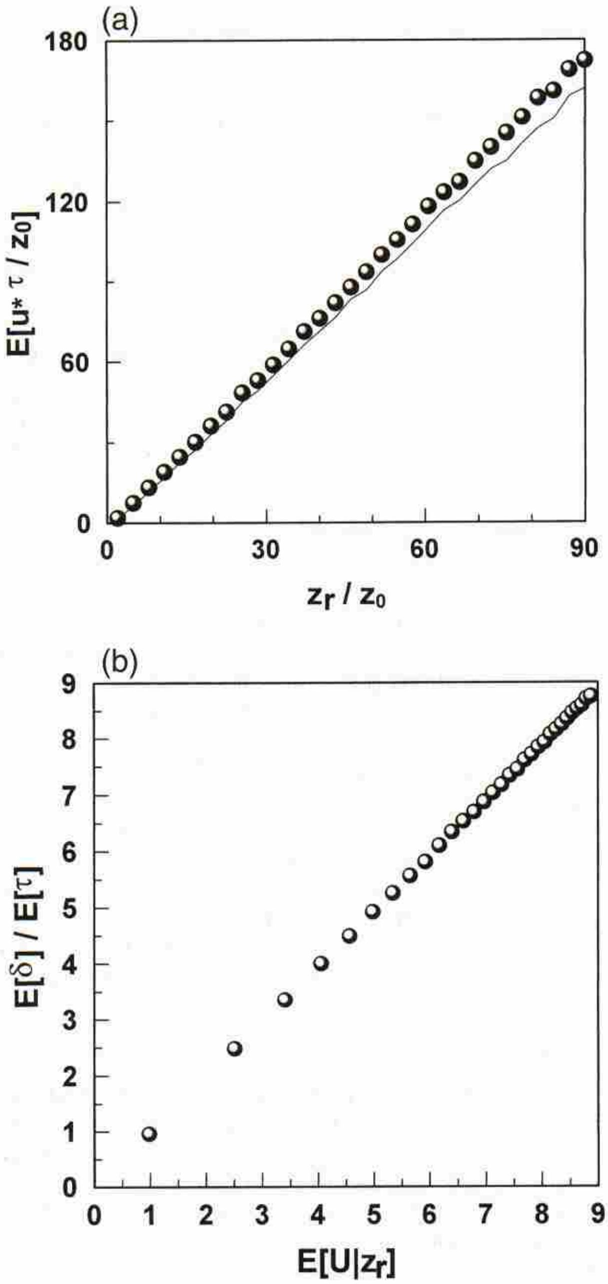

FIG. 3. Mean value (symbols) and std dev (line) of the normalized delay $u_* \tau / z_0$ below z_r vs reflection height z_r/z_0 for trajectory within a neutral surface layer (particle released at $z/z_0 = 500$, reflecting upper boundary at $z/z_0 = 10^3$). (b) Plot showing that the ratio $\overline{\delta}/\overline{\tau}$ of the mean drift to the mean delay is equal to the mean horizontal velocity $\langle \overline{u} \mid z_r \rangle$ in the waiting layer.

Eulerian velocity statistics that we assumed for canopy flow.

Figure 1 gives the calculated probability density function $g(\tau)$ for the case of reflection at $z_r/h = 2$. It is asymmetric because τ is necessarily positive, and many particles will reverse their direction and reemerge into the outer flow without a long passage below z_r. Perhaps

