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A critical examination of the random displacement model of turbulent dispersion

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Abstract Although the random displacement model (RDM) represents the "diffusion limit" of the first-order Lagrangian stochastic (or "Langevin") model of turbulent dispersion, we show that these provide distinct (numerical) solutions even for the case of a ground-level source, where intuition might suggest their solutions converge (i.e., the "far-field" model would suffice). We also demonstrate (analytically) that the discrete RDM does not preserve an initially well-mixed particle distribution—though the well-mixed 'test state' can be preserved to within an arbitrarily small error, by reducing the timestep. From a comparison with reference calculations calibrated to Project Prairie Grass, we conclude that the RDM provides in practice an *adequate* description of far-field dispersion, and so justifiably could be used as a replacement for grid-based Eulerian methods in simulation of medium- and long-range transport. However there can be an important loss of accuracy (for the test case examined, at least) if the timestep is not strictly limited, and we recommend instead the (generalized) Langevin treatment.

Keywords Air pollution · Dispersion models · Eddy diffusion · Lagrangian stochastic models · Long-range transport · Random displacement model · Well-mixed condition

1 Introduction

The random displacement model (RDM) of particle trajectories in turbulent flow, also known as the zeroth-order Lagrangian stochastic (LS) model, is a grid-free method that in the limit of

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infinitesimal steps is equivalent (e.g., Durbin 1983) to the Eulerian eddy-diffusion treatment of turbulent dispersion, i.e., first-order closure, or 'K-theory'. Although it shares the inability of K-theory to describe the non-diffusive near field of a source, the RDM nevertheless has appeal for the practical treatment of dispersion (e.g., Luhar and Rao 1994; Leone et al. 1997; Nasstrom and Pace 1998) because usually the region of interest lies in the far field, and the RDM method offers the convenience and flexibility of the Lagrangian approach without (or putatively so) the strict limitation on timestep Δt that would apply to a first-order LS model (i.e., there is no requirement that $\Delta t \ll T_L$, where T_L is the Lagrangian time scale of the turbulence).

The equivalence of the RDM to K-theory makes it an interesting complement to grid-based numerical Eulerian models[1] (e.g., of long-range transport, D'Amours, 1998), and is easily demonstrated in the case that the timesteps are of infinitesimal duration ($\Delta t \rightarrow \mathrm{d}t$) and if we overlook the possible necessity to intervene at domain boundaries. But what are the implications of the finite timestep of a realizable model? Thomson's (1987) well-mixed condition (w.m.c.) is the most powerful known constraint on Lagrangian models, and states that an acceptable model must have the property that, if applied to the motion of computational particles that are well mixed (in position *and* velocity space), it leaves those particles well-mixed. Just as 'well-mixed' first-order Lagrangian stochastic models are known potentially to fail the w.m.c. in their practical implementation (e.g., Wilson and Flesch 1993), the same deficiency (potentially) applies to the discrete RDM, a fact that may to some extent have motivated Ermak and Nasstrom (2000) to introduce their realizable (finite Δt) RDM based on a *non-Gaussian* distribution of the random displacements.

It is the purpose of this paper to examine the simplest RDM based on Gaussian forcing[2], in the context of the turbulence statistics of the horizontally-homogeneous and neutrally-stratified atmospheric surface layer ('hhNSL', or adiabatic wall-shear layer). In this regime the far-field eddy diffusivity $K \propto z$, where z is distance from the ground, a situation sufficiently complex to bring out the non-exactness of the discrete RDM when supplemented by a reflection scheme. We shall take as a "reference case" the situation of vertical dispersion (and streamwise advection) from a continuous ground-level source, for which the observations of Project Prairie Grass (PPG) (Barad 1958; Haugen 1959) provide a baseline, and show that simulations using the RDM are distinguishable from those of the more complex Langevin model, albeit by a margin that may not be of *practical* significance.

2 The RDM with infinitesimal steps

Considering motion on a single axis[3] z along which ensemble mean velocity vanishes (no mean flow), in general form the RDM is

$$\mathrm{d}Z = a\ \mathrm{d}t + b\ \mathrm{d}\xi, \tag{1}$$

where a, b are as yet unspecified model coefficients, and $d\xi$ is a random Gaussian variate with $\langle \mathrm{d}\xi \rangle = 0$, $\langle \mathrm{d}\xi^2 \rangle = \mathrm{d}t$. For now we suppose the timesteps are of infinitesimal duration, and we ignore domain boundaries.

[1] Of course such models carry their own discretization error, as a function of grid length and timestep.

[2] With some effort, the present analysis using the Chapman-Kolmogorov equation could be extended to cover Ermak and Nasstrom's (2000) zeroth-order model.

[3] Lagrangian coordinates will be represented in upper case.

To evaluate the coefficients we consider the Fokker-Planck equation

$$\frac{\partial p(z,t)}{\partial t} = -\frac{\partial}{\partial z}\,(a\ p) + \frac{1}{2}\,\frac{\partial^2}{\partial z^2}\left(b^2\ p\right) \tag{2}$$

corresponding to the stochastic Eq. 1, and which governs the evolution of the particle density distribution $p(z,t|\ldots)$ in phase space (entries to the right of the bar denote the conditioning of the ensemble, e.g., release time and place, but we shall often consider them implicit; elsewhere in this paper we label the particle density distribution generically as 'C', its dimensionality implied by the problem at hand). Consistency of Eq. 2 with the one-dimensional mass conservation equation (under eddy diffusion closure)

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial z}\left(K\,\frac{\partial p}{\partial z}\right) \tag{3}$$

demands that

$$a = \frac{\partial K}{\partial z}, \tag{4a}$$

$$b = \sqrt{2\,K} \tag{4b}$$

(Durbin 1983; Boughton et al. 1987). A criterion for how large the timestep might be allowed to be in practice stems from the fact that the root-mean-square step length is $\sqrt{2K\,\Delta t}$, implying that the specification

$$\sqrt{2K\,\Delta t}\,\frac{1}{(K)}\,\frac{\partial K}{\partial z} \ll 1 \tag{5}$$

should suffice.

