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DISPERSION BY TRANSITIONAL ATMOSPHERIC BOUNDARY LAYERS

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Abstract: The periods of time-varying turbulence in the atmospheric boundary layer, i.e. the morning and evening transitions, are often overlooked or highly idealised by dispersion models. These transitions make up a significant portion of the diurnal cycle and are known to affect the spread of pollution due to the different properties of turbulence in the residual and stable layers, resulting in phenomena such as lofting or fumigation.

Two main simulation techniques are presented for the purpose of modelling the dispersion of passive tracers in both convective and evening transition regimes: A 1-D Lagrangian stochastic model for inhomogeneous, non-Gaussian turbulence modified to include the additional condition that the turbulence be non-stationary, and a large-eddy particle model tracing pollutant paths using a combination of the resolved flow velocities and a random displacement model to represent sub-grid scale motions.

The benefit of representing skewness of vertical velocities in a Lagrangian stochastic model for convective turbulence is shown through comparison to observations and large-eddy simulation. The effect of the evening transition on the spread of pollution is investigated for different decay rates and initial atmospheric conditions through use of the large-eddy particle model, and the extent to which the results can be replicated by the Lagrangian stochastic model for non-stationary turbulence is explored.

Key words: *Lagrangian stochastic, large-eddy simulation, boundary-layer, convective, transition.*

INTRODUCTION

A large proportion of the pollution we produce is released into the atmospheric boundary layer, and with pollutants being harmful to the environment and people around them, the ability to predict their path is crucial. Industrial planning, air quality forecasting, and warning systems for disaster events, all depend on accurately predicting pollutant dispersion.

Through comparison to large-eddy simulation (LES) we investigate the extent to which Lagrangian stochastic (LS) modelling can accurately represent particle dispersion in the convective boundary layer (CBL). Starting with the Langevin equation for 1D diffusion in stationary inhomogeneous turbulence, we examine the benefit of more accurately representing the turbulence parameters, and including the skewness of vertical velocities present in the flow.

While there are a large number of studies concerning dispersion modelling in statistically stationary turbulence (e.g. deBaas et al. (1986), Mason (1992)), there are very few considering the case of non-stationary turbulence. This, however, occurs daily in the boundary layer during the morning and evening transitions corresponding with sunrise and sunset. We use LES to analyse the effect residual turbulence has on dispersion by examining an idealised evening transition (Nieuwstadt & Brost (1986)), and consider how LS models may be formulated to simulate such conditions.

A LAGRANGIAN STOCHASTIC MODEL

We begin with the Langevin equation to describe 1D (vertical) diffusion in non-stationary inhomogeneous turbulence:

$$dw = a(z,w,t)dt + b(z,w,t)dW(t). \qquad dz = wdt \tag{1}$$

where z, w, and t are vertical position, vertical velocity, and time respectively, and dW is an incremental Wiener process. Using Kolmogorov similarity theory, the Fokker-Planck equation and the well-mixed criteria of Thomson (1987) we may derive a model for the evolution of particle velocity based on the vertical velocity variance σ_w^2 and dissipation of kinetic energy ε of the turbulence:

$$dw = -\frac{C_0\varepsilon}{2\sigma_w^2}wdt + \frac{1}{2}\left(1+\frac{w^2}{\sigma_w^2}\right)\frac{\partial\sigma_w^2}{\partial z}dt + \frac{1}{2\sigma_w^2}\frac{\partial\sigma_w^2}{\partial t}dt + (C_0\varepsilon)^{1/2}\,dW(t) \tag{2}$$

where C_0 is the dispersion parameter. The profiles of σ_w^2 and ε as shown in figure 1 may be in the form of parameterized profiles fitted to observations and simulations (dashed) or profiles generated from LES at regular time intervals (solid).

Turbulence in the boundary layer can be defined more accurately, particularly in convective conditions, by using the third moment of vertical velocity $\overline{w^3}$ with the skewness of vertical velocities S equal to $\overline{w^3}/\sigma_w^3$. Skewness is a typical feature of convection driven by surface heating as warmed air close to the surface forms convective columns of comparatively fast moving, rising air surrounded by more slowly descending air. This feature of the CBL may be represented in a Lagrangian stochastic model by formulating it around a skewed probability density function for vertical velocity w at height z and time t, i.e.

$$P = \frac{A}{\sqrt{2\pi}\sigma_a}\exp\left[-\frac{1}{2}\left(\frac{w-w_a}{\sigma_a}\right)^2\right] + \frac{B}{\sqrt{2\pi}\sigma_b}\exp\left[-\frac{1}{2}\left(\frac{w+w_b}{\sigma_b}\right)^2\right] \tag{3}$$

where A, B, w_a, w_b, σ_a and σ_b are parameters to be determined. Given this form for P, the vertical velocity evolution equation for skewed turbulence is given by

$$dw = a(z,w,t)dt + b(z,w,t)dW(t) \tag{4}$$

where

$$a = \frac{1}{P}\left(-\frac{\sigma_w^2}{\tau}Q + \phi\right) \tag{5}$$

$$b = (C_0\varepsilon)^{1/2} \tag{6}$$

with Q defined as

$$Q = AP_a\left(\frac{w-w_a}{\sigma_a^2}\right) + BP_b\left(\frac{w+w_b}{\sigma_b^2}\right) \tag{7}$$