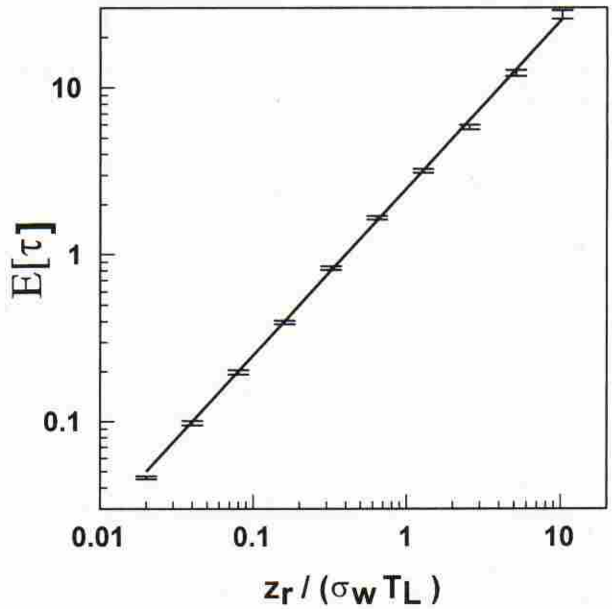

FIG. 4. Mean delay in the layer $0 \leq z \leq z_r$ of trajectories in homogeneous turbulence ($\sigma_w = T_L = 1$). Symbols give $\overline{\tau}$ (and std err in its estimation from 1000 reflections) from simulations; solid line is the formula $\overline{\tau} = 2z_r/\overline{|w|}$.

only few penetrate to ground ($z = 0$), where they experience reflection. The empirical pdf is plotted in comparison with the exponential $g(\tau) = (1/\overline{\tau}) \exp(-\tau/\overline{\tau})$, which, except for very small τ, is a reasonable approximation. However the exponential has maximum probability density at the origin ($\tau = 0$), whereas the clock starts for a surface delay when the particle crosses z_r in the downward direction (i.e., with $W < 0$), and finite Lagrangian autocorrelation (memory) implies that the pdf must satisfy $\mathrm{Lim}_{\tau \to 0} g(\tau) = 0$. A log-normal pdf has this property but is nevertheless a poorer overall representation than the exponential.

Figure 2a is a plot of our calculated mean value (and standard deviation) of the delay (per reflection) versus the choice of reflection height z_r. Evidently $\overline{\tau} \approx 2z_r/u_*$, so that it is as if the particle simply traversed the waiting layer twice at mean velocity u_* (the friction velocity based on the shear stress at $z = h$). Because in the atmospheric surface layer (above vegetation) $\sigma_w \approx 1.25u_*$, we may write $\overline{\tau} \approx 2.5z_r/\sigma_w(z_r)$.

The corresponding result for the average downwind displacement $\overline{\delta}$ during passages below z_r is given by Fig. 2b; Fig. 2c shows that $\overline{\delta} = \overline{\tau}\langle \overline{u} \mid z_r \rangle$, where

$$\langle \overline{u} | z_r \rangle = \frac{1}{z_r - z_b} \int_{z_b}^{z_r} \overline{u}(z)\, dz \qquad (14)$$

(in the present case $z_b = 0$).

The component δ_y of the waiting-layer drift per reflection that is due to the fluctuation velocity v' scatters randomly about its expected value ($\overline{\delta}_y = 0$). Figure 2d indicates that root-mean-square drift (per reflection; $\sigma_{\delta y}$) varies linearly with z_r, a line of best fit being $\sigma_{\delta y} =$

$1.9z_r - 0.4$. Of course, by the central limit theorem, as we add together many (say, M) independent displacements, each with expected value zero and rms value $\sigma_{\delta y}$, the expected value of the *net* displacement (due to the action of the fluctuation v' alone) scatters about zero with a much smaller standard deviation $\sigma_{\delta y}/M^{1/2}$. For long trajectories, the influence of the velocity fluctuations u', v' during the delays is negligible.

The mean delays and displacements proved to be insensitive to whether they were derived from N consecutive reflections of a single trajectory or from N independent trajectories from the source, each terminated after one reflection; they varied negligibly with simulation time step dt/T_L over the range $0.01 \leq dt/T_L \leq 0.1$. We can use the results to assess the practical significance of neglecting the delays. Suppose trajectories are calculated with reflection at $z_r = 2h$ ($\approx 20z_0$); taking $h = 25$ m, $u_* = 0.25$ m s^{-1}, we have that the mean delay is 400 s, that is, almost 7 min, and the mean displacement is about 250 m. For an agricultural canopy, mean delay would be much smaller, say about 30 s.

c. Surface delays in the neutral surface layer

To quantify the delays neglected in flow over smoother surfaces (small z_0) we again used the well-mixed LS model (appendix A) to calculate trajectories below z_r, in a manner identical to the previous section except that the mean wind profile was simplified to $\overline{u}(z)/u_* = 1/k_v \ln(z/z_0)$ and the Lagrangian timescale to $T_L(z) = 0.5z/\sigma_w$, where $\sigma_w = 1.25u_*$, and $k_v = 0.4$ is the von Kármán constant. Figure 3a gives the calculated mean delay. Again, the rule $\overline{\tau} \approx 2z_r/u_*$ applies. The waiting drift (Fig. 3b) is given very satisfactorily by $\overline{\delta} = \overline{\tau}\langle\overline{u} \mid z_r\rangle$, so it appears this connection between $\overline{\delta}$ and $\overline{\tau}$ may be exact, that is, independent of the particular regime of turbulence and mean wind.

As a numerical example, in the case that roughness length $z_0 = 0.05$ m, and if the boundary condition (reflection, or zero flux) is applied at $z_r = 5$ m, then if $u_* = 0.25$ m s^{-1}, mean surface delay is 40 s, and the mean displacement is about $2000z_0$, or 100 m.

d. Surface delay in homogeneous turbulence

The above results for the mean delay may be rewritten as $\overline{\tau} \approx 2z_r/(0.8\sigma_w)$. Given that the mean *magnitude* of a standardized Gaussian random variable is $(2/\pi)^{1/2} = 0.80$, could it be that the crucial velocity for the surface delays is $\overline{\mid w \mid}$?

To check whether this is so, we calculated $\overline{\tau}$ for reflection in Gaussian homogeneous turbulence. This also provided the opportunity to examine the behavior of $\overline{\tau}$ over a wide range in the ratio z_r/L of the depth of the waiting layer to the turbulence length scale $L = \sigma_w T_L$. If the depth of the waiting layer is very much larger than the length scale of the turbulent motion within it, surface delays are the outcome of a "diffusion" process, whereas if the opposite is true, we have a memory-dominated ("near field") process.

In the atmospheric surface layer, the turbulence length scale varies with height, that is, $L(z) = \sigma_w(z)T_L(z)$. It is known that $L \sim 1/2\ (z - d)$, where the displacement length $d \approx 2/3\ h$ (and so can be significant in the case of a tall plant canopy). If $z_r \gg d$, then $L(z_r) \sim 1/2z_r$, and so it is neither true that $z_r \gg L(z_r)$, nor is it true that $z_r \ll L(z_r)$; statistics of surface delays are probably influenced by memory of the entry velocity.

In homogeneous turbulence, an artificial situation prevails, and one can make the adherence layer $0 \leq z \leq z_r$ arbitrarily large with respect to the (constant) length scale. Figure 4 gives the calculated mean delay for waiting layers whose depth spans the range $0.01 \leq z_r/(\sigma_w T_L) \leq 10$. For these calculations, the time step was set to $dt = 0.02 \min(T_L, z_r/\sigma_w)$. The mean delay $\overline{\tau}$ agreed with the estimate $\overline{\tau} \approx 2z_r/\overline{\mid w \mid}$, even for $z_r/(\sigma_w T_L)$ as small as 0.04, that is, the difference between the formula and the computed mean delay did not exceed the standard error of the mean (σ_τ, standard deviation of the N estimates of τ divided by $N^{1/2}$).

4. Surface delays in continental-scale transport

Are these surface delays and drifts worth accounting for, in time-dependent dispersion problems? The Canadian Meteorological Centre has implemented a long range, first-order LS model,[3] coupled to the resolved velocity fields of a global weather analysis/prediction model (the Canadian Global Environmental Multiscale model). Using that model, we simulated the European Tracer Experiment (ETEX) of 1994 in which tracer gas was released near Rennes, France, and the time series of concentration of that gas was reported over the following days from stations covering Europe and Western Asia. The paths of 10 000 particles, released over the 12-h source duration (1600 UTC 23 October–0400UTC 24 October), were tracked for the succeeding 57 h; upon each surface reflection, we imposed delay $2z_r/u_*$ and displacements $\overline{\delta}_x = \overline{\tau}\langle\overline{u} \mid z_r\rangle$, $\overline{\delta}_y = \overline{\tau}\langle\overline{v} \mid z_r\rangle$, where the local friction velocity u_* and the near-ground winds $\overline{u}$, $\overline{v}$ varied geographically and temporally.[4]