3 Discretization error of the RDM: surface source

It is outside our intended scope to establish the error due to discretization of the RDM across all conceivable turbulence systems and source distributions, and as indicated above we restrict our attention to sources in the hhNSL. Thus, we begin by comparing the discrete RDM against the solution $C = C(z,t)$ to the diffusion equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(\alpha\,z\,\frac{\partial C}{\partial z}\right) \tag{6}$$

with boundary conditions

$$(\alpha\,z\,\partial C/\partial z)_{(z=0)} = 0, \tag{7a}$$

$$C(\infty,t) = 0 \tag{7b}$$

for a unit release at $t = 0, z = 0$ (to connect this with the hhNSL, make the interpretation $\alpha = k_v\,u_*/S_c$, where k_v is the von Karman constant, u_* is the friction velocity, and S_c is the turbulent Schmidt number). The exact solution for the probability density function for position (i.e., mean concentration) $C(z,t)$ is:

$$C = \frac{1}{\alpha\,t}\exp\left(-\frac{z}{\alpha\,t}\right) \tag{8}$$

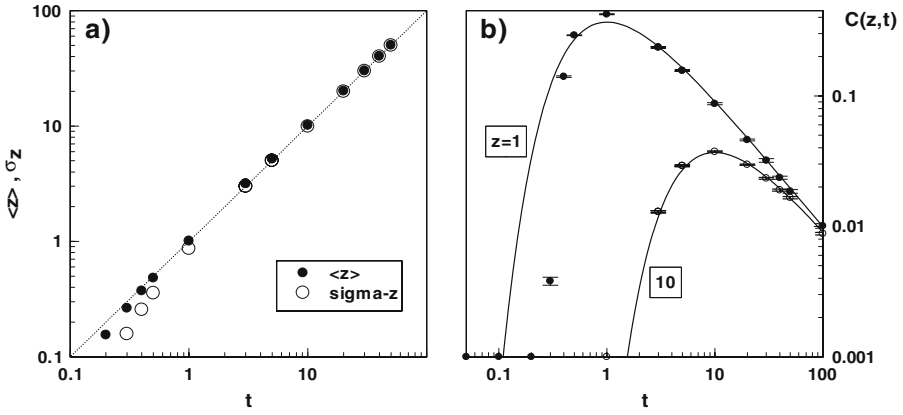

Fig. 1 Test of discrete RDM (timestep $\Delta t = 0.1$) against solution to the diffusion Eq. (8; $\alpha = 1$) for unit release at $z = t = 0$. Exact solution given by lines. Error bar on concentrations from the RDM gives standard error ($19 \times 256,000$ paths)

which satisfies

$$\int_0^\infty C(z,t)\ \mathrm{d}z = 1, \forall\, t, \tag{9a}$$

$$\int_0^\infty z\, C(z,t)\ \mathrm{d}z = \langle z(t)\rangle = \alpha\, t, \tag{9b}$$

$$\int_0^\infty (z - \langle z\rangle)^2\, C(z,t)\ \mathrm{d}z = \sigma_z^2(t) = \alpha^2\, t^2. \tag{9c}$$

Please note that perfect reflection has been imposed in the discretized RDM, either by rectifying any negative particle height $Z < 0$, or equivalently by permitting $-\infty \le Z \le \infty$ but using $|Z|$ to evaluate the diffusivity K.

The diffusion problem as defined above supplies a velocity scale (α), but no natural time scale — thus one has no criterion other than Eq. 5 for the timestep Δt of the discrete RDM. Figure 1 confirms the utility of Eq. 5, taking the particular case ($\alpha = 1$, $\Delta t = 0.1$). At fixed $t \gg \Delta t$, the discrete RDM simulation provides an accurate concentration transient $C(z,t)$ provided $\Delta t \ll z/2$, which is the condition expressed by Eq. 5 for this case. (We do not represent as novel this finding that the discrete RDM reproduces the continuous model to arbitrary accuracy as the timestep is decreased.)

4 Non-equivalence of RDM and Langevin models

In a later Section we shall compare RDM simulations with 'reference data' (Langevin simulations 'tuned' to the Project Prairie Grass observations) for streamwise advection and vertical diffusion from a surface source in the hhNSL. To clarify what might otherwise appear to be an inconsistency, here we wish to establish the non-equivalence of these (i.e., the RDM and Langevin) models. Of course they are *not expected* to be equivalent in the "near field" of a source (the spatial locus of their non-equivalence might be taken to define 'near field'). But does the near-field region in practice vanish, for a source placed on the ground? One might

imagine so, in view of the fact that at the ground we usually consider the turbulence length scale to be infinitely small[4].

Under the assumption that in the hhNSL the probability density function for the Eulerian velocity is Gaussian, the unique, well-mixed, one-dimensional, first-order Lagrangian stochastic model for vertical motion in the hhNSL is the 'Langevin' model

$$\mathrm{d}W = -\,W\,\frac{\mathrm{d}t}{T_L} + \sqrt{C_0\,\epsilon}\;\mathrm{d}\xi, \tag{10a}$$

$$\mathrm{d}Z = W\,\mathrm{d}t, \tag{10b}$$

(Thomson 1987), where T_L is the Lagrangian decorrelation time scale, ϵ is the turbulent kinetic energy dissipation rate, C_0 is a universal dimensionless constant, and (as earlier) $\mathrm{d}\xi$ is a Gaussian random variate with vanishing mean and variance $\mathrm{d}t$. The Langevin model is adapted to the hhNSL by choosing

$$T_L = \frac{2\sigma_w^2}{C_0\,\epsilon}, \tag{11a}$$

$$\epsilon = \frac{u_*^3}{k_v z}, \tag{11b}$$

$$\sigma_w = b\,u_*, \tag{11c}$$

$$dt = \gamma\,T_L \quad (\gamma \ll 1), \tag{11d}$$

where σ_w is the standard deviation of the Eulerian vertical velocity and $b \approx 1.3$. It can be shown that the eddy diffusion model implied by the Langevin model [Eqs. 10 and 11] in the 'diffusion limit' (Thomson 1987; Sawford and Guest 1988) is

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(K\,\frac{\partial C}{\partial z}\right), \tag{12a}$$

$$K = \frac{2}{C_0}\,b^4\,k_v\,u_*\,z, \tag{12b}$$

in which $k_v u_* z$ is the eddy viscosity of the hhNSL, and we may identify an effective turbulent Schmidt number

$$\frac{1}{S_c} = \frac{2}{C_0}\,b^4. \tag{13}$$

At the level of required practical accuracy, dispersion from a surface source in the hhNSL can adequately be treated by the advection-diffusion equation, the theoretical justification for which being that, since the time scale T_L tends to zero at the surface ($T_L \to T_L(0) \sim 0$), the mean travel time (scaled on timescale at the source) $\bar{t}\,/\,T_L(0)$ is large for any likely observation time/place. Alternatively put, in the far field of a source a first-order LS model should behave like an eddy diffusivity model— indeed (as noted earlier) this could be taken as effectively a *definition* of 'far field'.

[4] Corrsin (1974) outlines quite exhaustively the conditions under which an eddy diffusion treatment of turbulent convective transport is successful. Abbreviating, it is required that the mean convective flux at a point be uniquely determined by the mean concentration gradient at that point, and this (in turn) demands that plume dimension be large compared to the turbulence length scale (fine-grained transport mechanism). In the case at hand, near the source the plume dimension and turbulence length scale (evaluated, say, at the plume centroid) are *both* small, and both increase with increasing distance x (or time). Thus (Dr. B. Sawford, pers. comm. 2006), "whether or not the diffusion limit is a good approximation depends on the ratio of the coefficients in these growth laws".

