THE WELL-MIXED CONSTRAINT APPLIED TO RANDOM FLIGHT MODELS WITH REFLECTING BOUNDARIES

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1. INTRODUCTION

How should the ground be treated in random flight dispersion models? Rather than specify velocity statistics that prohibit particles from crossing $z = 0$, one usually introduces trajectory reflection, which, along with the finite timestep of the model, is not accounted for by Thomson's (1987) well-mixed constraint (w.m.c.). We will here express the w.m.c. in a discrete-time framework whose scope incorporates reflection. We show that no reflection algorithm can satisfy the w.m.c. when applied at a boundary where the probability density function is asymmetric in w, or locally inhomogeneous.

2. THE WELL-MIXED CONSTRAINT

The height (z) and velocity (w) of a tracer particle may be represented as a moving point in z-w space. The trajectory of the point (z,w) for an individual realization is stochastic, but by considering an ensemble of realizations, we may define a probability density function p(z,w,t), whose evolution is given by the Chapman-Kolmogorov (CK) equation (van Kampen, 1981):

$$p(z_2,w_2,t_2) = \int_\Omega p(z_2,w_2,t_2 \mid z_1,w_1,t_1)\ p(z_1,w_1,t_1)\ dz_1\ dw_1 \tag{1}$$

where Ω is the domain accessible to the particle, and $p(z_2,w_2,t_2 \mid z_1,w_1,t_1)$ is the transition density corresponding to the trajectory model (and any reflection scheme). Assuming stationarity, the transition density depends on $t_2 - t_1$, but not t_1.

Thomson's (1987) well-mixed constraint states that a trajectory model should have the property that passive tracer particles initially well-mixed in the flow (with respect to both position and velocity) must remain so. Assuming stationarity, constant fluid density, and denoting by $g_a(z,w)$ the Eulerian velocity pdf, the w.m.c. requires that the model (i.e. transition density) satisfies (for a suitably restricted timestep Δt):

$$g_a(z,w) = \int_\Omega p(z,w,\Delta t \mid z_0,w_0,0)\ g_a(z_0,w_0)\ dz_0\ dw_0 \tag{2}$$

This is true because, if the model is to fail the w.m.c., it must do so on the first time increment: if $p(z,w,\Delta t) = g_a(z,w)$, then $p(z,w,t) = g_a(z,w)$ for all t. Thus expressed, the well-mixed constraint is the criterion for a discrete-time Lagrangian stochastic model, including its reflection procedure; but it does not (alone) yield a unique solution for the transition density. Any reflection scheme results in non-equivalence of model and real time.

3. THE TRANSITION DENSITY

A suitable model for the increments in velocity and position is (Thomson, 1987): $dw = a(z,w,t)\ dt + b\ d\xi$, $dz = w\ dt$; where the $d\xi$ are independent and random, and have the Gaussian distribution with mean 0 and variance dt. We use this with finite increments Δt, etc., and add the specification $\Delta t << \tau$, where τ is the shortest significant timescale.

Suppose a particle goes from (z_0,w_0,t) to a subsequent disallowed state $(z^*,w^*,t+\Delta t)$, where $z^* < 0$. Then, under "perfect" or "smooth wall" reflection we correct the disallowed state $z^* < 0$ at $t + \Delta t$ by placing the particle in the state $(-z^*,-w^*, t+\Delta t)$. Introducing a unit step function C(z,w) that vanishes unless $w < -z/\Delta t$ we obtain a complete model algorithm:

$$\Delta w = a(z,w,t)\ \Delta t\ (1-2C) - 2Cw + b\ (1-2C)\ \Delta\xi, \qquad \Delta z = w\ \Delta t\ (1-2C) - 2Cz.$$

The corresponding transition density for position is $p_z(z,t+\Delta t \mid z_0,w_0,t) = \delta(z - z_0, w_0\Delta t\ (1-2C) - 2Cz)$, and, the transition density for velocity is:

$$p_w(w,t+\Delta t \mid z_0,w_0,t) = \frac{1}{\sqrt{2\pi}\ b\ \sqrt{\Delta t}} \exp\left[-\frac{(w - w_0 - a(z_0,w_0,t)\Delta t(1-2C) + 2Cw_0)^2}{2\ b^2\ \Delta t}\right]$$

The full transition density is $p = p_z p_w$. The evolution of $p(z,w,t)$ obtained by repeated integration of the CK Eq. (1) must, except as regards truncation- or stability-error (in numerical integration), equal the ensemble-mean evolution of the random flights.