and

$$\begin{aligned}\phi = &-\frac{1}{2}\left(1+\mathrm{erf}\frac{v_a}{\sqrt{2}}\right)\frac{\partial}{\partial z}(Aw_a) + \frac{1}{2}\left(1+\mathrm{erf}\frac{v_b}{\sqrt{2}}\right)\frac{\partial}{\partial z}(Bw_b) \\ &+ P_a\sigma_a\left\{\left(\frac{\partial}{\partial z}(A\sigma_a) + \frac{Aw_a}{\sigma_a}\frac{\partial w_a}{\partial z}\right) + \left(A\frac{\partial w_a}{\partial z} + \frac{Aw_a}{\sigma_a}\frac{\partial \sigma_a}{\partial z}\right)v_a + A\frac{\partial \sigma_a}{\partial \sigma_z}v_a^2\right\} \\ &+ P_b\sigma_b\left\{\left(\frac{\partial}{\partial z}(B\sigma_b) + \frac{Bw_b}{\sigma_b}\frac{\partial w_b}{\partial z}\right) - \left(B\frac{\partial w_b}{\partial z} + \frac{Bw_b}{\sigma_b}\frac{\partial \sigma_b}{\partial z}\right)v_b + B\frac{\partial \sigma_b}{\partial \sigma_z}v_b^2\right\}\end{aligned} \tag{8}$$

where

$$v_a = \frac{w-w_a}{\sigma_a} \qquad v_b = \frac{w+w_b}{\sigma_b} \quad .$$

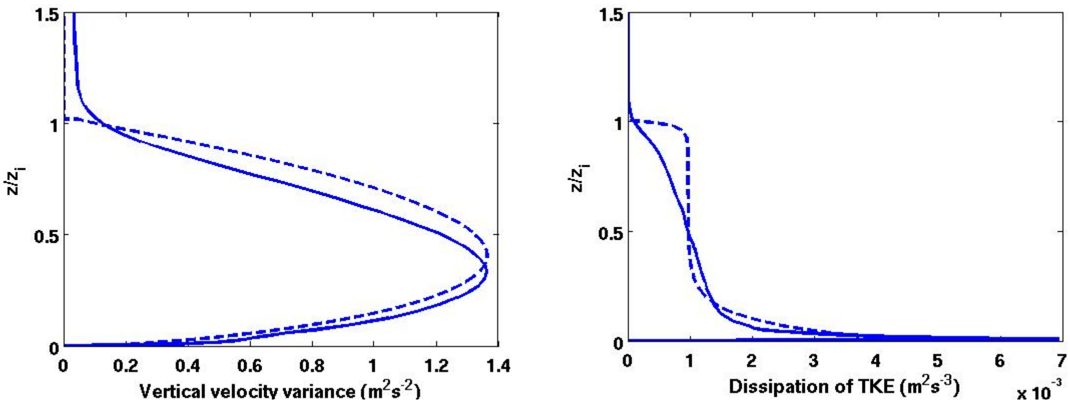

Figure 1: A comparison of vertical profiles of vertical velocity variance (left) and dissipation of TKE (right) as produced from the parameterizations of Weil (1990) (dashed), and the CBL large-eddy simulation at model time t = 10800s (solid).

LARGE-EDDY SIMULATION (LES)

Large-eddy simulation is a well-established technique for simulating turbulent flows such as the atmospheric boundary layer. Large-eddy models simulate turbulence in high Reynolds number flows through the numerical solution of the Navier-Stokes equations along with those for mass and momentum conservation. By separating turbulent eddies of different scales, LES efficiently resolves the large, energy-carrying eddies while smaller scale motions are parameterized according to some closure scheme. Such simulation methods produce detailed information about various aspects of the flow. Figure 2 shows an x-y cross section of the vertical velocity at $z = 50$ m with positive velocities in red and negative in blue.

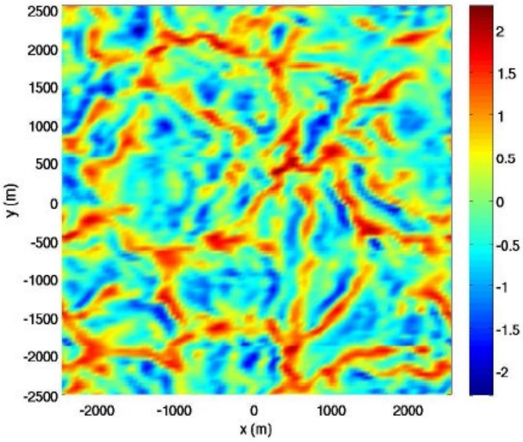

Figure 2: x-y cross section of vertical velocities in a large-eddy simulation of a typical daytime CBL.

In order to model dispersion using LES, particle paths are calculated using a combination of the resolved and sub-grid velocities of the simulated flow at their given position. The resolved part of each particle's 3D motion is calculated using an Euler forward step method from the current model time-step

$$d\mathbf{x} = \mathbf{u} \cdot dt \tag{9}$$

where the 3D velocity $\boldsymbol{u}$ at the current particle position is determined by linear interpolation of the resolved flow velocity at the surrounding grid points.

The motions due to sub-grid scale eddies are represented by random perturbations given to the particles in the x, y, and z direction at each model time-step. These random perturbations follow a Gaussian distribution with standard deviation

$$\sigma_d = (2K\Delta t)^{1/2} \tag{10}$$

where K is the interpolated model eddy diffusivity at the particle position, and Δt is the model time-step. The imposition of this random perturbation generates a mean drift velocity towards regions of small K and this is corrected for by adding a drift correction term ∇K.

At the lateral boundaries of the flow a periodic tiling of the domain is used, while particles reaching the surface are perfectly reflected and motion above the boundary layer top is restricted by a capping inversion.

DISPERSION IN A CONVECTIVE BOUNDARY LAYER (CBL)

In a daytime clear-topped CBL the approximately constant surface heating leads to the development of statistically stationary convective turbulence with a slowly increasing boundary layer depth over time. The large-eddy model is set-up to generate strong convective turbulence with a prescribed constant surface heat flux of 100 Wm^{-2}, uniform wind of 5 ms^{-1} and an initial potential temperature profile uniform with height up to 800 m and a capping inversion of strength 0.0025 Km^{-1} above 800 m. The domain consists of 100 X 100 points in the horizontal at 50 m spacing, and 70 points of variable spacing to a height of 4000 m in the vertical. After 3 hours model time the turbulence has become statistically stationary and the simulation represents a typical CBL, as shown in figure 3.

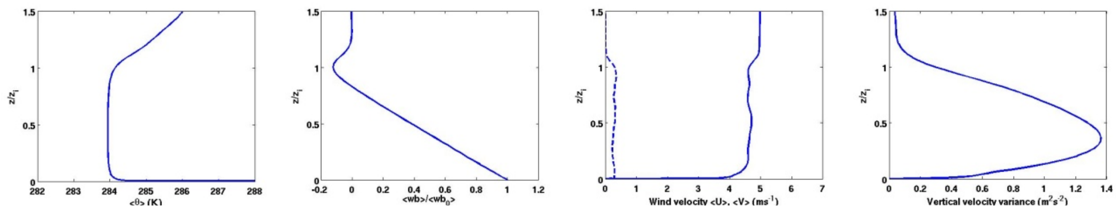

Figure 3: Vertical profiles of CBL properties calculated using a horizontal area average (represented by angular brackets) from large-eddy simulation, plotted against height non-dimensionalised by BL depth.

To generate dispersion statistics 90,000 particles are released over a uniform grid spanning the horizontal domain, and at a given initial height z. Their paths are calculated as described in the previous section for 10,000 seconds after the point of release.

Three variations of the LS model are used to simulate particle paths in the CBL. These treat one-dimensional, stationary, inhomogeneous turbulence initially using parameterized profiles of σ_w^2 and ε, moving on to be driven by profiles produced by LES, and finally including a representation of the skewness of vertical velocities, as described previously. 50,000 particles are released at initial height z and tracked for 10,000 seconds, as in the large-eddy simulations.

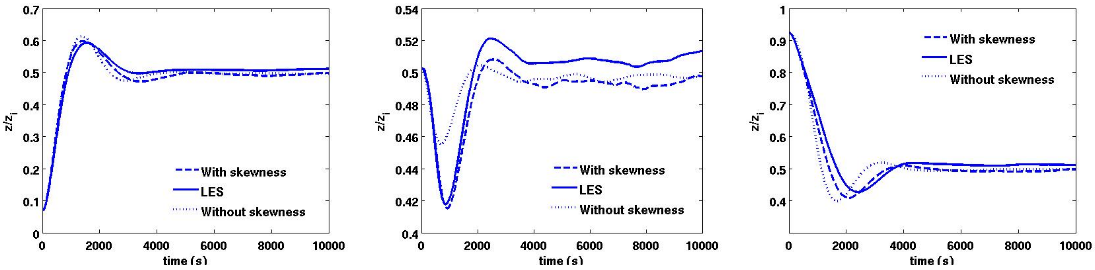

Figure 4: Comparison of mean plume heights in the CBL generated by: LS model not representing skewness (eq. 2), LS model including representation of CBL skewness (eq. 4); and large-eddy simulation.

As can be seen from the figures above, for all release heights the mean plume height tends to $z/z_i = 0.5$ as strong vertical mixing results in the particles becoming well-mixed over the entire depth of the CBL. For both the low and high particle releases, including a representation of skewness of vertical velocities slightly improves the magnitude and timing of the peak in mean plume height. In the mid-level particle release the short term agreement ($< 2000\ s$) between LS and LES is significantly improved in the case of the skewed model, at the cost of slightly reduced agreement in the long term.

DISPERSION IN AN EVENING TRANSITION

We investigate dispersion in an idealised evening transition based on the work of Nieuwstadt & