# Flow Boundaries in Random-Flight Dispersion Models: Enforcing the Well-Mixed Condition

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ABSTRACT

Lagrangian stochastic (LS) dispersion models often use trajectory reflection to limit the domain accessible to a particle. It is shown how the well-mixed condition (Thomson) can be expressed in the Chapman–Kolmogorov equation for a discrete-time LS model to provide a test for the validity of a reflection algorithm. By that means it is shown that the usual algorithm (perfect reflection) is exactly consistent with the wmc when used to bound Gaussian homogeneous turbulence, but that no reflection scheme can satisfy the wmc when applied at a location where the probability distribution for the normal velocity is asymmetric, or locally inhomogeneous. Thus, there is no well-mixed reflection scheme for inhomogeneous or skew turbulence.

## 1. Introduction

In numerical random-flight calculations, which mimic turbulent dispersion, one must often limit the domain accessible to the particles. This may be because a true flow boundary exists (e.g., the ground), or because we consider it unnecessary to calculate parts of the trajectory (e.g., within a forest), or simply because we are considering an artificial system (e.g., bounded homogeneous turbulence). Accordingly, there arise diverse specifications of velocity statistics near computational boundaries, and a boundary may or may not be crossable. If crossable, then we need to supplement the LS model with a reflection scheme—and this is a practice that has escaped anything but cursory investigation, despite the fact (which we will demonstrate here) that a bad reflection scheme tacked onto an otherwise "good" LS model may result in failure of an initially well mixed distribution of particles to remain well mixed, that is, violation of Thomson's (1987) "well-mixed constraint."

In this paper we are concerned with correct methods of restricting the particle domain. Our criterion will be that however this is achieved, the well-mixed constraint (wmc) must obtain. Failure of a trajectory model to satisfy the wmc implies a spurious growth of statistical order from disorder, and can lead to bad predictions of, for example, ground-level concentration from pollutant sources.

In order to bring the boundary treatment within the scope of the wmc, we impose the latter on the complete model algorithm (i.e., including reflection, if used), and in a discrete-time framework. This is achieved by enforcing the wmc in the Chapman–Kolmogorov equation, rather than (as did Thomson) in the (time continuous) Fokker–Planck equation derived therefrom. A complete specification of a discrete-time LS model, in our view, includes any reflection algorithm employed, and implies a transition density function that accounts for *all* motions of the particle, including reflection. The discrete-time probabilistic description is true to the underlying random-flight (RF) model: the only aspect that cannot be simulated (by repeatedly integrating the Chapman–Kolmogorov equation), is the use of a time step $\Delta t$ that varies along the trajectory, in response to the flow statistics encountered. But there is a penalty to the rigor of the discrete-time framework. Whereas the continuous-time description permits the *derivation* of a suitable model from the wmc, we are forced instead to *postulate* a model, then check (usually numerically) for satisfaction of the wmc.

We emphasize that it is not always possible to state whether an observed violation of the wmc is attributable to the means of boundary treatment, or to the implementation of a model derived from Thomson's criteria (i.e., a model that is well-mixed in the limit of an infinitesimal time step) with a finite time step. Criteria pertinent to the latter source of (discretization) error are briefly reviewed in the Appendix.

## 2. The "ground"

In engineering flows it is possible to imagine a flow boundary (say at $z = 0$) so smooth that one might have knowledge of velocity statistics arbitrarily close to $z = 0$. However, in the atmosphere this is almost never

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true. In atmospheric theories, whether concerned with the flow itself, or with motion of a tracer in the flow, there is normally a layer adjacent to ground within which the velocity statistics are unknown. A convenient parameterization is substituted for reality. We will call this the "unresolved basal layer" (UBL), and by way of example note the practice (usual in treating surface-layer dispersion) of extrapolating to ground the Monin–Obukhov surface-layer profiles, which in principle are valid only where $z \gg z_0$, $z_0$ (here) being the surface roughness length.

We are forced to ignore the structure of the UBL, and treat its statistics by extrapolation from the resolved profiles above, because the UBL itself is, for some or all of the following reasons, too complex to consider: measurements in the UBL (e.g., among the blades of grass, or between the clods, or at a different scale among the houses) are difficult if not impossible; the assumption of horizontal homogeneity is invalid [unless applied to suitably defined averages, e.g., Raupach and Shaw (1982)]; very close to ground, temperature gradients might be so large that conduction causes sufficiently rapid volumetric dilatation to invalidate the Boussinesq approximation [for a criterion see Batchelor (1985)]; and, the effective Reynolds number may not be infinite.

Sometimes the surface parameterization spans not just this truly unknown layer, but substitutes for known structure a simplification (we will still use the term UBL in this case). Thus to someone modeling dispersion in the convective boundary layer, details of motion within the forest may be irrelevant, and the entire forest layer may be treated as the UBL, even though it is feasible to specify velocity statistics within a canopy. But to someone modeling pollen dispersion in the forest, the UBL is likely to be a shallow layer covering, for example, the needle litter. Going further, one might (by design, and in many contexts legitimately) ignore the real structure of the entire atmospheric surface layer (ASL), replacing it with extrapolated mixed-layer profiles (e.g., Luhar and Britter 1989).

Are there severe consequences of our inevitable ignorance of velocity statistics in the UBL? Fortunately, it seems not. Let us focus on the horizontally uniform, neutrally stratified atmospheric surface layer (NSL). Sufficiently far from ground ($z \gg z_0$), turbulence in the NSL is characterized by a single velocity scale $u_*$, the friction velocity, and length scales $z$, $\delta$. Vertical dispersion is normally simulated by assuming the Lagrangian decorrelation time scale $\tau \propto z/\sigma_w$, and $\sigma_w = 1.3\, u_*$. This neglects the gradient of $\sigma_w$ across the UBL ($\sigma_w$ must vanish as $z \to 0$). Although the structure of the UBL is thus ignored, and the surface layer wrongly extrapolated to ground, simulations of this sort compare well with observations (e.g., Wilson et al. 1981).

Why? For example, by definition a ground-level source is within the UBL. Yet experience has shown that for any downstream distance likely to be of interest, continuous ground-level sources (release height $H$ nominally zero) of passive tracer may be treated as a release "near" ground with reflection of trajectories (in the context of Eulerian models, imposition of the no-flux boundary condition) at some "small" height $z = z_R$. Complete neglect of the actual structure of the UBL seems to be inconsequential, presumably for the following reasons: (i) horizontal velocities within the UBL are small, so trajectories enter and leave the UBL at roughly the same $(x, y)$ location; (ii) the UBL itself is disturbed by surface irregularities causing what may loosely be denoted turbulence, so that residence times therein are not long; (iii) the tracer mass residing in the UBL is usually small with respect to the total tracer mass; and (iv) all points in the UBL are located *close* to the ground, where the mean vertical flux vanishes; therefore the mean vertical concentration gradient in the UBL is small, resulting in an insensitivity of mean concentration near the wall to the exact placement of the model boundary.

The conclusion we reach is that the velocity statistics specified at the ground will never be demonstrably the "truth," and there is no barrier to pragmatism in their specification. A wide variety of surface boundary conditions are used in practice [e.g., for the convective boundary layer, compare Luhar and Britter (1989) with Weil (1990)].

## 3. Implementing a nonattainable boundary

As a real flow boundary (say at $z = z_R$) is approached, the probability density function $g_a(w)$ for the normal velocity $w$ along the $z$ axis must collapse,

$$\lim_{(z \to z_R)} g_a(z, w) = \delta(w, 0).$$

A real fluid element approaching the boundary is driven by eddies of ever smaller characteristic length, velocity, and time scales, and consequently is restricted to the flow domain. Accordingly, one might hope to implement an uncrossable (or unattainable) boundary in a trajectory model by specifying realistic profiles of the velocity statistics (e.g., velocity variance vanishing at the boundary) and a suitable time step (small compared with flow time scales, the latter essentially vanishing at the wall).

Suppose we wish the ground ($z_R = 0$) to be inaccessible to computational particles. This is guaranteed on the condition that whatever the present height $z$ of a particle whose present velocity $w$ is negative, the time step for the forthcoming step (usually and most naturally chosen as $\Delta t = \mu\tau(z)$, where $\mu \ll 1$) obeys

$$\Delta t(z) < \frac{z}{|w|},$$

which we can take to require

$$|w| < \frac{z}{\mu\tau}. \tag{1}$$

Since the magnitude of $w$ decreases with decreasing local velocity scale $\sigma_w(z)$, and since Eq. (1) is more likely to be satisfied with decreasing $\tau$, the natural way ("natural" in the sense that one imposes no additional constraint on the time step) to render the ground unattainable by model particles is to ensure that the turbulent velocity and time scales decrease as the ground is approached. Additional protection is available by reducing $\mu$.