4. GAUSSIAN TURBULENCE

The well-mixed one-dimensional model for stationary Gaussian turbulence is (Thomson, 1987):

$$dw = \frac{-w}{\tau(z)}\,dt + \frac{1}{2}\frac{\partial\sigma_w^2}{\partial z}\left(1 + \frac{w^2}{\sigma_w^2}\right) + b\,d\xi\,, \qquad b = \sqrt{\frac{2\,\sigma_w^2}{\tau}} \tag{3}$$

where τ is the decorrelation timescale. 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). But is it exactly well-mixed?

In the unbounded homogeneous case, it can easily be shown that the finite-increment model satisfies the w.m.c. provided $b^2 = \sigma_w^2/\Delta t(1-(1-\Delta t/\tau)^2)$. If $\Delta t \ll \tau$, this distinction regarding b is not important.

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 timestep $\Delta t \ll \tau$, the state $p(z,w,\Delta t)$ is still the well-mixed state. Splitting the integral in Eq. (1) into contributions $w_1 \leqq -z_1/\Delta t$ and $w_1 > -z_1/\Delta t$, and writing the delta functions that occur in the transition density as $\delta(z-z_1,w_1\Delta t) = (1/\Delta t)\ \delta(w_1,(z-z_1)/\Delta t))$, etc., it is confirmed that with the above specification of b, $p(z,w,\Delta t) = g_a(w)$. Smoothwall reflection satisfies the w.m.c. in Gaussian homogeneous turbulence. (LS = Lagrangian stochastic.)

Dispersion in the neutral surface layer is well-modelled by assuming Gaussian inhomogeneous turbulence, with $\sigma_w = 1.3\ u_*$ (u_* the friction velocity) and $\tau \sim z/\sigma_w$. We were unable to integrate analytically the Chapman-Kolmogorov equation for this case, so we integrated numerically over a single timestep. 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 timestep $\Delta t = 0.01$ s, which is less than a tenth of the smallest value taken on by τ 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 4th or 5th significant figure. A random flight simulation to $t=5$, with $\Delta t/\tau = .1$, distinctly violated the w.m.c.; but with $\Delta t/\tau = 0.01$, deviations from the well-mixed profile were of the order of the standard error, thus probably not significant. Reducing the time-step did not reduce the probability of reflection, because with σ_w constant, the boundaries remain attainable.

What about the general Gaussian case? It will normally be reasonable to assume the gradient in velocity variance $\partial\sigma_w^2/\partial z$ vanishes within a few length scales of ground (the usual assumption in simulating dispersion over a rough surface). With that proviso, anticipated by de Baas et al. (1986), smooth-wall reflection at ground will suffice in Gaussian turbulence.

5. SKEW TURBULENCE

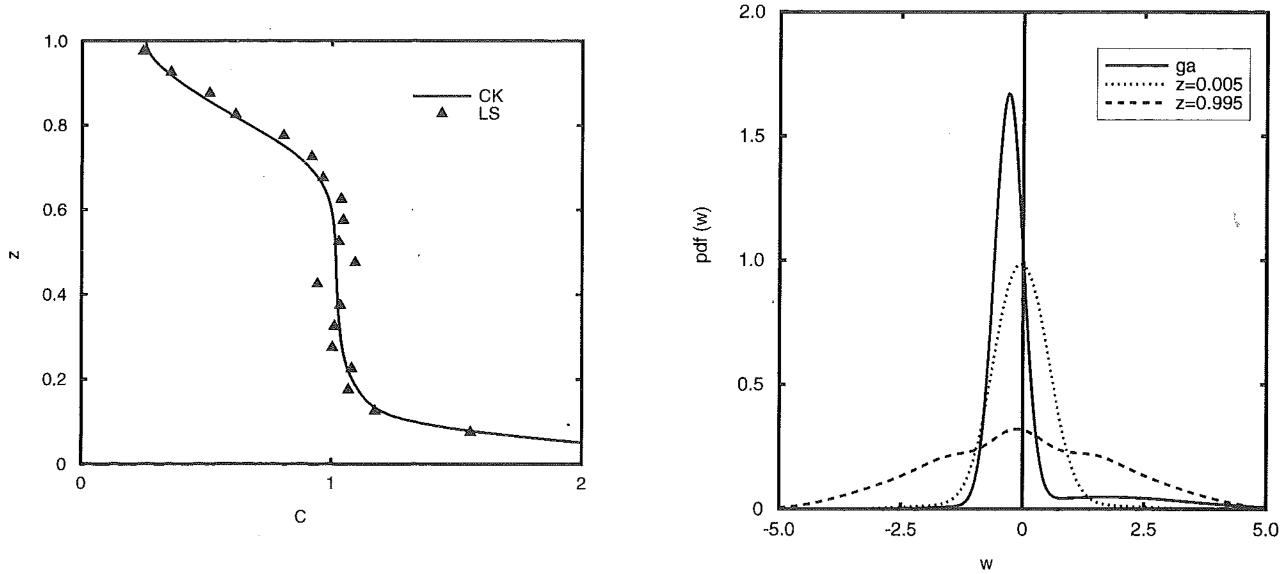
Following Baerentsen and Berkowicz (1984) we may form a skewed pdf, $g_a(z,w) = A(z)\ G_A(z,w) + B(z)\ G_B(z,w)$, where G_A and G_B are Gaussians having non-zero means. Corresponding to this is a unique well-mixed model for vertical motion, e.g. Luhar and Britter (1989).