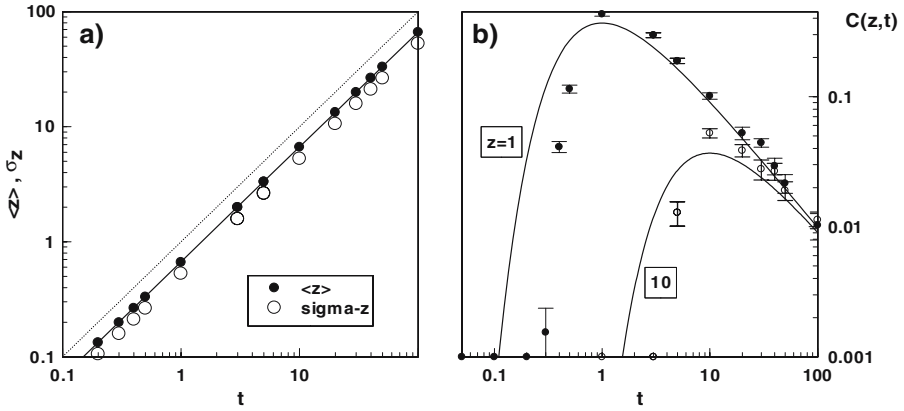

Fig. 2 Test of discrete Langevin model against solution to the diffusion Eq. (8; $\alpha = 1$) for unit release at $z = t = 0$. Diffusion solution given by lines. Langevin solution used $\gamma (= \Delta t / T_L) = 0.01$ except for case shown by heavy solid line for $\langle z \rangle (t)$, where $\Delta t / T_L = 0.001$. Error bar on concentrations from the Langevin model gives standard error ($19 \times 2,560$ paths)

It is expedient to determine whether the Langevin model and its diffusion limit provide *exactly* the same solution for a surface source, and for convenience we adopt the test case of the previous section. The choices $b = u_* = k_v = 1$, $C_0 = 2$ imply an effective tracer eddy diffusivity $K = z$, and setting $T_L = \epsilon^{-1} = z$ the Langevin equation reduces to

$$\mathrm{d}W = -\gamma\, W + \sqrt{2\gamma}\, r \tag{14}$$

where (here and later) r is a standardized Gaussian random number. (As a reminder, $\gamma = \Delta t(z)/T_L(z)$ is the dimensionless timestep. Please note that elsewhere, in the context of the RDM with height-independent timestep, we introduce an alternative dimensionless timestep $\nu = \Delta t\, u_*/z_0$.)

An explicit analytical solution to this Langevin model has not been found[5], thus we performed a random flight simulation using the discretized model. To prohibit particle migration to indefinitely small z, we imposed perfect reflection at z_{refl} (whereas in the continuous limit, the $z = 0$ boundary may well be unattainable; see Durbin 1983). Figure 2 compares against the analytical solution of the previous section (i.e., the diffusion limit of the Langevin model) the computed time evolution of the moments and the concentration transient from the Langevin model. Numerical parameters of the discrete model were $\gamma = \Delta t / T_L \leq 0.01$, $z_{src} = z_{refl} = 10^{-9}$ (same units as z, i.e. arbitrary), choices which suffice to render discretization error extremely small. What is evident from comparing Figs. 1 and 2 is that the Langevin equation and its diffusion limit are *not* equivalent, or more specifically, solutions of the Langevin model and the RDM model are distinct.

Although this may be surprising, it is not an entirely novel finding. Sawford (1985) had noted that (for a surface source in the hhNSL) "diffusion equation results match the Langevin solution only in the limit $b_2 = \partial(\sigma_w T_L)/\partial z \to 0$" and later Sawford (2001) identified a "systematic failure of the diffusion approximation[6] as the turbulence becomes increasingly

[5] Dimensional analysis easily establishes that $\langle z \rangle \propto z$, $\sigma_z \propto z$. However "when T_L is not constant [Eq. 10a] becomes horribly intractable" (Durbin 1980).

[6] Although Sawford (2001) documented a comparison of the one-dimensional RDM against a two-dimensional Langevin model (i.e., alongwind fluctuation U' included), he had identified the same anomaly between 1-D Langevin simulations and the RDM (pers. comm. 2006).

inhomogeneous". Similarly Mooney and Wilson (1993) compared a Langevin simulation with an exact solution to the advection-diffusion equation for a surface source in the hhNSL, and noted distinct outcomes at the upper edge of a plume.

5 Discrete RDM: evolution of a well-mixed initial distribution

As indicated above, the fate of an initially well-mixed particle distribution is a profoundly useful test of Lagrangian dispersion models, and we now examine whether the discrete RDM preserves a well-mixed initial state. We answer the question from two (self-consistent) perspectives, of which the more interesting is the following analytic approach.

The Chapman-Kolmogorov (CK) equation[7]

$$p(z_2, t_2) = \int_\Omega p(z_2, t_2 | z_1, t_1)\ p(z_1, t_1)\ \mathrm{d}z_1 \tag{15}$$

(where Ω represents the domain accessible to the particles) states that all the material present at time t_1 must be found somewhere, at later time t_2, where the step $\Delta t = t_2 - t_1$ is restricted only to be non-negative. The physics of the transport process (or model thereof) enters in the guise of the transition density $p(z_2, t_2 | z_1, t_1)$, which in the present case we may also identify with the distribution function for the random displacements.

Following Wilson and Flesch (1993), we may express the well-mixed condition[8] for a realizable (finite Δt) model as follows. Suppose z_r, L represent the lower and upper domain boundaries. We set $p(z_1, 0) = c$ where c is a constant (usually unity, or $(L - z_r)^{-1}$) signifying a well-mixed initial state, and we require of the transition density function that it should ensure the integral

$$p(z, \Delta t) = \int_{z_r}^{L} p(z, \Delta t | z_1, 0)\ p(z_1, 0)\ \mathrm{d}z_1 \tag{16}$$

evaluates to $p(z, \Delta t) \equiv p(z, 0) = c$. The transition density has to account explicitly for any intervention invoked at boundaries, in the form (for example) of perfect reflection:

$$\text{if } (z < z_r), \quad z \to 2\,z_r - z. \tag{17}$$

For the random displacement model (with finite Δt), and assuming we *do* impose perfect reflection at the lower boundary z_r, the transition density function is a summation

$$p(z, \Delta t | z_1, 0) = p_{nr}(z, \Delta t | z_1, 0) + p_r(z, \Delta t | z_1, 0) \tag{18}$$

of two Gaussians, corresponding to a step of length $|z - z_1|$ without reflection, and a step of length $|z + z_1 - 2z_r|$ *with* reflection. Specifically,

$$p_{nr}(z, \Delta t | z_1, 0) = \frac{1}{\sqrt{2\pi}\ \sqrt{2K(z_1)\Delta t}}\ \exp\left[-\frac{(z - z_1 - \mu)^2}{4K(z_1)\Delta t} \right], \tag{19a}$$

$$p_r(z, \Delta t | z_1, 0) = \frac{1}{\sqrt{2\pi}\ \sqrt{2K(z_1)\Delta t}}\ \exp\left[-\frac{(z + z_1 - 2z_r + \mu)^2}{4K(z_1)\Delta t} \right], \tag{19b}$$

[7] Strictly speaking, to legitimize naming Eq. 15 the 'Chapman-Kolmogorov equation' every factor must be interpreted as a conditional probability density (Gardiner 2004, Sect. 3.2.1). One may always regard some initial state (z_0, t_0) at time $t_0 < t_1 < t_2$ as being implicit.