When trajectories were reflected at $z_r \approx 10$ m, on average during its flight (of order 50 h) a particle experienced about 30 reflections, the average delay per

[3] Thomson's well-mixed 3D model for Gaussian inhomogeneous turbulence but with terms due to nonstationarity and local (horizontal) inhomogeneity of turbulence statistics neglected. The time step Δt along trajectories was held constant (i.e., height independent) at a value chosen in relation to the reflection height z_r; to be specific, Δt was required to be small relative to $1/2\ z_r/u_*$, the latter representing the *minimum* value of the Lagrangian timescale, which occurs at the boundary.

[4] We derived a formula for $\langle\overline{u} \mid z_r\rangle$ by integrating the composite mean wind profile of appendix B, from $z = 0$ to $z = z_r$, with the further assumption of an effective canopy height $h = 10z_0$, calculated from the roughness-length map employed in GEM.

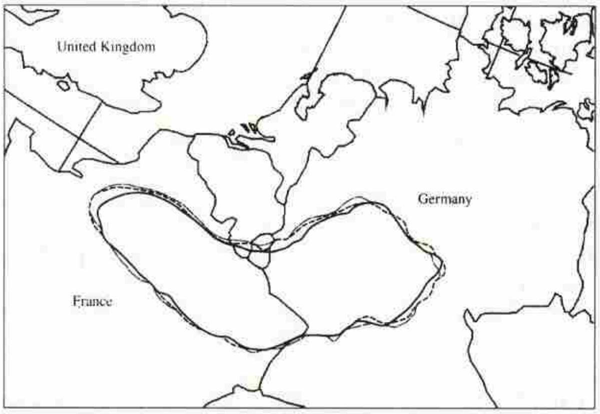

FIG. 5. ETEX plume position at 1500 UTC 24 Oct 1994, 11 h after the source was turned off, as indicated by the 0.5 ng m^{-3} concentration contour. Long-dashed line: $z_r \approx 2$ m, time step $\Delta t = 0.2$ s, surface effects (τ, δ) neglected; solid line: $z_r \approx 25$ m, $\Delta t = 2.5$ s, surface effects (τ, δ) neglected; short-dashed line: $z_r \approx 25$ m, $\Delta t = 2.5$ s, surface effects (τ, δ) parameterized.

reflection being about 40 s; thus, very roughly, 15 reflections occurred per particle per day, causing a net delay of about 10 min day^{-1}. The mean magnitude of the surface displacement was about 150 meters per reflection, resulting in a net displacement on the order of 1 km day^{-1} (direction of the displacements varies with surface wind direction). If the trajectories were instead reflected at $z_r \approx 25$ m, the average delay (displacement) per reflection increased to about 130 s (600 m), but the mean number of reflections (per particle per day) was virtually unchanged; in consequence, the net daily delay increased to about 30 min.

Figure 5 compares three simulations of the ETEX plume, giving a view of the 0.5 ng m^{-3} concentration contour, 11 h after the source was turned off. Owing to a more than tenfold increase in time step permitted, computation time is dramatically reduced when reflection height is increased from $z_r \approx 2$ m (reference simulation at high resolution, $\Delta t = 0.2$ s) to $z_r \approx 25$ m (low-resolution/high-reflection simulation, $\Delta t = 2.5$ s; surface delays uncorrected). Plume position, however, is degraded in the low-resolution calculation, most noticeably at the trailing (last arriving) edge of the plume, and by on the order of 10–20 km. As Fig. 5 shows, that deficiency is mitigated by parameterizing the mean surface delays and displacements.

5. Conclusions

No description of atmospheric transport will resolve motion on all scales, indefinitely close to the surface. Thus, in modeled trajectories there will always be a kind of discontinuity in which trajectories are reflected back to the interior of the flow; similar discontinuities are implicit in Eulerian models.

We calculated the neglected surface delays and drifts when particles passed below a nominal lower boundary, placed arbitrarily (at height z_r) within a horizontally uniform surface layer. We did not address the fact that, as the wind blows over fields, forests, and cities, particles will also temporarily be "lost" into wakes of windbreaks, urban canyons, forest clearings, and so on. According to our idealized calculations, mean delay per reflection $\overline{\tau} \approx 2.5 z_r/\sigma_w$ (where σ_w is the standard deviation of the vertical velocity at z_r) and mean alongwind displacement per reflection $\overline{\delta} \approx \langle \overline{u} \mid z_r \rangle \overline{\tau}$, where $\langle \overline{u} \mid z_r \rangle$ is the height average of $\overline{u}$ in the waiting layer. Net surface delays in continental-scale dispersion are neither dramatic nor negligible (on the order of 30 min day^{-1} for reflection at 25 m), and the delays and drifts, if *both* are neglected, do not compensate for each other.

These effects could also be parameterized in Eulerian models: one could add, below the (original) lower boundary z_r, an additional layer whose depth and eddy diffusivity would be adjusted to imply the desired mean residence time $\overline{\tau}$ and whose horizontal velocities would be specified as $\langle \overline{u} \mid z_r \rangle$, $\langle \overline{v} \mid z_r \rangle$.

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APPENDIX A

Lagrangian Stochastic Model

The components of the conditional mean acceleration for Thomson's well-mixed 3D model for the Lagrangian velocity fluctuations in horizontally uniform, stationary Gaussian turbulence are

$$
\begin{aligned}
a_u = {} & \frac{-b^2}{2\sigma^2}[U(\sigma_v^2\sigma_w^2 - \overline{v'w'}\,\overline{v'w'}) + V\overline{u'w'}\,\overline{v'w'} - W\sigma_v^2\overline{u'w'}] + \frac{1}{2}\frac{\partial\overline{u'w'}}{\partial z} \\
& + \frac{UW}{2\sigma^2}\left[\frac{\partial\sigma_u^2}{\partial z}(\sigma_v^2\sigma_w^2 - \overline{v'w'}\,\overline{v'w'}) - \frac{\partial\overline{u'w'}}{\partial z}\sigma_v^2\overline{u'w'}\right] + \frac{VW}{2\sigma^2}\left(\frac{\partial\sigma_u^2}{\partial z}\overline{u'w'}\,\overline{v'w'} - \frac{\partial\overline{u'w'}}{\partial z}\sigma_u^2\overline{v'w'}\right) \\
& + \frac{W^2}{2\sigma^2}\left(\frac{\partial\overline{u'w'}}{\partial z}\sigma_u^2\sigma_v^2 - \frac{\partial\sigma_u^2}{\partial z}\sigma_v^2\overline{u'w'}\right),
\end{aligned}
$$

$$a_v = \frac{-b^2}{2\sigma^2}[U\overline{u'w'}\,\overline{v'w'} + V(\sigma_u^2\sigma_w^2 - \overline{u'w'}\,\overline{u'w'}) - W\sigma_u^2\overline{v'w'}] + \frac{1}{2}\frac{\partial\overline{v'w'}}{\partial z} + \frac{UW}{2\sigma^2}\left(\frac{\partial\sigma_v^2}{\partial z}\overline{u'w'}\,\overline{v'w'} - \frac{\partial\overline{v'w'}}{\partial z}\sigma_v^2\overline{u'w'}\right)$$

$$+ \frac{VW}{2\sigma^2}\left[\frac{\partial\sigma_v^2}{\partial z}(\sigma_u^2\sigma_w^2 - \overline{u'w'}\,\overline{u'w'}) - \frac{\partial\overline{v'w'}}{\partial z}\sigma_u^2\overline{v'w'}\right] + \frac{W^2}{2\sigma^2}\left(\frac{\partial\overline{v'w'}}{\partial z}\sigma_u^2\sigma_v^2 - \frac{\partial\sigma_v^2}{\partial z}\sigma_u^2\overline{v'w'}\right), \quad \text{and}$$

$$a_w = \frac{b^2}{2\sigma^2}(U\sigma_v^2\overline{u'w'} + V\sigma_u^2\overline{v'w'} - W\sigma_u^2\sigma_v^2) + \frac{1}{2}\frac{\partial\sigma_w^2}{\partial z}$$