We specify: $\overline{w^2} = 0.5$, $\overline{w^3} = 1.0$, $\tau = 1.0$. Suppose particles are released at $t=0$, with random (skew) vertical velocity, at a random height in the range (0,1). We impose smoothwall reflection at $z=0,1$. Figure (1a) gives the concentration 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 Eq. (1); in both cases $\Delta t = 0.1$.

The agreement of these two simulations merely demonstrates that the transition probability corresponding to the random flight model has been correctly formulated, and the CK equation solved accurately. What is of interest, is that the well-mixed condition has been violated. This can only be due to the reflection scheme. Figure (1b), from the CK simulation, shows that the velocity pdf's near the walls differ grossly from g_a.

Can any reflection scheme be satisfactory in skew turbulence? We think not. Consider an arbitrary Eulerian velocity pdf $g_a(z,w)$ in domain $z \geqq 0$. 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 Δt is well mixed. Let $\varepsilon > 0$ be some small length. Particles that arrive at ε from initial position z_o either had velocity $w_o = -(z_o-\varepsilon)/\Delta t$ (no reflection) or $w_o = -(z_o+\varepsilon)/\Delta t$. The state at $z=\varepsilon$, $t=\Delta t$ is:

$$g_a(\varepsilon,w) = \frac{1}{\Delta t}\int_{z_o=0}^{\infty}\left(p_w^R\left(w,\Delta t\ \Big|\ z_o, -\frac{\varepsilon+z_o}{\Delta t}, 0\right) g_a\left(z_o, -\frac{\varepsilon+z_o}{\Delta t}\right) + p_w\left(w,\Delta t\ \Big|\ z_o, \frac{\varepsilon-z_o}{\Delta t}, 0\right) g_a\left(z_o, \frac{\varepsilon-z_o}{\Delta t}\right)\right) dz_o$$



(1a) (1b)

Figure 1. Application of smoothwall reflection in one-dimensional skew homogeneous turbulence. 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). Timestep for calculations (random flight = LS and Chapman-Kolmogorov = CK) was $\Delta t = 0.1$. Numerical integration of CK equation with $w \in (-5\sigma_w, 5\sigma_w)$, $\Delta w = 0.05\sigma_w$, $\Delta z = 0.01$.
(1a) Density profile at $t = 1$ according to random flights and integration of the CK equation.
(1b) Comparison of pdf of w at $t = 1.0$ with $g_a(w)$. Note increased symmetry of the distorted pdf's.

where p_w is the transition density for velocity and superscript R denotes the reflection path. Now, integrating 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, and letting $\varepsilon \to 0$, we have:

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

This is true only if g_a has median zero, and is independent of height over a distance above $z = 0$ that much exceeds $\sigma_w \Delta t$. Thus no reflection scheme is correct (consistent with the well-mixed constraint) at a boundary where the turbulence is skew, or locally-inhomogeneous.