We found (section 9) that when the convective boundary layer was parameterized with velocity and time scales vanishing at boundaries, and provided the ratio $\mu = \Delta t/\tau$ was small enough, boundaries were not crossed (and so were "naturally unattainable"); but great computational effort was involved to calculate short trajectory segments near the boundaries, and an alternative boundary treatment involving trajectory reflection was much more efficient.

*Artificial unattainability.* Suppose one wished to impose boundaries at $z = \mathrm{ZB}$, ZT. For a particle stepping on from state $(z_0, w_0)$, one might add an (additional) restriction on the time step

$$\Delta t \leqslant \frac{[(\mathrm{ZT} - \epsilon) - z_0]}{w_0}, \quad w_0 > 0$$

$$\Delta t \leqslant \frac{[z_0 - (\mathrm{ZB} + \epsilon)]}{|w_0|}, \quad w_0 < 0,$$

where $\epsilon > 0$ is an arbitrary small length. The infallible consequence of this strategy, we found, is violation of the wmc, attributable unambiguously to this means of bounding the domain.

## 4. Expressing the well-mixed constraint in the Chapman–Kolmogorov equation

In this section we will show how the well-mixed constraint can be imposed on discrete-time step LS models that may include a reflection algorithm.

The height $z$ and velocity $w$ of a single particle released into a turbulent flow may be represented as a moving point in $z$-$w$ phase space (the generalization to multiple dimensions is obvious). The trajectory of the point $(z, w)$ for an individual realization is stochastic, but by considering an ensemble of realizations of such a single particle release, we may define a position–velocity probability density function (or state function) $p(z, w, t)$, whose evolution is deterministic.

Suppose the fluid density is $\rho(z)$ and the Eulerian velocity pdf is $g_a(z, w)$ (we will restrict our attention to stationary flows). We may release the particles at random into the flow in such a way that the ensemble mean probability of release at $z$ is proportional to $\rho(z)$ (particles initially well mixed in position), and if the initial velocity is randomly chosen from the Eulerian pdf (release velocity well mixed) then $p(z, w, 0) \propto \rho(z)g_a(z, w)$. Thomson's well-mixed constraint states that a model for the calculation of trajectories should guarantee that passive tracer particles initially well mixed in the flow (in the sense defined above) *must remain well mixed, with respect to both position and velocity.*

Once released into the flow, a particle must thereafter exist *somewhere* and with *some velocity*; thus a conservation law applies to $p(z, w, t)$. Thomson showed that the wmc requires $g_a$ to be a solution to the Fokker–Planck equation, the differential equation that expresses probability conservation for the chosen trajectory model. Because we wish to impose the wmc for a practicable (i.e., time discrete) LS model, we will instead work with an integral statement of probability conservation, the Chapman–Kolmogorov equation (van Kampen 1981; Gillespie 1992).

Consider the phase space $z$-$w$ to have been divided into elementary volumes $d\Omega_j$ $(j = 1, \cdots, N)$. Then it is obvious that the probability $P(d\Omega_i, t_2)$ that a particle lies in $d\Omega_i$ at time $t_2$ is

$$P(d\Omega_i, t_2) = \sum_j T(d\Omega_i, t_2 | d\Omega_j, t_1)P(d\Omega_j, t_1),$$

where $t_2 > t_1$ and $T$ is the probability of transition in the given interval from $d\Omega_j$ to $d\Omega_i$. The specifics of the trajectory model (and any reflection procedure) define $T$. The corresponding expression for the evolution of the joint *density* function is the Chapman–Kolmogorov (CK) equation:

$$p(z_2, w_2, t_2) = \int_\Omega p(z_2, w_2, t_2 | z_1, w_1, t_1) \times p(z_1, w_1, t_1) dz_1 dw_1, \quad (2)$$

where $\Omega$ denotes the entire region of the $z$-$w$ domain that is accessible to a particle, and $p(z_2, w_2, t_2 | z_1, w_1, t_1)$ is the *transition density* [i.e., $p(z_2, w_2, t_2 | z_1, w_1, t_1) dz_2 dw_2$ is the probability of transition during interval $(t_2 - t_1)$ from $z_1$, $w_1$ into volume $z_2 \pm 1/2 dz_2$ and velocity interval $w_2 \pm 1/2 dw_2$]. Again, the trajectory model specifically defines the transition density, which will often be stationary, that is, will depend on $t_2 - t_1$ but not $t_1$ or $t_2$.

Imposition of the wmc in the Chapman–Kolmogorov equation is straightforward. Assuming the fluid density to be constant, we simply require that for all $t$, the transition density must satisfy

$$g_a(z, w) = \int_\Omega p(z, w, t | z_0, w_0, 0) g_a(z_0, w_0) dz_0 dw_0. \quad (3)$$

We can regard $g_a$ as known, so that this (novel) expression of the wmc is an integral equation for the transition density (in the terminology of integral equations, $g_a$ is an eigenvector of the transition density with eigenvalue 1). Unfortunately, there is no unique solution for the transition density [clearly $p(z_2, w_2, t_2 | z_1, w_1, t_1) = \delta(z_2, z_1)\delta(w_2, w_1)$ is *a* solution, though not a useful one: we are not interested in a trajectory model that leaves each particle in its initial state]. The well-mixed condition alone cannot fully determine the trajectory model. This is well known, and not surprising, since there is no dynamical content to the wmc. The wmc is rather a statement with respect to entropy, its satisfaction by a model prohibiting the spurious evolution of order from disorder.

In what follows we will sometimes make use of the fact that if a trajectory model is to fail the wmc, it must do so on the first time increment. For by the stationarity of the transition probability, provided $p(z, w, \Delta t) = g_a(z, w)$ then $p(z, w, t) = g_a(z, w)$ for all $t$. Thus, for stationary flows, one may impose the wmc by invoking Eq. (3) with the specialization $t = \Delta t$.

## 5. Criteria for reflection algorithms

For multidimensional LS models of non-Gaussian turbulence, the smooth-wall reflection scheme (see section 6) that has so far been employed without much scrutiny, will in general fail. The most complex reflection algorithm yet proposed seems to be that of Weil (1990), for turbulence having a skewed velocity pdf. In this section we consider whether there exist guidelines for the design or testing of a reflection scheme that are more restrictive than the "expanded" well-mixed criterion of the previous section (wherein the reflection algorithm is implicit in the transition density). We note that reflection schemes, no matter what their other merits, break the equivalence between model and real time (measured from release of the particle).

Any reflection scheme will be satisfactory in at least one respect—the mass (or number) flux across the boundary (we will for the present consider the vertical flux across a horizontal boundary at $z = 0$) will vanish. In terms of the state function, the vertical flux is (van Dop et al. 1985)

$$F_z(z, t) = \int_{w=-\infty}^{\infty} wp(z, w, t)dw = W(z, t)C(z, t),$$

where $C(z, t)$ is the mean concentration,

$$C(z, t) = \int_{w=-\infty}^{\infty} p(z, w, t)dw,$$

and the mean Lagrangian velocity $W(z, t)$ is defined by the above equation. One of the aims of reflection is to assure $F_z(0, t) = 0$ [or equivalently $W(0, t) = 0$], no matter what the preconditioning of $p(z, w, t)$, that is, no matter what the history of the particle trajectory. But is that all that is necessary of a reflection algorithm? Surely not. For if in our means of assuring $F_z(0, t) = 0$ we distort the velocity pdf in the region of $z = 0$, we fail the wmc.

The vertical flux of air is

$$F_{az}(z, t) = \int_{w=-\infty}^{\infty} wg_a(z, w)dw.$$

In many flows of interest (e.g., the horizontally uniform atmospheric surface layer) this will vanish. Clearly if it does so (and it will at any plane where we would wish to zero the flux of a passive tracer), then by definition so does the vertical flux of any well mixed tracer. Thus, satisfaction of the wmc by a complete LS algorithm guarantees vanishing vertical tracer flux at impermeable boundaries. Upholding the wmc seems to be a complete criterion for a reflection algorithm.

## 6. The transition probability and the trajectory model

We consider an LS model unambiguously defined only if the procedure at flow boundaries is specified and considered part of the model. In this section we will demonstrate by a simple one-dimensional example how to find the transition probability corresponding to a complete LS model.

We will again consider vertical motion, in a system bounded at $z = B$ and $z = T$ $(T > B)$. Provided only that $(z, w)$ evolves as Markov process, a suitable general model for the increments in velocity and position over an infinitesimal time increment $dt$ is

$$dw = a(z, w, t)dt + bd\xi, \quad dz = wdt,$$

where the increments $d\xi$ are independent and random, and have the Gaussian distribution with mean 0 and variance $dt$ (Thomson 1987). To obtain a practicable model, we will employ the above equations with finite increments $\Delta t$, etc., and add the specification $\Delta t \ll \tau$, where $\tau$ is to be regarded as the shortest significant time scale of the system. Our (arbitrary) practice is to calculate $\Delta z$ prior to incrementing $w$, which leads to a convenient factorization of the transition density into a product of independent transition densities for velocity and position (see below).

We must now face the possibility of a particle crossing $z = B$ or $z = T$. Suppose a particle goes from an allowed state $(z_0, w_0, t)$ to a subsequent disallowed state $(z^*, w^*, t + \Delta t)$, where $z^* < B$ or $z^* > T$. Then under "smooth-wall reflection" at the lower boundary we correct the disallowed state $z^* < B$ at $t + \Delta t$ by placing the particle in the state $(2B - z^*, -w^*, t + \Delta t)$, while in case of flight above the upper boundary the corrected state is $(2T - z^*, -w^*, t + \Delta t)$. We may incorporate these conditional reflection procedures into the generalized Langevin equations by introducing logical variables:

$$C_B(z_0, w_0) = \begin{cases} 0, & w_0 \geqslant -(z_0 - B)/\Delta t \\ 1, & w_0 < -(z_0 - B)/\Delta t, \end{cases}$$

$$C_T(z_0, w_0) = \begin{cases} 0, & w_0 \leqslant (T - z_0)/\Delta t \\ 1, & w_0 > (T - z_0)/\Delta t, \end{cases}$$

and

$$C_{BT}(z_0, w_0) = C_B \cup C_T.$$

In terms of these logical variables, the LS model may be expressed as

$$\Delta w = a(z_0, w_0, t)\Delta t(1 - 2C_{BT}) - 2C_{BT}w_0 + b(1 - 2C_{BT})\Delta\xi$$

$$\Delta z = w_0\Delta t(1 - 2C_{BT}) - 2C_{BT}z_0 + 2C_B B + 2C_T T.$$

This is a complete discrete-time LS model, in the sense that it contains a reflection algorithm, and is unambiguous with respect to the order of operations.

The corresponding transition density $p(z, w, t + \Delta t | z_0, w_0, t)$ for a single time step $\Delta t$ is composed of independent transition densities for position and velocity, $p = p_z p_w$. The transition density for position may be written

$$p_z(z, t + \Delta t | z_0, w_0, t) = \delta[z - z_0, w_0\Delta t(1 - 2C_{BT}) - 2C_{BT}z_0 + 2C_B B + 2C_T T],$$

meaning that given $z_0$, $w_0$, and $\Delta t$, the new position $z$ can take on only three possible values (the delta function for $p_z$ accords with the absence of diffusion along $z$ in the Fokker–Planck equation corresponding to the LS model). If reflection does not occur during $\Delta t$, the new position $z(t + \Delta t)$ must be $z_0 + w_0\Delta t$, that is, $p_z(z, t + \Delta t | z_0, w_0, t) = \delta(z - z_0, w_0\Delta t)$. On the other hand if reflection does occur, the new position is $2B - z_0 - w_0\Delta t$ (upward reflection at $B$), or $2T - z_0 - w_0\Delta t$ (downward reflection at $T$). We have assumed $T - B$ is sufficiently large to prohibit multiple reflections within a single time step.

Since the random forcing in velocity $b\Delta\xi$ is Gaussian, the transition density for velocity is also Gaussian, with variance $b^2\Delta t$:

$$p_w(w, t + \Delta t | z_0, w_0, t) = \frac{1}{(2\pi)^{1/2} b(\Delta t)^{1/2}} \times \exp\left\{-\frac{[w - w_0 - a(z_0, w_0, t) \times \Delta t(1 - 2C_{BT}) + 2C_{BT}w_0]^2}{2b^2\Delta t}\right\}.$$

The transition density for more complex cases (multidimensional, etc.) may be constructed by the same steps.

The evolution of the state function $p(z, w, t)$ obtained by repeated integration of the CK equation must, except as regards truncation or stability error caused by numerical integration, prove identical to the ensemble-mean evolution as calculated by random flights using the underlying model (provided the latter uses position-invariant time step). It would be pedantic to check this routinely, but an example of the expected consistency will be given (section 8). In the following sections we will test whether particular transition densities chosen to model motion in several bounded turbulence systems, including models of the lower atmosphere, satisfy the well-mixed condition.

## 7. Reflective boundaries for Gaussian turbulence

The well-mixed one-dimensional model for stationary Gaussian turbulence (i.e., turbulence in which the Eulerian velocity pdf is Gaussian) is (Thomson 1987):

$$dw = -\frac{w}{\tau(z)}dt + \frac{1}{2}\frac{\partial\sigma_w^2}{\partial z}\left(1 + \frac{w^2}{\sigma_w^2}\right)dt + b\,d\xi, \quad b = \left(\frac{2\sigma_w^2}{\tau}\right)^{1/2}, \quad (4)$$

where $\tau$ is the decorrelation time scale. A discrete implementation, with smooth-wall reflection at ground and with appropriate choices for $\tau(z)$ and $\sigma_w(z)$, gives good predictions of short-range dispersion in the atmospheric surface layer (e.g., Wilson et al. 1981).[1] But is it *exactly* well mixed?

In the unbounded homogeneous case, it can easily be shown that the finite-increment model satisfies the wmc Eq. (3), provided that

$$b^2 = \frac{\sigma_w^2}{\Delta t}\left[1 - \left(1 - \frac{\Delta t}{\tau}\right)^2\right]. \quad (5)$$

If $\Delta t \ll \tau$, this distinction regarding $b$ is not important.

### *a. Bounded Gaussian homogeneous turbulence*

Now suppose we use smooth-wall reflection at $z = 0$ to model the artificial system of bounded homogeneous turbulence. If the initial state is $p(z, w, 0) = g_a(w)$, then the entire LS algorithm is acceptable if, after a single time step $\Delta t \ll \tau$, the state $p(z, w, \Delta t)$ is still the well-mixed state. The state at $\Delta t$ is

$$p(z, w, \Delta t) = \int_{z_0=0}^{\infty}\left[\int_{w_0=-\infty}^{-z_0/\Delta t} p(z, w, \Delta t | z_0, w_0, 0) g_a(w_0)\,dw_0\right]dz_0 + \int_{z_0=0}^{\infty}\left[\int_{w_0=-z_0/\Delta t}^{\infty} p(z, w, \Delta t | z_0, w_0, 0) g_a(w_0)\,dw_0\right]dz_0.$$

Writing the delta functions that occur in the transition density (given earlier) as $\delta(z - z_0, w_0\Delta t) = (1/\Delta t)\delta[w_0, (z - z_0)/\Delta t)]$, etc., this is readily integrated to confirm that provided $b$ is given by Eq. (5), $p(z, w, \Delta t) = g_a(w)$. Our analysis (perhaps rather laboriously) proves that smooth-wall reflection exactly satisfies the wmc in Gaussian homogeneous turbulence. Random flight simulations confirm this. However, if instead of

[1] That this model was a discrete version of Eq. (4) is shown by Wilson et al. (1983).

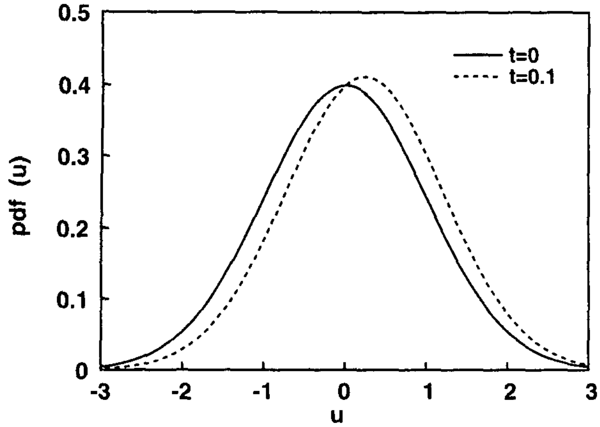


FIG. 1. Distortion of the wall-parallel ($u$) velocity pdf at $z = 0.01$ when smooth-wall reflection (with reversal of normal velocity only) is applied at $z = 0$ in two-dimensional, Gaussian, homogeneous turbulence. Velocity statistics $\sigma_U = \sigma_W = 1$, $\tau = 1$, and velocity correlation coefficient $\rho = -0.3$; pdf obtained by integrating the Chapman–Kolmogorov equation for a single time step $\Delta t = 0.1$ away from a well-mixed initial state. Numerical integration used $w \in (-5, 5)$, $\Delta w = 0.05$, $\Delta z = 0.01$. The pdf distortion does not occur far from the wall, nor if $\rho = 0$, nor if $u$ (as well as $w$) is reversed on reflection. The LS model is Thomson's (1987) multidimensional well-mixed model for Gaussian turbulence.

the smooth-wall reflection algorithm, "artificial unattainability" of the boundaries (section 3) is imposed, catastrophic violation of the wmc results.

What about other reflection algorithms? Suppose as an alternative to the smooth-wall reflection scheme we were to place any particle attaining $z < 0$ at $z = 0$. Then, whatever our strategy for treating the velocity, we must fail the well-mixed constraint: integration of the CK equation shows that at time $\Delta t$ after a well-mixed release, the marginal pdf for position will have the form $p(z, \Delta t) = c\delta(z, 0) + f(z)$, where $f(z)$ is some unspecified function; that is, the position pdf contains a weighted delta function. Another unacceptable reflection scheme is to map the disallowed position $z < 0$ to $-z$ and break the velocity correlation by adopting as the next velocity a random choice from the one-sided (positive only) Gaussian distribution $G^+(w)$. In that case, integration of the CK equation yields a marginal velocity pdf that contains a weighted term in $G^+(w)$.

The requirement that a reflection algorithm should satisfy the well-mixed constraint has implications that, on first sight, are surprising. Some two-dimensional models that include velocity covariance will require reversal upon reflection of both the normal velocity $w$ and the correlated along-wind velocity fluctuation $u$, although no "real world" significance can be attached to the need. For example, consider homogeneous turbulence, bounded at $z = 0, L$, in which the turbulent velocities $u$, $w$ have covariance $\langle uw \rangle = \rho\sigma_u\sigma_w$. Thomson (1987) gave a well-mixed multidimensional model for Gaussian turbulence that for the present case reduces to

$$dw = a_w dt + b_w d\xi_w, \quad du = a_u dt + b_u d\xi_u,$$

and if we choose

$$b_w = b_u = \left(2\frac{\sigma_w^2}{\tau}\right)^{1/2},$$

then the conditional mean particle acceleration components are

$$a_w = -\frac{\sigma_w}{\tau\sigma_u(1-\rho^2)}\left(-\rho u + \frac{\sigma_u}{\sigma_w}w\right)$$

$$a_u = -\frac{\sigma_w}{\tau\sigma_u(1-\rho^2)}\left(-\rho w + \frac{\sigma_w}{\sigma_u}u\right).$$

Now consider the motion of tracer particles that are initially well mixed in the $x$–$z$–$u$–$w$ space, that is, uniformly distributed in position and having for their velocity distribution the joint Gaussian. We will consider the evolution of the marginal distribution $p(z, u, w)$, that is, we will presume that the introduction of a reflection algorithm at boundaries at $z = 0, L$ does not affect the distribution of particles along $x$.

If only the normal velocity is reversed on reflection, an accumulation of mass results near $z = 0$ and a deficit results near $z = L$. Figure 1 compares the marginal pdf of $u$ with its initial value at the wall, as calculated by integrating the CK equation (1) over a single time step. The well-mixed condition is not satisfied.

This failure is readily understood. Let us consider an ensemble of possible *velocity* outcomes for a particle which, at time $n$ having state $(z_0, w_0)$, undergoes reflection (i.e., $w_0$ has such a value as will take the particle outside the flow domain). Then at time $n + 1$, after reflection, the velocities are $w^{n+1} = -(w_0 + \Delta w)$ and $u^{n+1} = (u_0 + \Delta u)$. Now noting that $\langle w_0 u_0 \rangle = \rho\sigma_u\sigma_w$, and that $\Delta\xi_u$ and $\Delta\xi_w$ are independent of each other and of the state at time $n$, we find that the velocity covariance at time $n + 1$ is $\langle w^{n+1}u^{n+1} \rangle = -\rho\sigma_u\sigma_w$, that is, the covariance has the wrong sign. The obvious fix is to reverse both $w$ *and* $u$ upon reflection. That necessity is confirmed both by random flights and by integration of the CK equation. In the Thomson model, failure to reverse $u$ upon reflection leads to an erroneous $u$ distribution near the wall, which impacts on the vertical motion and thus the vertical mass distribution through the coefficient $a_w$.

## *b. Bounded Gaussian inhomogeneous turbulence (e.g., neutral surface layer)*

Real turbulent flows are in general both inhomogeneous and non-Gaussian. But it is convenient, often the best we can do, and can be surprisingly successful (e.g., Flesch and Wilson 1992), to approximate non-Gaussian turbulence as Gaussian. We now consider whether smooth-wall reflection is acceptable for Gaussian inhomogeneous turbulence, noting that de Baas et al. (1986) have given an appealingly simple (but not rigorous) argument that smooth-wall (in their terminology, "perfect") reflection requires the velocity pdf near the boundary to have the property that odd moments vanish and even moments are constant.

Dispersion in the horizontally homogeneous, neutrally stratified atmospheric surface layer (NSL) is well modeled by assuming a height-independent Gaussian velocity pdf $g_a(w)$ with $\sigma_w \approx 1.3u_*$, and a time scale $\tau \propto z/\sigma_w$ (inhomogeneity arises solely through $\tau$). We were unable to integrate analytically the Chapman–Kolmogorov equation for this case, so we integrated numerically over a single time step. We specified that the tracer be well mixed initially over the range 0.1–5 m, and that $\tau = 0.5z/\sigma_w$. We used time step $\Delta t = 0.01$ s, which is less than a tenth of the smallest value taken on by $\tau$ within the system, $\tau(z_R)$. At the lower boundary the well mixed condition was satisfied to within 1%; while at $z = 2.5$ m differences with respect to the initial pdf occurred only in the fourth or fifth significant figure. Thus from our consideration of the CK equation, we see no problem with using smooth-wall reflection to bound "NSL" turbulence.

On the other hand, random flight simulations using smooth-wall reflection visibly violate the wmc, unless $\mu = \Delta t/\tau$ is very small. It is shown in the Appendix that this error is probably caused not by the reflection algorithm, but rather by the discretization of the asymptotically well-mixed model [Eq. (4)]; specifically, the cause is a bias in the random flight model due to using a finite, height-varying time step $\Delta t(z) = \mu\tau(z)$. As $\mu$ (thus the time step) is reduced, this "$\Delta t$ bias error" decreases, and a well-mixed release condition is more closely retained (though as $\mu$ decreases there is no reduction in the frequency of occurrence of reflection, because with $\sigma_w$ constant the boundaries remain attainable).

For a sufficiently small time step, then, smooth-wall reflection in conjunction with the RF model (Eq. 4) satisfies the well-mixed condition for Gaussian turbulence that is inhomogeneous only in its time scale. It seems probable (though is not proven) that the need for small $\Delta t/\tau$ is mandated by the RF model itself [Eq. (4)] through the Chapman–Kolmogorov condition (Appendix), rather than being a requirement for valid use of smooth-wall reflection. Since we cannot give an analytical solution to the CK equation, we are unable to state with certainty that smooth-wall reflection is exact, though we expect it is, given the height independence of $g_a(w)$ in this system. On the other hand, we found that imposing "artificial unattainability" (section 3) of the plane $z = z_0$ resulted in gross violation of the wmc.

What about application of smooth-wall reflection in the more general case of a Gaussian velocity pdf having height-dependent variance? In the context of the atmosphere, it will normally be reasonable to assume that the gradient in velocity variance $\partial\sigma_w^2/\partial z$ vanishes within approximately one length scale of ground (the normal assumption in simulating dispersion over a rough surface; we parameterize the UBL by setting $\sigma_w$ constant and $\tau \to 0$). With that proviso, anticipated by de Baas et al., smooth-wall reflection at ground will suffice in Gaussian turbulence.

## 8. Reflective boundaries for skewed turbulence

We begin this section by querying whether *any* reflection algorithm can rigorously satisfy our expanded wmc, when used to reflect particles at a (computational) boundary where the turbulence is skewed. The following argument suggests not.

Consider an arbitrary Eulerian velocity pdf $g_a(z, w)$ in the bounded flow domain $z \geqslant 0$. Suppose at $t = 0$ we have a well-mixed distribution of tracer, and that we calculate trajectories out to some small time $t = \Delta t$ with a well-mixed LS model, supplemented by a correct reflection scheme. Then the state at time $\Delta t$ is well mixed. Let $\epsilon > 0$ be some infinitesimal length. Particles that arrive at $\epsilon$ from initial position $z_0$ either had velocity $w_0 = -(z_0 - \epsilon)/\Delta t$ (no reflection) or $w_0 = -(z_0 + \epsilon)/\Delta t$. The state at $\Delta t$ is

$$g_a(\epsilon, w) = \frac{1}{\Delta t}\int_{z_0=0}^{\infty} p_w^R\left(w, \Delta t\left| -\frac{\epsilon + z_0}{\Delta t}, 0\right.\right) \times g_a\left(z_0, -\frac{\epsilon + z_0}{\Delta t}\right)dz_0 + \frac{1}{\Delta t}\int_{z_0=0}^{\infty} p_w\left(w, \Delta t\left|\frac{\epsilon - z_0}{\Delta t}, 0\right.\right) g_a\left(z_0, \frac{\epsilon - z_0}{\Delta t}\right)dz_0,$$

where $p_w$ is the transition density for velocity, and the superscript $R$ denotes the reflection path.

Now integrate both sides over all $w$, noting that $p_w$ and $p_w^R$ (which contain all the information about the hypothetical correct reflection scheme) have unit area

$$\int_{-\infty}^{\infty} g_a(\epsilon, w)dw = \frac{1}{\Delta t}\int_{z_0=0}^{\infty}\left[g_a\left(z_0, \frac{\epsilon - z_0}{\Delta t}\right) + g_a\left(z_0, -\frac{\epsilon + z_0}{\Delta t}\right)\right]dz_0.$$

Letting $\epsilon \to 0$, we have

$$1 = 2\int_{-\infty}^{0} g_a(-w'\Delta t, w')dw'. \qquad (6)$$

This can only be true if $g_a$ is symmetric in the velocity, and independent of height over a distance above the boundary that much exceeds $\sigma_w\Delta t$. Thus we anticipate that *no* reflection scheme can be correct (consistent with the well-mixed constraint) if it is applied at a boundary where the turbulence is skewed, or locally inhomogeneous.

We next show that smooth-wall reflection is certainly incorrect in skew turbulence. Following Baerentsen and Berkowicz (1984), we may form a skewed velocity pdf:

$$g_a(z, w) = A(z)G_A(z, w) + B(z)G_B(z, w), \qquad (7)$$

where $G_A$ and $G_B$ are Gaussians having nonzero means. According to Quintarelli (1990) this may be contrived to fit observed vertical velocity distributions in the convective boundary layer (CBL) quite well, and it has formed the basis for random-flight simulations of the CBL by Baerentsen and Berkowicz (1984), Luhar and Britter (1989; hereafter LB), and Weil (1990). Details for fitting Eq. (7) are given by these authors.

Corresponding to this specification of the Eulerian vertical velocity pdf, there is again a unique well mixed model for motion along that dimension. Rather than write down this model, for which the coefficient $a(z, w)$ is rather complicated even in the homogeneous case, we refer the reader to Luhar and Britter.

We examine the homogeneous case, and specify $\overline{w^2} = 0.5$, $\overline{w^3} = 1.0$, and $\tau = 1.0$. A single particle is released at $t = 0$ with a random vertical velocity (chosen from the specified skewed pdf) at a random height in the range (0, 1). We impose smooth-wall reflection at $z = 0, 1$. Figure 2a gives the concentration (pdf for position) at $t = 1.0$ according to two independent simulations, using on the one hand the random-flight method, and on the other, repeated integration of the Chapman–Kolmogorov equation (2); in both cases $\Delta t = 0.1$. Bearing in mind that for a finite number of trajectories the random-flight simulation gives only an estimate of the ensemble parameters, the two methods agree satisfactorily (as indeed they must).

The agreement of these two simulations merely demonstrates that the transition probability corresponding to the LS model has been correctly formulated, and the CK equation solved accurately. What is of greater interest in Fig. 2a is that, as anticipated by our earlier reasoning, the well-mixed condition has been violated. Since the LS model is "well mixed" in an unbounded domain, this failure can only be due to the reflection scheme.

Figure 2b, from the CK simulation, shows that the velocity pdf's near the walls at $t = 1$ differ grossly from the correct pdf $g_a$. We interpret the unmixed concentration profile as follows. Since $Sk_w > 0$, the mean *downward* velocity,

$$w\downarrow = \int_{-\infty}^{0} g_a(w)dw,$$

has a smaller magnitude than the mean upward velocity,

$$w\uparrow = \int_{0}^{\infty} g_a(w)dw,$$

yet zero mean velocity results because downdrafts predominate statistically. When smooth-wall reflection is used at $z = 0$, each arrival velocity $w^-$ is mapped to departure velocity $w^+ = -w^-$, and thus $w^+$ occurs with probability density $g_a(w^-)$ rather than $g_a(w^+)$. The resulting velocity pdf near the wall is more nearly symmetric than the proper (skewed) distribution $g_a(w)$, as can be seen in Fig. 2b. The result of this distortion

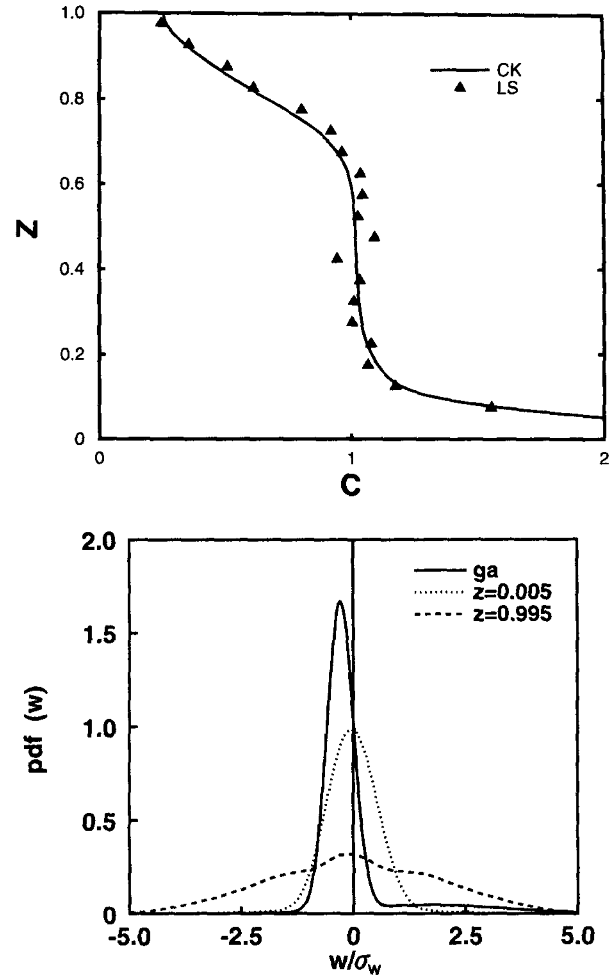


FIG. 2. Application of smooth-wall reflection in one-dimensional skew homogeneous turbulence with velocity statistics $\overline{w^2} = 0.5$, $\overline{w^3} = 1.0$, $\tau = 1$. Initial state well mixed, underlying LS model for skew turbulence that of Luhar and Britter (1989). Time step for calculations (random flight and Chapman–Kolmogorov) was $\Delta t = 0.1$. Numerical integration of CK equation with $w \in (-5\sigma_w, 5\sigma_w)$, $\Delta w = 0.05\sigma_w$, $\Delta z = 0.01$. (a) Density profile at $t = 1.0$ (calculated both by random-flight method and by integrating the CK equation), showing decay of the initially well-mixed state. (b) Comparison of pdf of $w$ at $t = 1.0$ with correct (well mixed) pdf, $g_a(w)$, showing that the pdf is distorted throughout the flow domain. Note the increased symmetry of the distorted pdf's.

is that the mean upward velocity near $z = 0$ is too small, causing surplus concentration at the wall. The opposite argument applies at the top boundary. Smooth-wall reflection, applied at a location where the pdf of the normal velocity is skewed, is incorrect.

