TRAJECTORY CURVATURE AS A SELECTION CRITERION FOR VALID LAGRANGIAN STOCHASTIC DISPERSION MODELS

JOHN D. WILSON and THOMAS K. FLESCH
Department of Earth & Atmospheric Sciences, University of Alberta, Edmonton, Alberta, T6G 2E3, Canada

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Abstract. Among well-mixed multi-dimensional Lagrangian stochastic (LS) dispersion models, we observe that those in poorest agreement with observations produce 'spiralling trajectories,' with an associated reduction in dispersion. We therefore investigate statistics of increments dθ' to the orientation $\theta' = \arctan(W'/U')$ of the Lagrangian velocity-fluctuation vector – as a possible means to distinguish the better LS models within the well-mixed class. 'Zero-spin' models, having $\langle d\theta' \rangle = 0$, are found to provide best agreement with observations. It is not clear however, whether imposition of the zero-spin property selects (in conjunction with the well-mixed condition) a unique model.

Key words: Trajectories, Turbulence, Dispersion, Diffusion, Numerical models

1. Introduction

The most important remaining problem for Lagrangian stochastic (LS) models of the paths of passive particles in turbulence, is to provide a criterion, further to Thomson's (1987) well-mixed condition (w.m.c.), that selects the *uniquely* correct model from the well-mixed class (Wilson and Sawford, 1996). Multi-dimensional LS models of first order are necessarily (Thomson, 1987; Gillespie, 1996) of the form*

$$\mathrm{d}U_i = a_i(U_i, X_i, t)\,\mathrm{d}t + b_{ij}(U_i, X_i, t)\,\mathrm{d}\xi_j, \tag{1}$$

where d$\mathbf{U}$ is the velocity increment over time increment dt, $\mathbf{a}$ (the conditional mean acceleration) and $\mathbf{b}$ are coefficients to be determined (and whose specification depends on the nature of the turbulence), and the dξ_j provide Gaussian random forcing. Thomson provided rational constraints on the specification of $\mathbf{a}$, $\mathbf{b}$, but in the multi-dimensional case his w.m.c. constrains $\mathbf{a}$ only to within an unknown vector $\boldsymbol{\phi}$, whose divergence in velocity space is (however) known. For example, for a two-dimensional (2-D) model defining trajectories in steady-state and horizontally-homogeneous turbulence,

$$\frac{\partial \phi_u}{\partial u} + \frac{\partial \phi_w}{\partial w} = -\frac{\partial}{\partial z}(w\, g_a(u, w, z)), \tag{2}$$

* U_i denotes the *total* Lagrangian velocity. In this paper we follow meteorological convention: U will be the x-('alongwind') component, and W the 'vertical' (z) component. In the simplest atmospheric flows, turbulence statistics are invariant in the horizontal plane, but vary with z.

where g_a is the Eulerian joint velocity probability density function (p.d.f.). It has been shown (Sawford and Guest, 1988) and we show here, that different models within the well-mixed class can give substantially differing rates of dispersion. As the LS model arguably provides the best treatment of dispersion to hand, the non-uniqueness problem needs to be solved.

It is an interesting observation that, among a class of well-mixed models, some have the propensity to produce 'spiralling trajectories', with an associated suppression of the rate of dispersion. Corresponding to this deficiency, such models produce trajectories exhibiting a Lagrangian autocorrelation function characterised by a **shorter timescale** than is implied by the 'input' or 'design' timescale

$$T_L = \frac{2\sigma^2(z)}{C_0\epsilon(z)}, \tag{3}$$

that is implicit in the usual specification of the model coefficients b_{ij} (in Equation (3), σ^2 is the turbulent velocity variance, ϵ is the turbulent kinetic energy dissipation rate, and C_0 is a universal dimensionless constant). This observation spawned an investigation by Borgas et al. (1997; BFS) of dispersion in (minimally) non-isotropic homogeneous turbulence, wherein statistical properties were taken to involve a special direction ($\boldsymbol{\Omega}$), with respect to which the turbulence was axisymmetric. BFS gave a non-unique, well-mixed LS model for this flow, and derived the implied Lagrangian velocity covariance function $\langle U_i(t)U_j(0)\rangle$ and the pattern of dispersion $\langle X_i(t)X_j(t)\rangle$. Dispersion in directions normal to the axis of symmetry was suppressed, due to the tendency of trajectories to spiral around that axis. BFS related their asymmetry vector $\boldsymbol{\Omega}$ to the mean angular momentum of a particle,

$$\langle \underline{L} \rangle = \langle \underline{X} \times \underline{U} \rangle. \tag{4}$$

The present paper stems from our feeling that a more direct criterion of trajectory curvature is needed. $\langle \mathbf{L} \rangle$ is not a local property of the trajectory, because it involves reference to a coordinate origin. Since an LS model by definition provides the Lagrangian velocity (or velocity-fluctuation) vector, it is straightforward to examine statistics of changes in the orientation of that vector, as implied by alternative models.

2. Statistics of Trajectory Curvature

The well-mixed condition selects a unique model for motion in a single dimension, but not so for two- and three-dimensional motion. Our discussion will be focused on 2-D trajectory models, but carries over easily to three dimensions. To avoid irrelevant complexity we consider stationary, horizontally-uniform turbulence.

In the atmospheric boundary layer, trajectories exhibit curvature due to the vertical wind shear $\partial\bar{u}/\partial z$. We quantify that curvature in Appendix A, but as regards construction of proper LS models in two (or more) dimensions, it is fruitful to focus not on that process, but on the rotation entailed by the *fluctuations*, (U', W'). And although in what follows we give statistics of the change in trajectory orientation, the mean *rate* of change (turning-rate) of the velocity vector is implied, and is (in principle) a measurable Lagrangian property.

2.1. Lagrangian stochastic model for velocity fluctuations

While it is more usual to formulate LS models for the *total* Lagrangian velocity, it is convenient for our purposes to split the velocity increment over time interval dt, writing

$$\mathrm{d}U_i = \mathrm{d}\bar{u}_i + \mathrm{d}U_i', \tag{5}$$

where the increment in the mean velocity over dt is just

$$\mathrm{d}\bar{u}_i = (\bar{u}_j + U_j')\,\mathrm{d}t\,\frac{\partial \bar{u}_i}{\partial x_j}. \tag{6}$$

Accordingly we adopt the generalised Langevin equation

$$\mathrm{d}U_i' = a_i(U_i', X_i, t)\,\mathrm{d}t + b_{ij}(U_i', X_i, t)\,\mathrm{d}\xi_j, \tag{7}$$

where the random forcing dξ_j is drawn from a Gaussian distribution with vanishing mean and variance dt. Consistency of this model with Kolmogorov's similarity theory of locally-isotropic turbulence requires (Thomson, 1987) that $b_{ij} = \delta_{ij} b$ where $b = (C_0\epsilon)^{1/2}$. In what follows, the meaning of $\mathbf{a}$ will be as according to Equation (7) – and $\boldsymbol{\phi}$ will represent the corresponding partially-constrained component of $\mathbf{a}$. In the Fokker–Plank equation that defines $\boldsymbol{\phi}$, the velocity pdf g_a is the pdf for velocity *fluctuation*.

2.2. Definition of rotation angles

The orientation of the Lagrangian velocity-fluctuation vector is

$$\theta' = \arctan\frac{W'}{U'}, \tag{8}$$

while its rotation $\Delta\theta'$ over a finite (realisable) model timestep Δt is

$$\Delta\theta' = \arctan\left(\frac{U'\Delta W' - W'\Delta U'}{U'^2 + W'^2 + U'\Delta U' + W'\Delta W'}\right). \tag{9}$$

However the finite difference is not very tractable, and so we instead analyse statistics of the differential. Now $\theta' = \theta'(U', W')$, but because the velocities are stochastic, the differential dθ' is to be obtained not by the ordinary chain rule of Calculus, but by application of Ito's formula* (see Gardiner, 1983; or for application in the context of LS models, Thomson, 1987). Accordingly

$$\mathrm{d}\theta' = \left(a_u \frac{\partial\theta'}{\partial U'} + a_w \frac{\partial\theta'}{\partial W'} + \frac{b^2}{2}\frac{\partial^2\theta'}{\partial U'^2} + \frac{b^2}{2}\frac{\partial^2\theta'}{\partial W'^2} \right) \mathrm{d}t + \frac{\partial\theta'}{\partial U'} b\,\mathrm{d}\xi_u + \frac{\partial\theta'}{\partial W'} b\,\mathrm{d}\xi_w, \tag{10}$$

and carrying out the differentiations we obtain:

$$\mathrm{d}\theta' = \frac{U'(a_w\,\mathrm{d}t + b\,\mathrm{d}\xi_w) - W'(a_u\,\mathrm{d}t + b\,\mathrm{d}\xi_u)}{U'^2 + W'^2} + \frac{(b^2 - b^2)U'W'\,\mathrm{d}t}{(U'^2 + W'^2)^2}. \tag{11}$$

The second term on the rhs stems from the Ito correction, and obviously vanishes, but only because we have adhered to Kolmogorov similarity, i.e., scaled the random forcing equally in the two stochastic equations. As we consider stationary, horizontally-homogeneous turbulence, we henceforth drop the prime on W, assuming $\bar{w}$ = 0.

We may decompose dθ' into deterministic and random parts, $\mathrm{d}\theta' = \mathrm{d}\theta'_d + \mathrm{d}\theta'_r$. The deterministic part is

$$\mathrm{d}\theta'_d \equiv \langle \mathrm{d}\theta'; U, W, Z\rangle = \frac{U'a_w - W a_u}{U'^2 + W^2}\,\mathrm{d}t, \tag{12}$$

and is the expected rotation, given the particle's preceding values of velocity and position. The 'fluctuating rotation' is

$$\mathrm{d}\theta'_r = b\frac{U'\,\mathrm{d}\xi_w - W\,\mathrm{d}\xi_u}{U'^2 + W^2}. \tag{13}$$

The latter is 'model-independent' (no dependence on the $\boldsymbol{\phi}$ vector), with vanishing mean value since $\langle \mathrm{d}\xi_i\rangle = 0$, and has variance

$$\langle \mathrm{d}\theta_r'^2\rangle = \frac{b^2\,\mathrm{d}t}{U'^2 + W^2}, \tag{14}$$

(the variance of dθ' about the mean value dθ'_d for *prescribed* U', W). Given that we shall later suggest a new selection constraint (for well-mixed LS models) that specifies only the *mean* rotation angle, it is reassuring that the 'fluctuating rotation' is model-independent.

* We are indebted to an anonymous reviewer for correcting us on this important point.

Unconditional statistics of $\mathrm{d}\theta'$ are obtained by taking the probability-averaged integrals over $U' - W$ space. For example, the expected value for $\mathrm{d}\theta'$, *given* that particle position $Z = z$, is:

$$\langle \mathrm{d}\theta'; z\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle \mathrm{d}\theta'; U', W, z\rangle \;\; g_a(U', W, z)\, \mathrm{d}U'\, \mathrm{d}W, \tag{15}$$

and in view of Equation (12),

$$\langle \mathrm{d}\theta'; z\rangle = \mathrm{d}t \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{U' a_w - W a_u}{U'^2 + W^2} \;\; g_a(U', W, z)\, \mathrm{d}U'\, \mathrm{d}W. \tag{16}$$

The well-mixed condition gives for the $\mathbf{a}_i$:

$$\begin{aligned} a_u &= \frac{\phi_u}{g_a} + \frac{b^2}{2}\frac{\partial \ln g_a}{\partial U'} = \frac{\phi_u}{g_a} + \frac{b^2}{2}\frac{1}{g_a}\frac{\partial g_a}{\partial U'} \\ a_w &= \frac{\phi_w}{g_a} + \frac{b^2}{2}\frac{\partial \ln g_a}{\partial W} = \frac{\phi_w}{g_a} + \frac{b^2}{2}\frac{1}{g_a}\frac{\partial g_a}{\partial W} \end{aligned}\;. \tag{17}$$

Substituting into Equation (16) we have:

$$\begin{aligned} \langle \mathrm{d}\theta'; z\rangle \; = \; & \mathrm{d}t \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{U'\phi_w - W\phi_u}{U'^2 + W^2}\, \mathrm{d}U'\, \mathrm{d}W \\ & + \frac{b^2\, \mathrm{d}t}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\frac{U'}{U'^2 + W^2}\frac{\partial g_a}{\partial W} - \frac{W}{U'^2 + W^2}\frac{\partial g_a}{\partial U'}\right) \mathrm{d}U'\, \mathrm{d}W. \end{aligned} \tag{18}$$

Equation (18) provides the basis upon which we may diagnose mean trajectory rotation $\langle \mathrm{d}\theta'; z\rangle$, as implied by various Lagrangian stochastic models, for various types of turbulence. For simplicity we shall call LS models for which $\langle \mathrm{d}\theta'\rangle = 0$, that is, models in which there is no preferred direction of rotation of the velocity-fluctuation vector, ‘zero-spin’ models – admitting that this is a misuse of the term ‘spin’. In Section (3) we shall examine well-mixed 2-D models for the wind-tunnel dispersion data of Legg et al. (1986), showing that those doing the best job of calculating spread are zero-spin models.

3. Trajectory Curvature in Multi-Dimensional Gaussian Turbulence

By definition, in two-dimensional Gaussian turbulence the Eulerian velocity fluctuation pdf is

$$g_a(u', w) = \frac{1}{2\pi\sigma} \exp\left(-\frac{u'^2\sigma_w^2 + w^2\sigma_u^2 + u'wu_*^2}{\sigma^2}\right), \tag{19}$$

where $\sigma^2 = \sigma_u^2 \sigma_w^2 - u_*^4$, $u_*^2 = -\langle u'w \rangle$. It is of significance to the integrations which will follow that g_a is either (when $u_* = 0$) perfectly even (symmetric) on the u', w axes, or at least ($u_* \neq 0$) has opposite quadrant symmetry in $u' - w$ space.

3.1. Axi-symmetric, homogeneous, Gaussian turbulence

Borgas et al. (1997) considered dispersion in 3-D Gaussian turbulence, for which the turbulence was assumed to be minimally anisotropic, the departure from isotropy owing to the existence of a 'special direction', $\boldsymbol{\Omega}$, here taken to be aligned along the y axis, $\boldsymbol{\Omega}$ = (0, Ω, 0). They introduced a particular (but not unique) well-mixed model,

$$a_i = -\frac{U_i}{T} + \epsilon_{ijk} \Omega_j U_k = -\frac{U_i}{T} + (\underline{\Omega} \times \underline{U})_i, \tag{20}$$

wherein the additional component of the conditional mean acceleration acts perpendicular to the plane containing $\boldsymbol{\Omega}$ and U_i. With Ω_i = (0, Ω, 0) the conditional mean acceleration reduces to,

$$a_u = -\frac{U}{T_L} + \Omega W, \quad a_v = -\frac{V}{T_L}, \quad a_w = -\frac{W}{T_L} - \Omega U. \tag{21}$$

Now suppose we look at projections of the motion onto the $x - z$ and $y - z$ planes, and define

$$\theta = \arctan \frac{W}{U}, \quad \beta = \arctan \frac{V}{U}. \tag{22}$$

It is easy to show that:

$$\langle \mathrm{d}\theta; U, V, W \rangle = \frac{U a_w - W a_u}{U^2 + W^2} \,\mathrm{d}t = -\Omega \,\mathrm{d}t, \tag{23}$$

whence it follows at once upon averaging in velocity space that there is non-zero spin, $\langle \mathrm{d}\theta \rangle = -\Omega \,\mathrm{d}t$. Similarly,

$$\langle \mathrm{d}\beta; U, V, W \rangle = \frac{U a_v - V a_u}{U^2 + V^2} \,\mathrm{d}t = -\Omega \,\mathrm{d}t \frac{VW}{U^2 + V^2}. \tag{24}$$

Since this is odd in V (and W) it vanishes upon averaging over V (or W): $\langle \mathrm{d}\beta \rangle = 0$. This provides a perspective on the novel aspect of the Borgas et al. model for axisymmetric turbulence: the chosen $\boldsymbol{\phi}$ results in mean curvature of trajectories, which manifests as spiralling about the axis defined by the special direction $\boldsymbol{\Omega}$. If we reduce to the fully isotropic case ($\boldsymbol{\phi}$ = 0), we have $\langle \mathrm{d}\theta \rangle$ = $\langle \mathrm{d}\beta \rangle$ = 0, and more-rapid dispersion results.

3.2. Gaussian Inhomogeneous Turbulence

We retain the earlier-given (general) forms for a_u, a_w (which involve the only partly constrained non-uniqueness vector with components ϕ_u, ϕ_w), but adopt specifically the Gaussian pdf $g_a(U', W)$ for substitution into Equation (18). It can be shown by a tedious but straightforward integration that **any** well-mixed model (for U', W) in Gaussian turbulence, provided it is consistent with the Kolmogorov similarity theory, has:

$$\langle \mathrm{d}\theta'; z\rangle = \mathrm{d}t \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{U'\phi_w - W\phi_u}{U'^2 + W^2}\, \mathrm{d}U'\, \mathrm{d}W. \tag{25}$$

To obtain this result it is helpful to transform to polar coordinates $s = (U'^2 + W^2)^{1/2}$, arctan(W/U'), and to bear in mind the symmetry of g_a, namely $g_a(-U', -W) \equiv g_a(U', W)$. In view of this symmetry, any term in $(U'\phi_w - W\phi_u)/g_a$ that involves a factor $(U')^m W^n$ with $(m+n)$ *odd* will make no contribution to $\langle \mathrm{d}\theta'; z\rangle$ through the integral in Equation (25).

Now, several well-mixed models (varying in their specification of $\boldsymbol{\phi}$) have been proposed for multi-dimensional Gaussian turbulence.

3.2.1. *Thomson's (1987) Model for Gaussian Turbulence*

Thomson's model for the total velocity (U, W) corresponds (to first order in dt) to the following model* for the velocity fluctuation (U', W):

$$\frac{\phi_u}{g_a} = -\frac{1}{2}\frac{\partial u_*^2}{\partial z} + \frac{1}{2\sigma^2} \times \left(U'W\left(\sigma_w^2 \frac{\partial \sigma_u^2}{\partial z} - u_*^2 \frac{\partial u_*^2}{\partial z}\right) + W^2\left(u_*^2 \frac{\partial \sigma_u^2}{\partial z} - \sigma_u^2 \frac{\partial u_*^2}{\partial z}\right)\right), \tag{26}$$

$$\frac{\phi_w}{g_a} = \frac{1}{2}\frac{\partial \sigma_w^2}{\partial z} + \frac{1}{2\sigma^2} \times \left(U'W\left(u_*^2 \frac{\partial \sigma_w^2}{\partial z} - \sigma_w^2 \frac{\partial u_*^2}{\partial z}\right) + W^2\left(\sigma_u^2 \frac{\partial \sigma_w^2}{\partial z} - u_*^2 \frac{\partial u_*^2}{\partial z}\right)\right). \tag{27}$$

Multiplying by the velocities, substituting into Equation (25), and integrating, it follows that $\langle \mathrm{d}\theta'; z\rangle = 0$ (this is because in each term of the integrand $(U')^m W^n$ appears with $m+n$ odd). Thomson's well-mixed multi-dimensional LS model for Gaussian turbulence is a 'zero-spin' model.

3.2.2. *Borgas' Model for Gaussian Turbulence*

Rodean (1996) has provided a derivation of the following well-mixed model for Gaussian turbulence – here simplified to the steady-state, horizontally-homogen-

* Obtained by subtracting the term $W\,\partial\bar{u}/\partial z$ from Thomson's a_u, which follows from the fact over the interval dt, $d\bar{u} = (W\,\mathrm{d}t)\partial\bar{u}/\partial z$.

eous case; this model was first given by Sawford and Guest (1988), and attributed to M. Borgas. The $\boldsymbol{\phi}$ vector in 2-D is:

$$\begin{aligned}\frac{\phi_u}{g_a} = & -\frac{\partial u_*^2}{\partial z} + \frac{u_*^2}{\sigma^2}\frac{\partial \sigma^2}{\partial z} - \frac{u_*^2}{\sigma^2}\frac{\partial \bar{u}}{\partial z}(\sigma_w^2 U' + u_*^2 W) \\ & -W\frac{\partial \bar{u}}{\partial z} + \frac{u_*^2}{2\sigma^2}\left(\frac{\partial \sigma_w^2}{\partial z} - \frac{\sigma_w^2}{\sigma^2}\frac{\partial \sigma^2}{\partial z}\right)U'^2 \\ & +\frac{u_*^2}{\sigma^2}\left(\frac{\partial u_*^2}{\partial z} - \frac{u_*^2}{\sigma^2}\frac{\partial \sigma^2}{\partial z}\right)U'W \\ & +\frac{u_*^2}{2\sigma^2}\left(\frac{\partial \sigma_u^2}{\partial z} - \frac{\sigma_u^2}{\sigma^2}\frac{\partial \sigma^2}{\partial z}\right)W^2, \end{aligned} \tag{28}$$

$$\begin{aligned}\frac{\phi_w}{g_a} = & \frac{\partial \sigma_w^2}{\partial z} - \frac{\sigma_w^2}{2\sigma^2}\frac{\partial \sigma^2}{\partial z} + \frac{\sigma_w^2}{\sigma^2}\frac{\partial \bar{u}}{\partial z}(\sigma_w^2 U' + u_*^2 W) \\ & +\frac{\sigma_w^2}{2\sigma^2}\left(\frac{\sigma_w^2}{\sigma^2}\frac{\partial \sigma^2}{\partial z} - \frac{\partial \sigma_w^2}{\partial z}\right)U'^2 \\ & +\frac{\sigma_w^2}{\sigma^2}\left(\frac{u_*^2}{\sigma^2}\frac{\partial \sigma^2}{\partial z} - \frac{\partial u_*^2}{\partial z}\right)U'W \\ & +\frac{\sigma_w^2}{2\sigma^2}\left(\frac{\partial \sigma_u^2}{\partial z} - \frac{\sigma_u^2}{\sigma^2}\frac{\partial \sigma^2}{\partial z}\right)W^2. \end{aligned} \tag{29}$$

Multiplying by the appropriate velocities for evaluation of Equation (25), we obtain a non-vanishing contribution to $\langle \mathrm{d}\theta'; z\rangle$. The Borgas well-mixed model for Gaussian turbulence is not a zero-spin model. As we shall show, this correlates with its giving generally the poorest agreement (among LS models we studied) with observed rates of dispersion.

3.2.3. *Flesch and Wilson Model*

In the more general context of non-Gaussian turbulence, Flesch and Wilson (1992) introduced a well-mixed model designed to have the property that $\boldsymbol{\phi}$ should act so as not to change the orientation of the velocity-fluctuation vector (this model has been generalised to three dimensions by Monti and Leuzzi, 1996). Since the Flesch-Wilson model has

$$U'\phi_w - W\phi_u = 0, \tag{30}$$

it follows immediately from Equation (25) that it is a zero-spin model, in the case of Gaussian turbulence. But Flesch and Wilson noted the possibility (however improbable) of very large accelerations occurring according to this model. While that may not in practise be important, it remains a troublesome point.

3.3. Comparison of Well-Mixed Gaussian Models with Disersion Experiments

We have applied two-dimensional Thomson, Borgas, and Flesch–Wilson LS models to simulate dispersion in and above a model plant canopy, in wind tunnel flow (Legg et al., 1986; hereafter LRC). We have elsewhere (Flesch and Wilson, 1992) given our choice of flow statistics, derived from the data provided by the authors. We must point out that velocity statistics of this flow are highly non-Gaussian, and that it is therefore inappropriate to apply LS models intended for Gaussian flows. However Flesch and Wilson have already shown that Gaussian models provide, in fact, a very good simulation of the experiments. The Flesch–Wilson model here assumes Gaussian velocity statistics, like the other models.

Figure 1 compares the observed rate of spread, from a line source in the flow, with the predictions of each of the LS models. Also shown are the unique 1-D LS model for Gaussian turbulence, which incidentally is in poor agreement with the observations near the source; and another model, described in the next section. Figure 1 indicates that available 2-D well-mixed models differ in their prediction of the rate of dispersion in the LRC flow, and that the zero-spin models both provide excellent agreement with the observations, whereas the Borgas model, not a zero-spin model, underestimates the rate of spread. This is similar to what has been found in the case of homogeneous turbulence: spiralling of trajectories reduces the rate of dispersion. Figure 2 shows that the ϕ fields of the Thomson and the Borgas models are very different for the LRC flow. This brings us to the question, is there a constraint on ϕ, in addition to the w.m.c., that ensures a zero-spin model?

4. Tailoring ϕ to Minimize Trajectory Looping

Many atmospheric flows involve 'organised' rotation – tornados, building wakes, the convective boundary-layer, etc. Presumably however, that rotation would enter LS models through the *mean* velocity field. It is not obvious that one would ever wish to 'design in' a 'biased' rotation of the Lagrangian velocity – *fluctuation* vector – although possibly criteria with respect to (e.g.) $\langle d\theta'^2 \rangle$, the variance of the fluctuating rotation, might prove useful (at present we have no observations of that statistic). Then supposing one wished to tailor ϕ to obtain a zero-spin model, how to proceed? In general, Equation (18) provides an implicit specification constraining ϕ to ensure spinless velocity-deviation.* But we have been unable to extract from it an explicit (and therefore usable) condition.

* Recall that in LS models for the *total* Lagrangian velocity, ϕ is to be augmented by the amount

$$(U_j - \bar{u}_j)\frac{\partial \bar{u}_i}{\partial x_j} g_a .$$

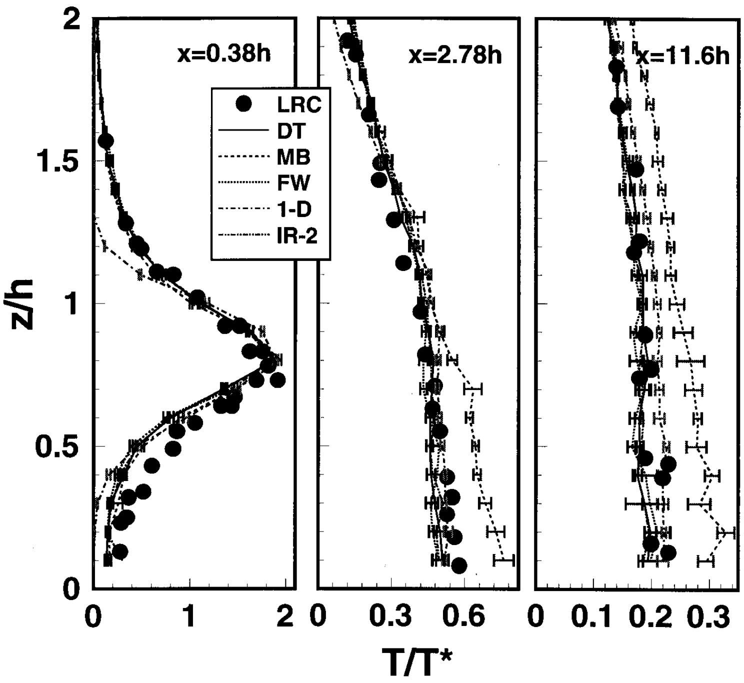

Figure 1. Lagrangian stochastic simulations of dispersion of heat from an elevated line source within a model plant canopy in a wind tunnel, in comparison with observations (●) by Legg et al. (1986). The length scale h is canopy height. The temperature scale $T^* = Q/(\rho c_p h_s U_s)$, where Q is the source strength [W m^{-1}], h_s is the source height, and U_s is the mean windspeed at source height. Error bars give the standard error of the mean resulting from a set of independent simulations with each model. Legend identifies these models: 1-D, The unique well-mixed LS model for 1-D Gaussian turbulence; DT, Thomson model for multi-dimensional Gaussian turbulence; MB, Borgas model for multi-dimensional Gaussian turbulence; FW, Flesch–Wilson model; IR-2, Well-mixed model for Gaussian turbulence based on irrotational ϕ/g_a.

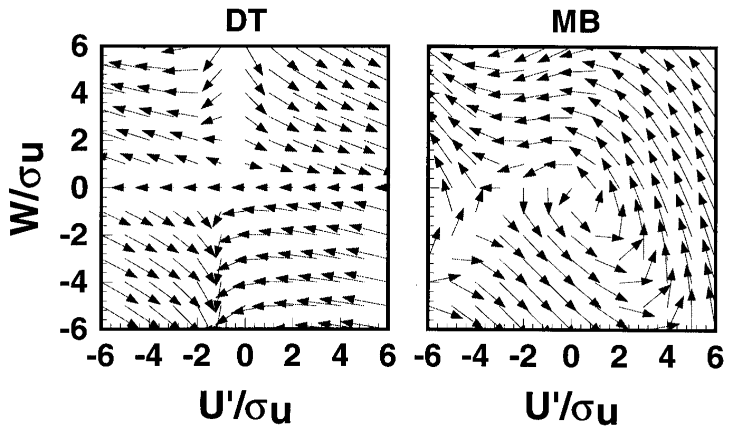

Figure 2. The ϕ/g_a fields of the Thomson (DT) and Borgas (MB) well-mixed LS models for Gaussian turbulence, evaluated at height $z/h = 0.85$ in the wind-tunnel flow of Legg et al. (1986).

On the other hand we note that an arbitrary non-divergent but rotational vector $\boldsymbol{\phi}_S/g_a$ (i.e. having zero divergence but non-zero curl; such a vector is called ‘solenoidal’) can be added to $\boldsymbol{\phi}/g_a$ without altering the value of $\nabla \cdot (\boldsymbol{\phi}/g_a)$, which is constrained by the wmc. Accordingly we hypothesize (but have not proven) that LS models having $\boldsymbol{\phi}/g_a$ irrotational, will be ‘zero-spin’ models. But even if this is true, the relationship is generally not reciprocal: for although (as shown earlier) the Thomson multi-dimensional Gaussian model is a zero-spin model, the solenoidal component of its $\boldsymbol{\phi}$ field is non-zero. In the case of steady-state, two-dimensional, horizontally-uniform, Gaussian turbulence, even were the shear stress to vanish, Thomson’s specification for $\boldsymbol{\phi}/g_a$ has non-vanishing curl:

$$\nabla \times \frac{\boldsymbol{\phi}}{g_a} = \frac{U'}{2}\frac{\partial \ln \sigma_u^2}{\partial z}. \tag{31}$$

4.1. Numerical determination of an irrotational $\boldsymbol{\phi}/g_a$ field

We invoke the Helmholtz decomposition theorem,* and determine an (irrotational) $\boldsymbol{\phi}$ as

$$\frac{\phi_i}{g_a} = -\frac{\partial \psi}{\partial u_i'}. \tag{32}$$

Application of the w.m.c. results in an equation

$$\frac{\partial^2 \psi}{\partial u_i'^2} = \frac{1}{g_a}\left(\frac{\partial g_a}{\partial t} + \frac{\partial}{\partial x_i}(u_i' g_a) - \frac{\partial \psi}{\partial u_i'}\frac{\partial g_a}{\partial u_i'}\right), \tag{33}$$

for the scalar field ψ (g_a is the pdf for the velocity fluctuation). We solved Equation (33) numerically, to obtain the field of $\boldsymbol{\phi}/g_a$ at each of 300 levels on the range $0 \le z \le 6h$ (h the canopy height) for the LRC flow. The integration was performed on a rectangular domain:

$$\begin{array}{ll} -10\sigma_u \le U - \bar{u} & \le 10\sigma_u \\ -10\sigma_w \le W & \le 10\sigma_w \end{array}, \tag{34}$$

with resolution $0.2\sigma_u$, $0.2\sigma_w$, specifying that the normal gradient $\mathbf{n} \cdot \nabla\psi$ of ψ at the boundaries ($\mathbf{n}$ being a unit vector normal to the boundary) should vanish.** During the subsequent LS simulations, $\boldsymbol{\phi}$ was determined at any location (U', W, Z) by interpolation from the grid.

A simulation of the LRC dispersion experiment using this irrotational $\boldsymbol{\phi}/g_a$ model is shown on Figure 1. There is no (statistically) significant difference between

* With some reservation as to its applicability, for the theorem is predicated on some conditions.

** It is not clear which are the correct boundary conditions. However we found that except very close to the boundaries, the solution is not very sensitive to the choice made.

this simulation and those of the zero-spin models* (Thomson, Flesch-Wilson), and, all three provide quite good agreement with the measurements – whereas the Borgas model does not. It is characteristic of the non-zero-spin Borgas model, that particles move on counter-clockwise looping trajectories.

5. Conclusion

Well-mixed LS models for which there is a preferred direction of rotation ($\langle \mathrm{d}\theta'; z\rangle \neq 0$) of the Lagrangian velocity-*fluctuation* vector give rise to looping trajectories, and a reduced rate of dispersion. In a particular case we examined (dispersion in a model plant canopy within a wind tunnel), zero-spin models provided good (and generally indistinguishable) agreement with observations. Thus we suggest that a supplementary specification (beyond enforcing consistency with g_a by imposing the wmc) to reduce membership of the class of well-mixed multi-dimensional LS models, is the requirement that $\langle \mathrm{d}\theta'; z\rangle = 0$. However as far as we can tell, this does not select a *unique* well-mixed, zero-spin model. Nor are we able to provide an explicit recipe for $\boldsymbol{\phi}$ that results in the zero-spin property, though it is plausible that the requirement $\boldsymbol{\phi}/g_a$ be irrotational might suffice.

Finally, an unambiguous definition of 'looping' of particle trajectories is needed. Let $P(\mathbf{x}_2, t_2 \mid \mathbf{x}_1, t_1)$ be the transition probability density, from position $\mathbf{x}_1$ at time t_1 to the region of $\mathbf{x}_2$ at later time t_2. Then $P(\mathbf{x}, t \mid \mathbf{x}, t_0)$ is the probability density for a *return* at time $t > t_0$ to a location earlier occupied, and quantifies the probability density for 'looping' relative to fixed coordinates. The requirement that

$$\frac{\partial P(x_i, t \mid x_i, t_0)}{\partial t} \leq 0 \quad \forall t,\ \forall x_i, \tag{35}$$

seems one possible mathematical prescription for 'no-looping' (again, relative to fixed coordinates). Now, $P(\mathbf{x}, t \mid \mathbf{x}, t_0)$ is just the concentration at $(\mathbf{x}, t)$ due to the release of unit mass at $\mathbf{x}$ at time $t = t_0$. It follows immediately from the mass conservation equation that condition (35) requires

$$\frac{\partial F_i}{\partial x_i} \geq 0 \quad \forall\, t > t_0, \tag{36}$$

where F_i is the mean flux density subsequent to a unit release at $(\mathbf{x}, t_0)$. This seems a sensible result, requiring that the spatial field of the mean vector mass flux density which results from the release of unit mass at the point $\mathbf{x}$ should be such as to *never increase* the concentration at $\mathbf{x}$. Unfortunately, Equation (36) raises no explicit constraint on the coefficients of the LS model. But in any case, it is probably more relevant to prohibit trajectory 'looping' as seen in a drifting frame of reference. In the highly restrictive case of a flow having a constant and spatially-uniform mean

* The ϕ/g_a fields for the other models are analytical, so need not be obtained numerically.

velocity field (**U**), the probability density for 'looping' in a coordinate frame that moves with the mean flow is $P(\mathbf{x}+\mathbf{U}(t-t_0), t \mid \mathbf{x}, t_0)$: it seems unlikely that an explicit constraint on model coefficients would ensue from constraining this density function.