[8] Some readers may feel the qualification "well-mixed" is misrepresented or misapplied, when attached as a property of (or criterion for) a *discretized* Lagrangian model. However it seems to us a legitimate and useful terminology.

where

$$\mu = \Delta t \ (\partial K/\partial z)_{z=z_1} \tag{20}$$

(in the case of the hhNSL, μ is a constant and $K(z_1) \propto z_1$). One simply substitutes this transition density into Eq. 16 with $p(z_1, 0) = c$, and integrates to determine whether the particle distribution $p(z, \Delta t)$ remains uniform, after the one finite timestep (note that the components of the transition density are Gaussians in z, but *not* in z_1, which is the variable over which one must integrate). It may be worth emphasizing that (with the restriction of Gaussian forcing) the single-step transition density corresponding to the discretized RDM is *exactly* the indicated Gaussian, no matter how large or small (and no matter how suitable or unsuitable, physically) the chosen timestep $\Delta t = t_2 - t_1$. However, it is to be distinguished from the "real" transition density that is implicit in the *continuous* RDM, which in general is *not* Gaussian.

If we reflect trajectories at both a lower and an upper boundary, and if the forcing is Gaussian, then an infinite number of possible paths connect two subsequent positions z_1, z and $p(z, \Delta t|z_1, 0)$ involves an infinite sum that is not difficult to write down. However it appears that analytical solutions to the necessary integral are unknown, preventing the application of Eq. 16 to test for satisfaction of the w.m.c.

5.1 Unbounded or bounded homogeneous turbulence

We set $L = \infty$ and $K(z) = \text{const.}$, and we set the lower reflecting boundary at arbitrary z_r or even $z_r = -\infty$. The transition density simplifies and (in either case) it is straightforward to integrate Eq. 16 to show that the well-mixed condition is satisfied identically.

5.2 RDM for neutral surface layer: $z_r = 0$, $\Delta t = \text{const.}$

If we define the 'von Karman constant for mass' $k_m = k_v/S_c$, then the tracer eddy diffusivity for the hhNSL is $K = k_m u_* z$. By Eq. 4a the drift term in the RDM [Eq. 1] equates to

$$\mu = \Delta t \ (\partial K/\partial z) = k_m \, u_* \, \Delta t \tag{21}$$

(note that $\mu \, z \equiv K \ \Delta t$) and it will be convenient to define the dimensionless height

$$\eta = \frac{z}{\mu} = \frac{z}{k_m u_* \, \Delta t}. \tag{22}$$

The RDM for a single step from position Z_1 to a new (random) position Z over a single (uniform, i.e., height-independent) timestep Δt is

$$Z - Z_1 = \mu + \sqrt{2 \, \mu \, Z_1} \quad r \tag{23}$$

(as earlier, r is a standardized Gaussian random variate). Equation 5 for the limit to the timestep evaluates to $\Delta t \ll z/(2k_m u_*)$, which obviously (for any constant Δt) cannot be assured at all heights $z = Z_1$.

We would like to know whether this model preserves a well-mixed state, and we can answer the question in either of two ways, viz. by integrating the CK equation, or by performing a stochastic simulation. For the analytical solution ('CK') we set

$$p^{CK}(z_1, 0) = \ 1, \quad 0 \le z_1 \le \infty, \tag{24}$$

whereas in the random flight ('RF') experiment we release particles uniformly on $0 \le z \le L$, i.e.,

$$p^{RF}(z_1, 0) = \begin{cases} 1 & 0 \le z_1 \le L, \\ 0 & L < z_1. \end{cases} \tag{25}$$

Integrating Eq. 16 with Eqs. 19 and 24 is straightforward (Gradshteyn and Ryzhik 1980), and yields

$$p^{CK}(\eta, \Delta t) = \exp\left[\frac{z - \mu - |z - \mu|}{2\mu}\right] + \exp\left[\frac{-(z + \mu)}{\mu}\right], \tag{26}$$

where the notation on the left-hand side emphasizes that the solution (after one step) is universal (i.e., independent of Δt) in $\eta = z/(k_m u_* \Delta t)$. An alternative expression of Eq. 26 is

$$p^{CK}(\eta, \Delta t) = \begin{cases} 2e^{-1} \cosh \eta & \eta \le 1 \\ 1 + e^{-1-\eta} & \eta \ge 1 \end{cases} \tag{27}$$

and limiting values are:

$$p^{CK}(\eta, \Delta t) \to \begin{cases} 2e^{-1} \approx 0.73 & \eta \ll 1 \\ 1 + e^{-2} \approx 1.14 & \eta \to 1 \\ 1 & \eta \gg 1 \end{cases} \tag{28}$$

Figure 3 compares $p^{CK}(\eta, \Delta t)$ with the outcome of a stochastic simulation ($k_v = 0.4$, $S_c = 0.63$). In the random flight simulation, paths were reflected at $z/\mu = (0, 5)$ and the upper reflection, not accounted for in p^{CK}, explains the small discrepancy between the solutions aloft. As is obvious from the analytical solution, the realizable RDM model Eq. 23 does not preserve a well-mixed distribution, but the error decays above $z/\mu = 1$ on length scale μ, and so can be made arbitrarily small at given z by decreasing the timestep. This last point suggests a possible criterion for the timestep. Supposing one wished to be sure that discretization error can be neglected (after a *single* step, away from a well-mixed initial state) at a particular height ℓ and above, one might choose (say) $3\mu \le \ell$ which translates to

$$\Delta t \le \frac{\ell}{3 k_m u_*} \tag{29}$$

(if ℓ were specified so as to lie within the lowest 'sampling bin' used in conjunction with the RDM, the error due to this violation of the w.m.c. would vanish). Figure 3 also shows the discretization error (computed by random flight simulation) after $n = 100$ timesteps, at which time $p(\eta, t)$ closely approximates the asymptotic ($n \to \infty$) steady state profile for given Δt and upper reflection height. Taken at face value, this profile appears to suggest the discretization error (for given Δt) is larger at larger time, however it needs to be remembered that the error aloft at $\eta > 1$ is (in a reviewer's words) "a reaction to error below $\eta = 1$" and would be smaller if the upper reflection height were raised (mass deficit below $\eta = 1$ compensated by a small excess on $1 \le \eta \le \infty$).