$$+ \frac{UW}{2\sigma^2}\left[\frac{\partial\overline{u'w'}}{\partial z}(\sigma_v^2\sigma_w^2 - \overline{v'w'}\,\overline{v'w'}) + \frac{\partial\overline{v'w'}}{\partial z}\overline{u'w'}\,\overline{v'w'} - \frac{\partial\sigma_w^2}{\partial z}\sigma_v^2\overline{u'w'}\right]$$

$$+ \frac{VW}{2\sigma^2}\left[\frac{\partial\overline{u'w'}}{\partial z}\overline{u'w'}\,\overline{v'w'} + \frac{\partial\overline{v'w'}}{\partial z}(\sigma_u^2\sigma_w^2 - \overline{u'w'}\,\overline{u'w'}) - \frac{\partial\sigma_w^2}{\partial z}\sigma_u^2\overline{v'w'}\right]$$

$$+ \frac{W^2}{2\sigma^2}\left(\frac{\partial\sigma_w^2}{\partial z}\sigma_u^2\sigma_v^2 - \frac{\partial\overline{u'w'}}{\partial z}\sigma_v^2\overline{u'w'} - \frac{\partial\overline{v'w'}}{\partial z}\sigma_u^2\overline{v'w'}\right).$$

In the current simulations, for which it was assumed that $\overline{v'w'} = 0$ and that $\sigma_v^2 = \sigma_u^2$, $\sigma^2 = \sigma_v^2(\sigma_u^2\sigma_w^2 - \overline{u'w'}\,\overline{u'w'})$.

APPENDIX B

Normalized Velocity Statistics for a Generic Plant Canopy

We specified the profile of mean wind speed as

$$\frac{\overline{u}(z)}{u_*} = \begin{cases} \dfrac{\overline{u}(h)}{u_*}\exp\left[\beta_u\left(\dfrac{z}{h} - 1\right)\right], & z \le h \\ \dfrac{\overline{u}(h)}{u_*} + \dfrac{1}{k_v}\log\left(\dfrac{z - d}{h - d}\right), & z > h, \end{cases}$$

where the friction velocity u_* is based on the shear stress at $z = h$, the von Kármán constant $k_v = 0.4$, and the displacement length $d/h = 2/3$. The extinction parameter β_u may be defined in terms of the ratio of the wind speeds at $z = h$ and $z = 0$:

$$\beta_u = \ln\left[\frac{\overline{u}(h)/u_*}{\overline{u}(0)/u_*}\right],$$

where we set $[\overline{u}(h)/u_*, \overline{u}(0)/u_*] = (3.0, 0.15)$ so that $\beta_u = 3.0$. For the standard deviation of the vertical velocity, we wrote

$$\frac{\sigma_w(z)}{u_*} = \begin{cases} \dfrac{\sigma_w(h)}{u_*}\exp\left[\beta_{\sigma w}\left(\dfrac{z}{h} - 1\right)\right], & z \le h \\ \dfrac{\sigma_w(h)}{u_*}, & z > h, \end{cases}$$

where $[\sigma_w(h)/u_*, \sigma_w(0)/u_*] = (1.25, 0.3)$ so that $\beta_{\sigma w} = 1.43$. The same form was used for σ_u (assumed to be equal to σ_v) with $[\sigma_u(h)/u_*, \sigma_u(0)/u_*] = (2.0, 0.5)$, and similarly the normalized shear stress was constant (equal to $-u_*^2$) above the canopy, with an exponential extinction in the canopy to a value on ground of $-0.03u_*^2(\beta_{u_*^2} = 3.5)$. Last, the Lagrangian timescale was specified as

$$\frac{u_* T_L(z)}{h} = \begin{cases} 0.3, & z \le h \\ \max\left[0.3, \dfrac{0.5(z/h - d/h)}{\sigma_w/u_*}\right], & z > h \end{cases}$$

[a calculation with $u_*\ \tau/h = 0.3(z/h)/0.15$ for $z/h \le 0.15$ yielded a negligibly different outcome].

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