We have reasoned that there is no rigorous reflection algorithm to bound skewed and/or inhomogeneous turbulence. However, that fact does not prohibit the existence of reflection algorithms that, for suitably small (but finite) $\Delta t$, are acceptable in practice. Unfortunately, we are unable to make any general statement about the magnitude of errors that are liable to result from invalid reflection rules; there are simply too many factors: the nature of the turbulence profiles near the wall, the source location, etc. To illustrate these factors we will look at the behavior of the error that arises from using perfect reflection in the doubly bounded domain (reflection at $z = 0, L$) of homogeneous skew turbulence considered above.

We again use the well-mixed initial condition, eliminating release height as a factor in the reflection error. Then if we define $C^*$ to be the correct concentration $(1/L)$, that is, that which would be observed if the reflection scheme caused no error, then on the basis of a dimensional analysis the functional dependence of the fractional error is

$$\frac{C - C^*}{C^*} = F\left[\frac{t}{L/\sigma_w}, \frac{\overline{w^3}}{\sigma_w^3}, \frac{\Delta t}{\tau}, \frac{\tau}{L/\sigma_w}\right].$$

For the present system it is found that for sufficiently large $t$ the concentration error approaches a steady state (Fig. 3). The steady-state fractional error is larger, and is achieved more slowly, when the domain size is increased relative to the turbulent length scale. This suggests that the existence of a bound to the reflection-induced error is a consequence of complementary reflection errors (as discussed above) at the two walls, rather than inherent self-compensation of the error. This is significant, because when we first noted the steady-state limit, we suspected self-compensation might be arising by the mechanism that the very invalidity of the perfect reflection rule results in some particles near the wall (those that have been reflected) having a velocity pdf that is closer to being symmetric than would otherwise be the case, and for which consequently the reflection rule is closer to being valid.

We found that the steady-state reflection error in the present simple system depends linearly on skewness Sk (rather than on $\mathrm{Sk}^{1/3}$). We also noted a dependence of the steady-state error on $\Delta t/\tau$, which is surprising, because in homogeneous turbulence the velocity pdf of hitting particles does not vary with the distance from which they arrive, nor does the frequency of occurrence of reflection per unit time change with $\Delta t$.

We believe that, in general, there is no asymptotic limit to the reflection error, but that at any time the magnitude of the error, as well as depending on release position and flow properties, will depend upon the skewness of the Eulerian velocity pdf at the mean position of occupancy of particles immediately preceding the distance step that brings them to the boundary. A similar situation must obtain with respect to inhomogeneity in velocity variance. Considering the infinity of possible selections of turbulence profiles near a boundary, we can give no general quantitative bound to the reflection error that might arise.

We have noted that the nonexistence of an exact reflection scheme for the case of skew turbulence does not prevent the existence of schemes that are better than perfect reflection. We end this section by comparing results using perfect reflection with results of a

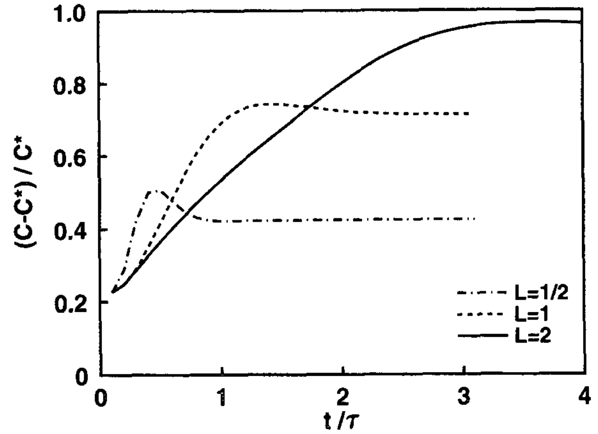


FIG. 3. Evolution of the fractional error in near-boundary concentration caused by using smooth-wall reflection at $z = (0, L)$ to bound a domain of homogeneous skew turbulence. Turbulence properties $\sigma_w = \mathrm{Sk}_w = \tau = 1$, time step $\Delta t = 0.1$, several values of domain depth $L$.

scheme proposed for homogeneous skewed turbulence by Weil (1990).

Suppose a particle crosses $z = 0$ with velocity $w^-$. Then under Weil's scheme it is reflected with velocity $w^+$ as defined implicitly by

$$\frac{\int_{w^-}^{0} g_a(w)dw}{\int_{-\infty}^{0} g_a(w)dw} = \frac{\int_{0}^{w^+} g_a(w)dw}{\int_{0}^{\infty} g_a(w)dw}.$$

We tested Weil's algorithm in homogeneous skewed turbulence in the domain $z \geq 0$, using a simplification of the Luhar–Britter model to the homogeneous case. The scales of motion were specified to be $\sigma_w = 1$, $\mathrm{Sk}_w = 1$, $\tau = 1$. We numerically integrated the Chapman–Kolmogorov equation over a single time step $\Delta t = 0.1$, to obtain the state function $p(z, w, \Delta t)$ for an initially well mixed distribution. Our velocity discretization was $(-5\sigma_w \leq w \leq 5\sigma_w, \Delta w = 0.01\sigma_w)$. Since we were interested in $p(z, w, \Delta t)$ very close to $z = 0$, we limited the height integration to contributions from initial heights $z_0 \leq 5\sigma_w\tau$, using resolution $\Delta z_0 = 0.01$.

Both Weil's scheme and perfect reflection gave incorrect density and velocity pdf (Fig. 4) at the wall after only a single time step. The irregularity of our calculated pdf for the Weil scheme is due to imperfect numerical integration of the CK equation. We do, however, feel confident that the velocity pdf exhibited by a population of particles in a random-flight model would be a smoothed version of what we have calculated, so we believe that Weil's reflection scheme, though not correct, does a better job of retaining the proper pdf asymmetry than does the smooth-wall reflection scheme.

## 9. Bounding the convective boundary layer

In the CBL, $g_a(w)$ is inhomogeneous and skewed. Therefore CBL dispersion models using reflection to

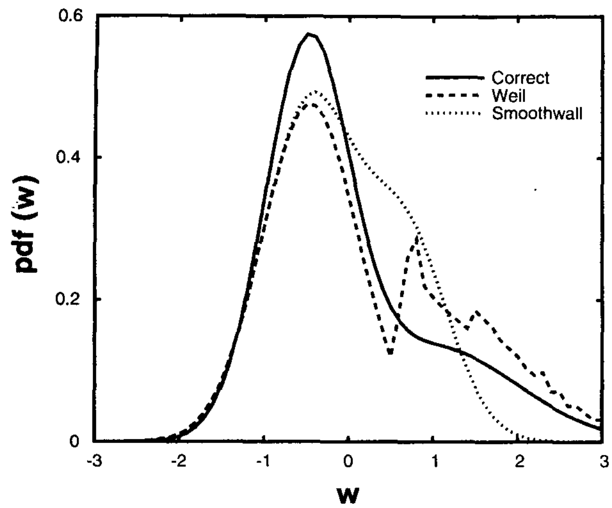


FIG. 4. Erroneous normal velocity pdf's at $z = 0.005$ resulting from application at $z = 0$ of smooth-wall reflection or of Weil's reflection scheme for skew turbulence. Homogeneous skew turbulence, with $\sigma_w = \mathrm{Sk}_w = \tau = 1$. Integration of the CK equation from an initially well mixed state to $t = 0.1$, using $w \in (-5, 5)$, $\Delta w = 0.01$, $\Delta z = 0.002$. Final pdf's block averaged over $\delta w = \pm 0.1$.

bound the particle domain will only satisfy the wmc if profiles of the velocity moments, time scale, and time step are appropriately tailored at the boundaries. In this section we examine how particles are confined to the flow domain in two recently reported random-flight models of the CBL.