6 Advected plume from a surface source: performance of the discrete RDM

Now in practice we seldom have to do with computing the future of a well-mixed tracer (except in the context of testing models). What do the above results imply for performance in relevant dispersion problems? It is impossible to provide a general answer. For example, consider the case of an elevated line source, and in which one's interest is the concentration

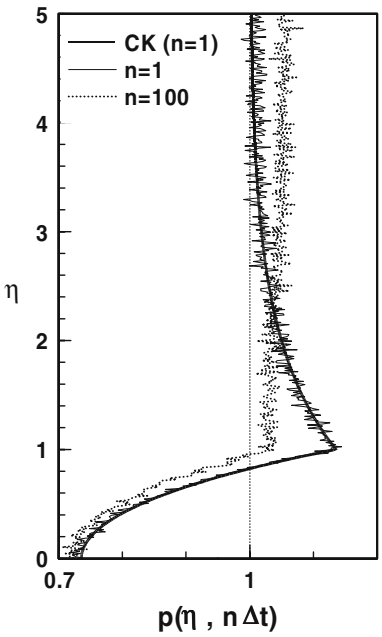

Fig. 3 Test of a realizable RDM (finite timestep Δt, perfect reflection at $\eta = 0$ and at $\eta = 5$) relative to the well-mixed condition. The flow regime is the horizontally-uniform, neutrally-stratified atmospheric surface layer. The initial state is well-mixed, $p(\eta, 0) = 1$, i.e., particles released evenly on $0 \leq \eta \leq 5$. The random flight simulations move a single step ($n = 1$) or 100 steps ($n = 100$) forward in time away from the initial state, with timestep Δt, and the figure shows the new particle distribution $p(\eta, n\Delta t)$. Also shown is the solution obtained by integrating the Chapman-Kolmogorov equation for a single step with $L = \infty$ (Parameters $k_v = 0.4$, $S_c = 0.63$; $19 \times 320,000$ particles.)

profile at a sufficiently short downwind distance that the plume has not yet interacted with the ground, or more generally, with that region of the flow where the chosen timestep Δt fails to be small relative to the criterion of Eq. 5. Then the discreteness of the model can have negligible impact on the solution. Conversely, when the source is at the ground, presumably we have to deal with the most taxing circumstance, i.e., that *most* likely to reveal the consequences of discretization.

In view of this, we take as an indicative case that of a continuous ground-level point source in the horizontally-homogeneous, neutrally-stratified atmospheric surface layer. We compute the crosswind-integrated concentration[9] C within samplers of physical depth d (correcting the lowest sampler's depth for surface reflection at z_{refl}, in any case that $z_{refl} > 0$). It is convenient to adopt the roughness length z_0 as an 'external' length scale (though it has no relevance to vertical dispersion, per se) and normalize using u_*, z_0 so that the RDM transforms to

$$\Delta Z/z_0 = \mu/z_0 + \sqrt{2\,\mu\, Z\, z_0^{-2}} \quad r, \tag{30a}$$

$$\Delta X/z_0 = \nu/k_v \, \ln\left(1 + Z/z_0\right), \tag{30b}$$

where (for the RDM, unless otherwise specified) the mean streamwise velocity has been formulated as

$$\overline{u}(z) = \frac{u_*}{k_v} \ln\left(\frac{z + z_0}{z_0}\right) \tag{31}$$

[9] By symmetry, and provided both are normalized on the appropriate source strength, crosswind-integrated concentration due to a point source is equivalent to the natural concentration from a line source oriented along the crosswind axis.

for compatibility with reflection at $z = 0$ ($< z_0$). The key dimensionless parameters of the simulation will be

$$\nu = \frac{\Delta t\, u_*}{z_0}, \tag{32a}$$

$$\frac{\mu}{z_0} = k_m \nu, \tag{32b}$$

$$\frac{d}{\mu} = \frac{1}{k_m \nu}\,\frac{d}{z_0}. \tag{32c}$$

Figure 4 gives computed transects of mean crosswind-integrated concentration at ground level (C_0): the simulations correspond exactly with those of Fig. 1, the only difference being the different release condition, and the fact that here we continue timestepping until the lateral displacement specified. The RDM solutions are compared with corresponding values tabulated by Wilson[10] (1982b; Table 1) from Langevin simulations, and also with an approximate analytical solution to the advection-diffusion equation given by Wilson (1982a; summarized in the Appendix). Here taken as a criterion for accuracy of the RDM in the problem at hand, these solutions can be considered as 'calibrated' back to Project Prairie Grass (e.g., see Figs. 8 and 9 of Wilson 1982a) by virtue of a choice of the turbulent Schmidt number S_c, and so we take them to represent the reference case (surface point source in hhNSL). It is important, however, to remember that an uncertainty of order 5% attaches to them—and more importantly, to remember that (as established in Sect. 4) the RDM can be expected *not* to exactly reproduce a Langevin simulation, even in this case of a ground-level source.

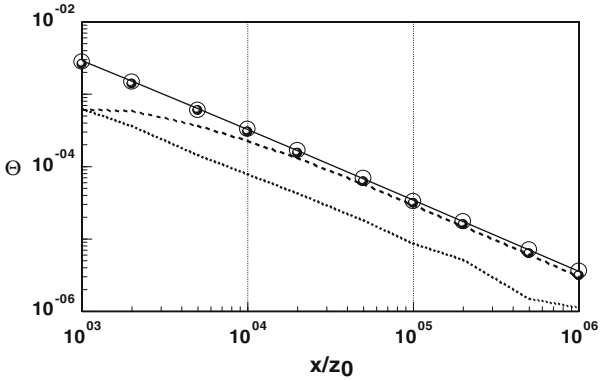

Fig. 4 Test of a realizable RDM (finite and constant timestep; perfect reflection at $z_r = 0$) relative to the benchmark of dispersion from a continuous ground-level source of strength Q in the horizontally-homogeneous, neutrally-stratified atmospheric surface layer (hhNSL). Figure shows the computed transect of crosswind-integrated ground-level concentration $\Theta = z_0 u_* C_0/(k_v Q)$. ◯, tabulation of Wilson (1982a) based on 1-D Langevin simulations; solid line, approximate analytical solution to the advection-diffusion equation (Wilson 1982a); solid beads, RDM with $\nu = 1, d/z_0 = 10$ ($d/\mu = 15.75$); heavy dashed line, RDM with $\nu = 50$ and $d/z_0 = 0.01x/z_0$ ($d/\mu \geq 0.315$); fine dashed line, RDM with $\nu = 50$ and $d/z_0 = 10$ ($d/\mu = 0.315$). Solutions correspond with $S_c = 0.63$

[10] The tabulation of Wilson (1982b) stems from a well-mixed, first-order Lagrangian stochastic model, previously calibrated against Project Prairie Grass, e.g., Wilson et al. (1981b).

On the view provided by Fig. 4, the RDM with constant timestep $\nu = 1$ *appears* to agree adequately with the reference data, although a deviation is evident for the larger (timestep) ν. In interpreting Fig. 4 one needs to consider the sampler-depth d/z_0 (which should not be so large as to cause unwanted smoothing of a rapidly height-varying concentration profile at short range x/z_0) and of the ratio d/μ (which should be sufficiently large as to smooth out the discretization error observable on Fig. 1). The RDM with $\nu = 50$, $d/z_0 = 10$ provides a uniformly bad outcome, presumably because with $d/\mu = 0.315$ the sampling is done in the region where the imperfection of the finite Δt model plays a role (i.e., inadequate depth of smoothing). Given a variable sampler depth $d = x/100$, beyond about $x/z_0 = 5 \times 10^3$ a simulation with $\nu = 50$ is close to, though still distinguishable from, that with $\nu = 1$.

However a more revealing view is provided by Fig. 5, where the cross-wind integrated concentration has been re-scaled as $\Phi = C_0\, u_*\, x\, (k_v\, Q)^{-1}$ and is more nearly independent of distance x/z_0. On the narrow linear scale needed to display $\Phi = \Phi(x/z_0)$, the distinction between the reference data (to repeat for clarity, equivalent to a Langevin simulation that has been tuned to PPG; see either Wilson (1982b), or more recently Wilson (2007), Figs. 2, 3) and the RDM is more easily seen. Even with a small timestep and even at long range, the RDM is distinctly *not* equivalent to a Langevin model—which was anyway to be expected in view of the demonstration of Sect. 4. Concentrations computed by the RDM are lower (at given x/z_0) than those from the Langevin model, which is consistent with the RDM's larger $\langle z \rangle$ for given time t since release than the Langevin model (compare Figs. 1, 2). Also emphasized by Fig. 5 is the poor performance of the RDM for ground-level concentration when the latter is estimated in bins whose depth d is shallow compared to the length scale $\mu = k_m u_* \Delta t$ over which the boundary reflection error is important.

Finally, in the simulation shown on Fig. 5 the Langevin model imposed reflection at $z/z_0 = 1$ with the streamwise velocity formulated as $\overline{u} \propto \ln(z/z_0)$, rather than (as for all but

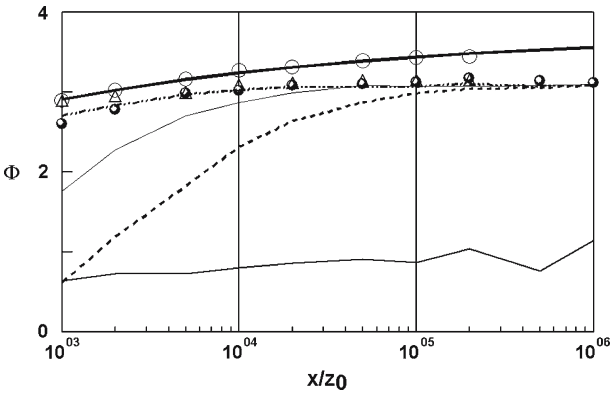

Fig. 5 Test of the RDM relative to the benchmark of dispersion from a continuous ground-level source of strength Q in the hhNSL. Figure shows the computed transect of crosswind-integrated ground-level concentration scaled as $\Phi = u_* C_0 x/(k_v\, Q)$. Heavy solid line, approximate analytical solution to the advection-diffusion equation (Wilson 1982a); ◯ one-dimensional Langevin simulation ($dt/T_L = 0.02$; for other details see Wilson 2007) also equivalent to tabulation of Wilson (1982a); solid beads and chain-dash line, RDM with constant timestep $\nu = u_* \Delta t/z_0 = 1$ and sampler depth $d/z_0 = 0.01 x/z_0$ (beads, reflection at $z = 0$; chain-dash line, reflection at $z/z_0 = 1$); light solid line, RDM with $\nu = 10$ and $d/z_0 = 0.01 x/z_0$ ($d/\mu \geq 1.575$); heavy dashed line, RDM with $\nu = 50$ and $d/z_0 = 0.01 x/z_0$; fine dashed line, RDM with $\nu = 50$ and $d/z_0 = 10$ ($d/\mu = 0.315$). Also shown (triangle) is a simulation using an RDM formulated in $\lambda = \ln(z/z_0)$, for which case $\gamma = \Delta t/T_L = 0.01$, $d/z_0 = 0.01 x/z_0$. All solutions correspond with $S_c = 0.63$

one of the RDM simulations shown) reflection at $z = 0$ with $\overline{u} \propto \ln(1 + z/z_0)$. This small distinction does not account for the manifest difference between RDM simulations and the Langevin equation, for one of the RDM simulations [chain-dash line on Fig. 5] was run with reflection at z_0 and $\overline{u} \propto \ln(z/z_0)$, as in the Langevin simulation; the difference in outcome is negligible.

6.1 Transformation of the hhNSL to unbounded homogeneous turbulence

It is usual with first-order Lagrangian stochastic models to specify the timestep $\Delta t = \gamma\, T_L(z)$ with $\gamma \ll 1$, where in the hhNSL the Lagrangian velocity autocorrelation time scale is

$$T_L = \frac{a\ z}{\sigma_w} \tag{33}$$

(a is a constant and $\sigma_w = b\, u_*$ is the velocity standard deviation). With the identification $K = \sigma_w^2 T_L = k_v u_* z/S_c$, it follows that best consistency with PPG is obtained with $a \approx 0.5$, which corresponds to $S_c \approx 0.63$ (Wilson et al. 1981b). But this is not the key point: the point is that with $\Delta t \propto z$ we have consistent resolution of particle paths, the timestep tracking the changes in the time scale as the particle moves along the vertical. This was the spirit of the original Lagrangian similarity theory of Batchelor (1957), although not all Lagrangian stochastic models have been formulated this way, with an evolving timestep: and especially not zeroth-order models, for understandable reasons.

To set $\Delta t \propto T_L$ in the zeroth-order model may seem spurious and uneconomical; this is a diffusion model and (as such) treats the motion as a sequence of uncorrelated steps, so that it is appropriate that Δt should exceed, but be unrelated to, the velocity autocorrelation time scale. Nevertheless, the previous section showed that the zeroth-order model in fact requires a small timestep ($\Delta t \lesssim 10\, z_0/u_*$) to secure even passably good agreement with the reference data (ground-level source in hhNSL), and so an implementation of the RDM with $\Delta t = \gamma\, T_L$ does not, in that light, seem absurd.