6. THE CONVECTIVE BOUNDARY-LAYER

In the CBL, $g_a(w)$ is inhomogeneous and skewed. Luhar and Britter (1989; hereafter LB) and Weil (1990) simulated dispersion from sources in the CBL, using essentially the same well-mixed 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, though in both cases skewness vanished at $0, \delta$. LB did not resolve a surface layer, but imposed at $z = 0$ (and $z = \delta$) vanishing σ_w and τ, and an infinite $\partial\sigma_w/\partial z$. Had $\partial\sigma_w/\partial z$ been finite at $0, \delta$ the LB scheme would have implied theoretically that boundaries were non-crossable, even with finite timestep, and indeed in our simulation (see below) with $\Delta t/\tau = 0.001$, no particles crossed the boundaries (reflection never occurred). On the other hand, Weil's parameterization gave a normal surface layer near ground ($\sigma_w = 1.3u_*$, and a small and linearly-increasing length scale) and requires a reflection algorithm, no matter how small Δt (reducing $\Delta t/\tau$ does not reduce the frequency of occurrence of reflection).

Using these models, we calculated the evolution of an initially well-mixed distribution of particles (Figure 2). In both cases, the well-mixed distribution was retained for a sufficiently small choice of the timestep. With the LB model, because of the infinite gradient in velocity scale at $z = 0$, inadmissible 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) timestep $\Delta t = (0.01, 0.02, 0.05)\delta/w_*$ exceeding $\tau(z)$ near boundaries, and imposed a numerical constraint $g_a(w) \geq g_{min}$ to prevent unrealistic velocities (A. Luhar, pers. commun.).

There is no way to tell whether the unmixed profiles that result when $\Delta t/\tau$ is only modestly small (e.g. 0.1) result principally from reflections (in both cases reflection is less valid with increasing Δt), or from the size per se of the timestep in relation to the inhomogeneity of the velocity statistics. Perhaps the very question is meaningless. What is certain is that for one reason or other (reflection - strong inhomogeneity), the timestep needs to be very small (in relation to $\tau(z)$, in both parameterizations. That implies a much longer computation time for the LB scheme, due to its vanishing σ_w and τ at $0, \delta$ (unattainable boundary).

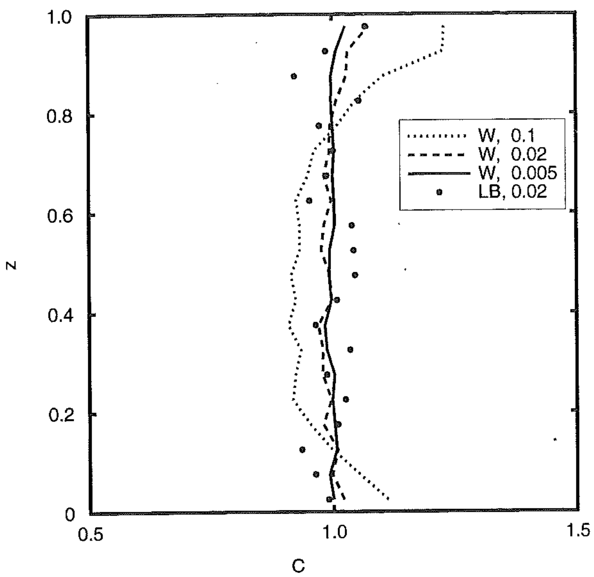


Figure 2. Random flight simulations of the evolution of an initially well-mixed concentration profile ($C = 1$) in the convective boundary layer. Profiles at $t = \delta/w_*$ according to the Weil (W) and Luhar-Britter (LB) models. Legend gives $\Delta t/\tau$.

7. DISCUSSION AND CONCLUSION

Trajectory reflection is an efficient means to bound the particle domain. And since there is always a layer at ground in which velocity statistics are unknown, one is free to design profiles of velocity statistics (and the timestep) that validate 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. Since w is stochastic, this is a complex criterion, and involves the timestep.

Assuming skewness vanishes at the boundaries, the simplest approach is to make the timestep as small as necessary to satisfy the w.m.c. Alternatively, one might place at ground a homogeneous Gaussian layer (spanning $z = 0$ to $z = \lambda$, say), and ensure by restriction of the timestep ($w\Delta t \geqq -z$ when $z > \lambda$ and $w < 0$) that no particle starting above λ can strike ground. The timescale and velocity scale specified within the homogeneous layer should ensure that any reflected particle makes at least one stop in the homogeneous layer on its way to and from ground. An objection at once occurs: the required profiles may necessitate the tiny timestep one hoped to avoid.

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