Luhar and Britter (1989; hereafter LB) and Weil (1990) both presented random flight simulations of dispersion from sources in the CBL, using essentially the same well mixed (as $\Delta t \rightarrow 0$) model, and with perfect reflection at $z = 0$ and at the top of the boundary-layer $z = \delta$. Their parameterizations for the turbulence statistics differed markedly near the boundaries. In both cases $\langle w^3 \rangle$ vanished at $z = (0, \delta)$, but LB used $\mathrm{Sk}_w = 0.8$ (for all $z$), while Weil's parameterization had $\mathrm{Sk}_w = 0$ at the boundaries due to nonzero $\langle w^2 \rangle$ at those points. LB did not resolve a surface layer, but imposed at $z = 0$ (and $z = \delta$) vanishing $\sigma_w$ and $\tau$ and a very large gradient $\partial \sigma_w / \partial z$. In our LB simulation (see below) with $\Delta t / \tau = 0.001$, no particles crossed the boundaries (reflection never occurred; presumably this was fortunate, since with drastic inhomogeneity of the velocity pdf near the boundary, perfect reflection is incorrect). In contrast to the LB parameterization, Weil's gave the semblance of a normal surface layer near ground ($\sigma_w = 1.3 u_*$, and a small and linearly increasing length scale), and *required* a reflection algorithm no matter how small $\Delta t$ (reducing $\Delta t / \tau$ did not reduce the frequency of occurrence of reflection).

Using these models, we calculated the evolution of an initially well mixed distribution of particles (Fig. 5). In both cases, the well-mixed distribution was retained for a sufficiently small choice of the time step. With the LB model, because of the infinite gradient in velocity scale at $z = (0, \delta)$, inadmissable velocities (exceeding $\delta / \Delta t$) sometimes occurred unless $\Delta t \ll 0.1\, \tau(z)$, a stronger limitation than expected. Luhar and Britter used a much larger (and constant) time step $\Delta t = (0.01, 0.02, 0.05) \delta / w_*$ exceeding $\tau(z)$ near boundaries and imposed a numerical constraint $g_a(w) \geq g_{\min}$ to prevent unrealistic velocities (A. Luhar 1992, personal communication).

There is no way to tell whether the unmixed profiles that result when $\Delta t / \tau$ is only moderately small [e.g., 0.1, which value in homogeneous turbulence would result in discretization errors of less than about 2%; Wilson and Zhuang (1989)] result principally from reflections (in both cases reflection is less valid with increasing $\Delta t$), or from the size per se of the time step in relation to the inhomogeneity of the velocity statistics. Perhaps the very question is meaningless. What is certain is that for one reason or the other (reflection—strong inhomogeneity) the time step needs to be very small [in relation to $\tau(z)$] in both parameterizations, even though "inhomogeneity time scales" such as

$$\tau_*^v = \left( \sigma_w \frac{\partial \ln \overline{w^2}}{\partial z} \right)^{-1}, \quad \tau_*^{\mathrm{Sk}} = \left( \sigma_w \frac{\partial \ln \overline{w^3}}{\partial z} \right)^{-1}$$

are not substantially smaller than $\tau$. Computation time for the LB scheme, due to its vanishing $\sigma_w$ and $\tau$ at 0, $\delta$ (unattainable boundary for small-enough $\Delta t$), is much longer than for the Weil scheme.

Thus in both models, boundaries have been successfully imposed (i.e., in such a way as to preserve the well-mixed property of the random flight algorithms). In the case of the LB model (which has here been im-

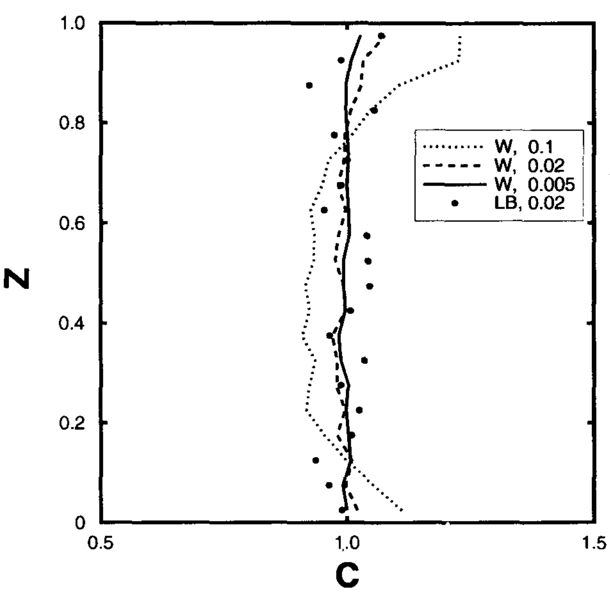


FIG. 5. Random flight simulations of the evolution of an initially well mixed concentration profile ($C = 1$) in the convective boundary layer. Profiles at $t = \delta / w_*$ according to the Weil (W) and Luhar–Britter (LB) models. Legend gives $\Delta t / \tau$.

plemented so as to make $\Delta t/\tau$ everywhere small), confinement resulted from making the boundaries unattainable (reflection, which would be invalid, did not occur). On the other hand Weil's near-wall flow statistics are such that, though reflection did occur, it was applied to particles coming from such close proximity to the boundary that neither inhomogeneity nor skewness in that shallow region compromised excessively the use of perfect reflection.

## 10. Conclusions

One way to test whether a discrete-time (i.e., practicable) Lagrangian stochastic model obeys the well-mixed criterion is to simply calculate the evolution of an initially well mixed particle distribution. We have shown that it can be a useful alternative to formulate that test probabilistically, using the Chapman–Kolmogorov equation to calculate the evolution of the particle position–velocity distribution. This requires construction of the transition density corresponding to a chosen LS model, by steps that we have demonstrated, and our approach results in a novel expression of the wmc that shows that if an LS model (for stationary flow) is to fail the wmc, it must do so on the first time step.

In this framework, which we believe is uniquely appropriate to the task, we have examined the device of particle reflection. We have proven that perfect reflection is in restricted circumstances rigorous, but that where it fails, no alternative and rigorous reflection scheme exists. This is not to say there are not schemes that are *better* than perfect reflection, and that for suitably limited time steps might be acceptable in practice; indeed, Weil's scheme for reflection in skew homogeneous turbulence performs better than smooth-wall reflection for that case.

Imposing an unattainable boundary (i.e., incorporating realistic profiles of velocity statistics right to the boundary) may require a prohibitively small time step, whereas trajectory reflection is an efficient means to bound the particle domain. We have noted that velocity statistics at true boundaries (e.g., the ground) are unknown, since there is *always* an unresolved basal layer (UBL) implicit in atmospheric simulations. Therefore one is free to design profiles of velocity statistics (and the time step) that legitimize the reflection algorithm.

What is required, if reflection is to be used, is that the velocity pdf be both symmetric about $w = 0$, and height independent over the largest distance (from the boundary) that might be traversed by a particle during the step over which reflection occurs. Assuming skewness vanishes at the boundaries, the simplest approach is to make the time step as small as necessary to satisfy the wmc. Alternatively, one might place at ground a homogeneous Gaussian layer (spanning $z = 0$ to $z = \lambda$, say) whose time scale and velocity scale ensure that any reflected particle makes at least one stop (at $z < \lambda$) on its way to and from ground. An objection at once occurs: the required profiles may necessitate the tiny time step one hoped to avoid.

*Acknowledgments.* We thank Dr. A. K. Luhar for providing details of the simulations reported by Luhar and Britter (1989). JDW acknowledges support from NSERC and AES/Environment Canada.