Let $\Lambda = \ln(Z/z_0)$ and define

$$\mathrm{d}t^* \equiv \frac{u_*}{z}\ \mathrm{d}t\ = \gamma\ \frac{a}{b}. \tag{34}$$

Then by virtue of the Ito formula, it can be shown that the stochastic differential of Λ is

$$\mathrm{d}\Lambda = \sqrt{\frac{2K}{Z^2}}\ \mathrm{d}\xi \equiv \sqrt{2k_m}\ \mathrm{d}\xi^*, \tag{35}$$

where (as before) $\langle \mathrm{d}\xi \rangle = 0$, $\langle \mathrm{d}\xi^2 \rangle = \mathrm{d}t$, and where $\langle (\mathrm{d}\xi^*)^2 \rangle = \mathrm{d}t^*$. The transformation to steps in $\ln(z/z_0)$ gives a description of surface-layer dispersion in terms of pure diffusion, in an unbounded regime of homogeneous turbulence; for there is no need (in principle) to introduce surface reflection because $\lambda \to -\infty$ merely corresponds to $z \to 0$, and we may represent the mean horizontal wind speed as a function of λ,

$$\overline{u} = \frac{u_*}{k_v}\ \ln\left(1 + \ e^{\lambda}\right), \tag{36}$$

where $\lambda \equiv \ln(z/z_0)$. This mapping of the inhomogeneous surface-layer turbulence of physical space to an unbounded regime of homogeneous turbulence in λ-space is analogous to a

transformation used by Wilson et al. (1981a) for first-order LS simulations, i.e., their 'z_*, t_H' coordinate system[11].

Since the physics of dispersion is independent of the coordinate system employed and the stochastic equations implemented for dZ and for $d\Lambda$ are mathematically equivalent, Eq. 35 enjoys the same status as a well-mixed model (in the limit $\Delta t \to 0$) as does Eq. 1. As for whether that property attaches also to the practical implementation with finite Δt, the question cannot be answered by integration of the Chapman-Kolmogorov equation (the latter does cast an interesting light on the distribution of particles on the true height axis as a function of 'computational time' $n\Delta t^*$ since commencement in a well-mixed state, a distribution which is *not* uniform).

Figure 6b indicates that simulations of the surface-layer advection-diffusion problem (nominally, Project Prairie Grass) using Eq. 35 with $\Delta t / T_L(z) = 0.1$ are in excellent agreement with the reference data (misleadingly so, in view of the findings of the previous section), and slightly superior to simulations (Fig. 6a) using the constant Δt formulation [Eq. 30a] in the sense of not showing the irregularity near the ground incurred as a consequence of the (inescapable) need to implement a boundary reflection. The simulation using the λ-system released particles at $\lambda = 0$ (i.e., $z/z_0 = 1$; outcome was insensitive to exact placement of the source) and applied perfect reflection at $\lambda = 0$. The latter step was needed only to avoid tracking particles towards $\lambda \to -\infty$, and other choices (e.g., reflection at $\lambda = -\ln 4000$) did not affect the outcome, but only the computation time (with the choice to reflect at $\lambda = 0$, computation time was comparable with that of the constant Δt simulation that used $\nu = u_* \Delta t / z_0 = 1$). Concentration was estimated in bins of constant depth $\Delta\lambda = 2\ln(4000)/201 \approx 0.083$ such that the depth of the lowest bin $\Delta z/z_0 < 0.1$, explaining the larger stochastic error in the λ-space simulation (Fig. 6b) than in the z-space simulation (Fig. 6a), which used $\Delta z/z_0 = 2$.

Figure 6a emphasizes the error of the constant-Δt RDM near the reflecting boundary, and that this error (as expected) decreases with decreasing Δt. Recall that for a simulation with constant $\Delta t = \nu z_0/u_*$ the length scale for decay of the boundary error is $\mu/z_0 = k_m \nu$. Thus (as we have set $k_m = k_v/S_c = 0.4/0.63$) for the case $\nu = 10$, $\mu/z_0 = 6.35$, while for $\nu = 1$ this reduces to $\mu/z_0 = 0.635$: this explains the differing scales of the region of discrepancy, for constant-Δt RDM simulations with $\nu = 1, 10$. Two (otherwise identical) simulations with $\nu = 10$ demonstrate a weak sensitivity to whether one sets $z_{refl}/z_0 = 0$ with $\overline{u} \propto \ln(1 + z/z_0)$ or $z_{refl}/z_0 = 1$ with $\overline{u} \propto \ln(z/z_0)$.

A simulation of the ground-level concentration transect with the RDM formulated in λ-space (with $\gamma = 0.01$) is shown alongside results from the z-space RDM, on Fig. 4. The λ-space formulation (shown with $\Delta t / T_L = 0.01$, but choices 0.1, 1 provided negligibly different outcomes) proves superior to the constant timestep RDM at very short range, and equivalent to it at long range. The clear distinction of the RDM relative to the Langevin solutions is the basis for the 'misleadingly so' in an earlier paragraph above, for when the RDM and Langevin equation are compared at $x/z_0 = 2 \times 10^3$ (as on Fig. 6) the difference is smaller than it is at larger range (as evidenced by Fig. 5).

[11] The equivalent Eulerian description, for a continuous unit line source at $x = 0$, $z/z_0 = 1$, is

$$\frac{1}{k_v}\,\lambda\, e^{\lambda}\,\frac{\partial C}{\partial x} = k_m\,\frac{\partial^2 C}{\partial \lambda^2} + \delta(x-0)\,\delta(\lambda - 1).$$

If this could be solved with boundary conditions at infinity, one would have the (as yet unfound) exact solution to this prototypical surface-layer dispersion problem.

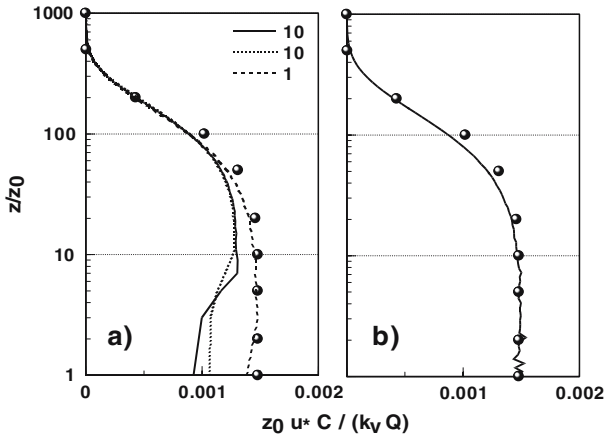

Fig. 6 Vertical profiles of crosswind-integrated concentration at a distance $x/z_0 = 2 \times 10^3$ downstream from a ground-level point source in the neutral surface layer. Symbols show the tabulation of Wilson (1982b). (**a**) RDM formulated in z/z_0 with constant timestep $u_*\Delta t/z_0 = \nu = (1, 10)$. For $\nu = 10$ (solid line) and for $\nu = 1$, perfect reflection was applied at $z = 0$ and $\overline{u} \propto \ln[(z + z_0)/z_0]$, whereas for $\nu = 10$ (fine dashed line), perfect reflection was applied at $z/z_0 = 1$ and $\overline{u} \propto \ln(z/z_0)$. In all cases sampler depth constant ($d/z_0 = 2$; $\mu/z_0 = \nu k_v/S_c = 0.635\nu$) except where (fine dashed line) lowest sampler corrected for reflection at $z/z_0 = 1$. (**b**) RDM formulated in $\lambda = \ln(z/z_0)$ space with $\Delta t(z)/T_L(z) = 0.1$, and constant sampler depth $\Delta\lambda$ such that the depth of the lowest bin is $\Delta z/z_0 < 0.1$ (All simulations 19×10^6 paths. $S_c = 0.63$)

7 Conclusion

We have demonstrated the usefulness of the Chapman-Kolmogorov formulation in the context of testing a discrete Lagrangian model against the well-mixed condition, and that a discrete RDM that is not well-mixed nevertheless may provide an adequate simulation of real world dispersion — provided that its timestep is suitably chosen. Perhaps more importantly, we have also shown that, although it represents the "diffusion limit" of the corresponding Langevin model, the RDM provides an appreciably different solution for the concentration due to a ground-level source, a case for which it had often been assumed that the far-field description (i.e., diffusion treatment) is adequate; this conclusion is independent of specific choices we made here for the coefficient C_0 and the Schmidt number. For our reference case of a ground level source, the magnitude of the difference in predictions between the RDM and Langevin models is fairly small relative to experimental uncertainties, so that the distinction will seldom be of practical importance.

As to what constitutes a 'suitably small' timestep for the RDM, by concentrating on the plume not far downwind from a ground-level source we have taken the most demanding case, for here trajectories are confined to the very region near the ground where Eq. 5 is most restrictive: perhaps, then, it is not too surprising that this case demands a stringent timestep limitation $\Delta t \lesssim 10\, z_0/u_*$, sufficiently small to more or less erase the computational advantage of the simpler RDM relative to the first-order Lagrangian stochastic (i.e., Langevin) model (note: other formulations of the RDM can alleviate this severe limitation on the timestep, in particular that introduced by Ermak and Nasstrom 2000). More generally, what will constitute an adequately small timestep for the RDM will depend on the specifics of the atmospheric flow regime, and the geometry of the source and detector (viz., their height, volume, separation). All in all, there would appear to be little to recommend use of the RDM in lieu of the more natural first-order Lagrangian stochastic (i.e., generalized Langevin) simulation, even for

far-field dispersion problems. Admittedly for the test case examined here, the magnitude of the RDM model's error can be arranged to be small (i.e., unimportant in view of realistic levels of experimental precision), but the necessity to fret over details such as the relationship of sampler depth to chosen timestep (even in this well-defined case) is disconcerting. Unless a modest saving in computation time outweighs a potential (and probably in most cases, unquantifiable) loss of accuracy, Langevin simulations are to be preferred.

In closing, and in the context of the previous sentence, it seems appropriate to recall that empirical micrometeorological relationships, such as the purported $b = \sigma_w/u_* = 1.3$ (in the neutral limit), originate as a curve fitted through scattered observations but tend to gather an aura of being 'the right value.' Taking 'b' as an example, even at ideal sites and during neutral stratification, its measured values from individual sampling intervals of normal length (say, 15 – 60 min) scatter quite widely around 1.3 (e.g., Panofsky 1973; Pasquill 1974, Table 2. VI; Stull 1988; Pahlow et al. 2001; and many others) and there is no profound reason to *expect* it to be constant—it would be amazing if there were not meteorological (or surface) factors lying outside the (by design, limited) scope of Monin-Obukhov similarity theory that bear on σ_w, u_* and their ratio. It is a merit of the Langevin model, therefore, that it is based on observable velocity statistics and rationally assimilates their specific values, if known. Rather than take the pragmatist's view that experimental uncertainties or inaccuracies of meteorological inputs (like b) render meaningless a ranking (such as the present one) of meteorological theories, we believe the more rational and general of two theories is to be preferred in principle.

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Appendix: Analytical solution for ground-level source in the neutral surface layer

The following approximate analytical solution to the advection-diffusion equation

$$\frac{u_*}{k_v}\,\ln\left(\frac{z}{z_0}\right)\,\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(\frac{k_v u_* z}{S_c}\,\frac{\partial C}{\partial z}\right) \tag{37}$$

for a continuous surface line source was given by Wilson (1982a; his Eqs. 23N, 24N, 28N, 29N). As shown in Fig. 9 of that paper, it provides a good fit to Project Prairie Grass with parameters $N = 0.25$ (which implies a choice of meteorological parameters including the von Karman constant and the Schmidt number) and $r = 0.5$ (this r should not be confused with the Gaussian random variate appearing earlier). Here we briefly re-capitulate. The dimensionless variables are the downstream distance $\xi = x/z_0$, height $\lambda = z/z_0$ and the crosswind-integrated concentration $z_0\,u_*\,C\,(k_v\,Q)^{-1}$.

The first step in evaluating the solution is to determine the plume depth $\delta = \delta(\xi)$ from the implicit equation

$$(\delta - 2)\,e^{\delta} + \delta = (N/r)\,\xi - 2, \tag{38}$$

which is easily done by stepping forward from $\delta = 0$ with a suitably small increment, to the zero-crossing of the difference between left- and right-hand sides. Then evaluate the slope

$\dot{\delta} = \partial\delta/\partial\xi$ and curvature $\ddot{\delta}$ of the plume boundary from

$$\dot{\delta} = \frac{N/r}{e^{\delta}\ (\delta - 1) + 1}, \tag{39a}$$

$$\ddot{\delta} = -\,(r/N)\,\delta\ \left(\dot{\delta}\right)^3\ e^{\delta}, \tag{39b}$$

and the (crosswind-integrated) concentration profile is given (for $\lambda \leq \delta$) by

$$\frac{z_0\, u_*\, C}{k_v\, Q} = \frac{r\,\ddot{\delta}}{N^2}\ \left[\left(\lambda\, e^{\lambda} - \delta\, e^{\delta}\right) - 2\ \left(e^{\lambda} - e^{\delta}\right) + (\lambda - \delta)\right]. \tag{40}$$

As was shown by Wilson, this solution is in excellent agreement with a Langevin simulation of the same problem. This begs explanation, however—in view of the finding of Sect. 4 that the Langevin model and the RDM (or diffusion equation) implied by it are *not* equivalent (even for a surface source). There seems no alternative to the proposition that the approximation error of this solution (distinction between Eq. 40 and the unknown exact solution) compensates the distinction between the Langevin and diffusion-equation descriptions, such that fortuitously, the approximate solution is better than it 'deserves' to be.

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