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Appendix A: Trajectory Curvature in 1-D Turbulence

In the case of atmospheric turbulence, fluctuations u' in horizontal windspeed are much smaller than the mean wind $\bar{u} = \bar{u}(z)$, except very close to the ground. It is therefore common to construct one-dimensional LS models of atmospheric dispersion in the x–z plane, models that ascribe to the particle the velocity vector $(\bar{u}, W)$, i.e., exclude the alongwind fluctuation. We shall consider the trajectory rotation that arises in such treatments. The change dU in (total) Lagrangian alongstream velocity over dt is just

$$\mathrm{d}U = \mathrm{d}Z \frac{\partial \bar{u}}{\partial z} = W\,\mathrm{d}t \frac{\partial \bar{u}}{\partial z}, \tag{37}$$

while the (stochastic) increment in vertical velocity is

$$\mathrm{d}W = a_w(W, Z)\,\mathrm{d}t + b\,\mathrm{d}\xi_w. \tag{38}$$

Then the conditional mean rotation of the $(\bar{u}, W)$ vector is easily shown to be

$$\langle \mathrm{d}\theta; W, Z\rangle = \frac{\bar{u} a_w(W,Z) - W^2 \dfrac{\partial \bar{u}}{\partial z}}{\bar{u}^2 + W^2}\,\mathrm{d}t + \frac{b^2 \bar{u}\,\mathrm{d}tW}{(\bar{u}^2 + W^2)^2}, \tag{39}$$

where the second term on the rhs stems from the Ito correction.

For example we may consider Gaussian 1-D turbulence, for which the Eulerian vertical velocity pdf is:

$$g_a(w, z) = \frac{1}{\sqrt{2\pi}\sigma_w(z)} \exp\left(-\frac{w^2}{2\sigma_w^2(z)}\right). \tag{40}$$

The implied (and unique) well-mixed 1-D model is (Thomson, 1987)

$$a_w(W, Z) = -\frac{W}{T_L(z)} + \frac{1}{2}\frac{\partial \sigma_w^2}{\partial z}\left(1 + \frac{W^2}{\sigma_w^2}\right), \tag{41}$$

where we note that the drift correction part of this is even (symmetric) in W. Then,

$$\begin{aligned}\langle \mathrm{d}\theta; W, z\rangle \;=\; & \frac{\bar{u}\left(-\frac{W}{T_L(z)} + \frac{1}{2}\frac{\partial \sigma_w^2}{\partial z}\left(1 + \frac{W^2}{\sigma_w^2}\right)\right) - W^2\frac{\partial \bar{u}}{\partial z}}{\bar{u}^2 + W^2}\,\mathrm{d}t \\ & + \frac{b^2 \bar{u}\,\mathrm{d}t W}{(\bar{u}^2 + W^2)^2}.\end{aligned} \tag{42}$$

Now,

$$\langle \mathrm{d}\theta; z\rangle = \int_{-\infty}^{\infty} \langle \mathrm{d}\theta; W, z\rangle\;\, g_a(W, z)\,\mathrm{d}W. \tag{43}$$

Since g_a is even in W and $\langle \mathrm{d}\theta; W, Z\rangle$ is a sum of even and odd contributions, the integral decomposes into the integrals of even and odd functions of W: only the even part is non-zero, and it follows that:

$$\begin{aligned}\frac{\langle \mathrm{d}\theta; z\rangle}{\mathrm{d}t} \;=\; & A(z) - \exp\left(\frac{\bar{u}^2}{2\sigma_w^2}\right)\,\mathrm{erfc}\left(\frac{|\bar{u}|}{\sqrt{2}\sigma_w}\right) \\ & \times\left[\sqrt{\pi}A\frac{|\bar{u}|}{\sqrt{2}\sigma_w} - \frac{\sqrt{\pi}}{2\sqrt{2}\sigma_w}\frac{\bar{u}}{|\bar{u}|}\frac{\partial \sigma_w^2}{\partial z}\right],\end{aligned} \tag{44}$$

where

$$A(z) = -\frac{\partial \bar{u}}{\partial z} + \frac{\bar{u}}{2\sigma_w^2}\frac{\partial \sigma_w^2}{\partial z}. \tag{45}$$

In the neutrally-stratified and horizontally-homogeneous atmospheric surface layer (NSL), the verical profile of the mean wind is

$$\bar{u}(z) = \frac{u_*}{k_v}\ln\left(\frac{z}{z_0}\right), \tag{46}$$

where k_v (=0.4) is von Karman's constant, u_* is the friction velocity and z_0 is the surface roughness length. Thus for the NSL, $A = -u_*/(k_v z)$.

Random flight simulations (for the NSL, and for linearly-sheared Gaussian homogeneous turbulence) have confirmed Equations (44, 45). Not surprisingly, according to our analysis, and believably in reality, trajectories preferentially curve (clockwise) in the mean shear. An interesting case would be the region at the top of a crop canopy: where there are large positive values of both $\partial_z \bar{u}$ and $\partial_z \sigma_w$.

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