## APPENDIX

### Discretization Error Due to Turbulence Inhomogeneity

Gillespie (1992) has analyzed formally the discretization error resulting from "noninfinitesmal" approximation of a continuous Markov process. Consider a one-dimensional Langevin equation for the vertical motion of a particle:

$$dw = A(z, w)dt + B(z)\sqrt{dt}N$$
$$dz = (w + dw)dt,$$

where $N$ is a Gaussian random number (mean zero, unit variance). Gillespie requires that the noninfinitesmal model should satisfy the "Chapman–Kolmogorov condition,"

$$dw(t, t+\Delta t) = dw(t, t + a\Delta t) + dw[t + a\Delta t, t + a\Delta t + (1 - a)\Delta t],$$

where $0 \leqslant a \leqslant 1$ and the notation $dw(t, t + \Delta t)$ indicates the increment in $w$ over interval $(t, t + \Delta t)$. Substituting the Langevin equation into this condition, then expanding $A$ and $B$ in their Taylor series (truncated at first order), and conservatively simplifying, one obtains the following restrictions on the magnitude of the time step $\Delta t$, due to inhomogeneity:

$$|\partial_z A|\Delta t^2 < \epsilon, \quad |\partial_z B|\Delta t^{3/2} < \epsilon, \quad |\partial_w A|\Delta t < \epsilon,$$
$$|w\partial_z(\ln A)|\,dt < \epsilon, \quad |wA^{-1}\partial_z B|\,dt^{1/2} < \epsilon,$$

where $0 \leqslant \epsilon \ll 1$.

### *a. Application to the neutral surface layer (NSL)*

In the usual treatment of dispersion in the horizontally uniform NSL, inhomogeneity arises solely through a height-dependent decorrelation time scale, $\tau = \beta z/\sigma_w$ (best agreement of random flight simulations with experimental data is obtained with $\beta \approx 0.5$, Wilson et al. 1981). Gillespie's analysis, applied to the well-mixed model [Eq. (4)], $A = -w/\tau$ and $B = (2\sigma_w^2/\tau)^{1/2}$, requires a time step satisfying

$$\frac{\Delta t}{\tau} \leqslant \min\left[\epsilon, \left(\frac{\epsilon\sigma_w}{|w|\beta}\right)^{1/2}, \frac{\epsilon\sigma_w}{|w|\beta}, \frac{\sqrt{2}\epsilon}{\beta}, \frac{2\epsilon^2}{\beta^2}\right],$$

where $\epsilon \ll 1$.

### *b. Unmixed concentration profile in NSL due to discretization*

How small $\epsilon$ actually needs to be depends how large a departure from an initially well-mixed concentration

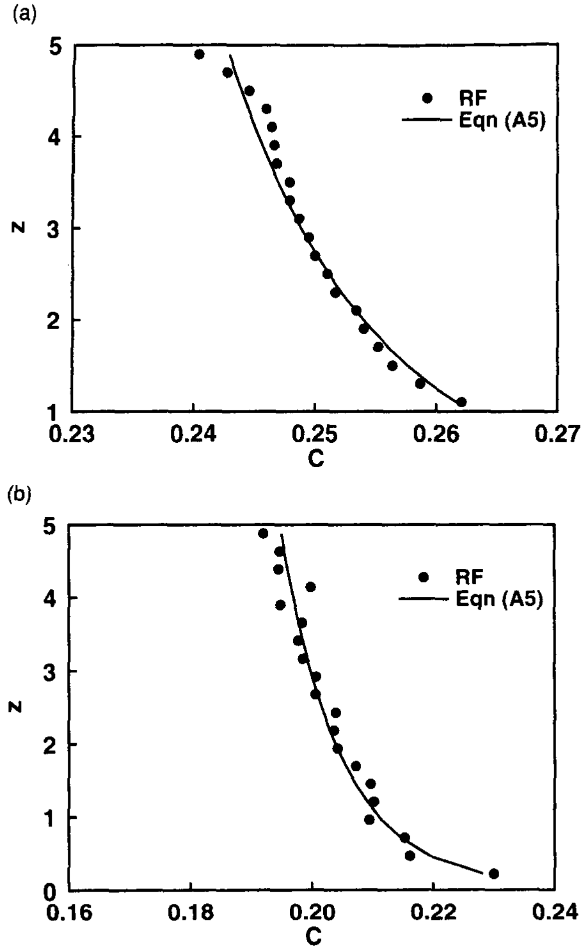


FIG. A1. Violation of the well-mixed condition by an asymptotically well mixed random flight model [Eq. (4)], due to a finite, biased time step. Evolution of an initially well mixed concentration profile $C = C^* = (\mathrm{ZT} - \mathrm{ZB})^{-1}$ in the neutral surface layer, with perfect reflection at (ZB, ZT). Time step $\Delta t = 0.1\tau$ ($\mu = 0.1$), time scale $\tau = 0.5z/\sigma_w$, $u_* = 0.3$ m s$^{-1}$. RF concentration profile is compared with Eq. (A5), with $\alpha = 1/2$. (a) (ZB, ZT) = (1.0, 5.0) m, $C^* = 0.25$. Random-flight profile at $t = 10$ s. Discrepancy between RF and Eq. (A5) near the top boundary is probably a near-field effect, not accounted for in Eq. (A5), whose derivation assumes a far field diffusivity. (b) (ZB, ZT) = (0.1, 5.0) m, $C^* = 0.204$. Random-flight profile at $t = 100$ s. Agreement of the RF profile with Eq. (A5) strongly suggests the violation of the wmc is due to $\Delta t$ bias error, and not a consequence of the smooth-wall reflection algorithm.

field we regard as significant. For present purposes, we do not want to spuriously conclude that a reflection algorithm is to blame, if there arises a violation of the wmc due to failure to impose the above conditions sufficiently rigorously. It will help in this regard if we can anticipate the form taken by any violation of the wmc due to a too large time step.

Whenever a finite time step $\Delta t(z) = \mu\tau(z)$ is employed in an RF model in a region where $\partial\tau/\partial z$ is nonzero, a model bias arises. Suppose $\partial\tau/\partial z > 0$, as in the NSL. At location $z_1$ a time step $\mu\tau(z_1)$ is chosen, and the particle moves from $z_1$ to $z_2$. Then for upward-moving particles ($z_2 > z_1$), the time step $\mu\tau(z_1)$ is smaller than the average of $\mu\tau(z)$ along the step $z_2 - z_1$. The opposite is true for downward-moving particles; thus the bias.

A typical value for $z_2 - z_1$ is $\sigma_w\Delta t$, so we can estimate the bias in time step as

$$\Delta t\!\downarrow - \Delta t\!\uparrow \approx \sigma_w \Delta t \frac{\partial(\Delta t)}{\partial z}. \tag{A1}$$

In the NSL, $\tau = \beta z/\sigma_w$. It follows that (assuming equality in the above approximation)

$$\frac{\Delta t\!\downarrow - \Delta t\!\uparrow}{\Delta t} = \mu\beta, \tag{A2}$$

which has the necessary property of vanishing as either $\mu$ or $\beta$ vanish. The consequence of this biased time step is that when we consider an ensemble of many trajectories, a velocity bias arises, its value in the case of the NSL being $w_B = -\alpha\mu\beta\sigma_w$, where $\alpha$ is expected to be of order 1 (from Fig. A1 we conclude $\alpha = 1/2$). This bias is not to be considered as acting causally at any instant in the trajectory of a single particle, but rather as arising in the sense of a law of large numbers.

Now if we start from a well-mixed initial condition and calculate the paths of many particles in a bounded region of the NSL, this bias will cause violation of the wmc. At large times after release, we can expect that a steady-state error will exist such that diffusion along the erroneous concentration gradient will balance the bias flux $w_BC$:

$$w_B C - K\frac{\partial C}{\partial z} = 0. \tag{A3}$$

In the NSL, $K = \sigma_w^2\tau = \beta\sigma_w z$, and it follows that

$$\frac{\partial \ln C}{\partial \ln z} = -\alpha\mu. \tag{A4}$$

Assuming the domain is bounded at $z_T$ and $z_B$ and that the total mass is 1 [so that the well-mixed concentration is $C^* = 1/(z_T - z_B)$], we expect the long-time unmixed concentration profile, arising from the time step bias, to be approximately

$$C(z) = \frac{1 - \alpha\mu}{z_T^{1-\alpha\mu} - z_B^{1-\alpha\mu}} \frac{1}{z^{1-\alpha\mu}}. \tag{A5}$$

Figure A1 shows the outcome of random-flight simulations [asymptotically well mixed LS model, Eq. (4)] of the dispersion of initially well-mixed particles in the NSL, using smooth-wall reflection to bound the domain. Equation (A5) (with $\alpha = 1/2$) agrees so closely with the unmixed concentration profiles of the RF model, that we conclude the RF error is "$\Delta t$ bias error," and not a consequence of the reflection algorithm. The bias velocity causing violation of the wmc in Fig. A1 is small, $w_B/\sigma_w = -0.025$.

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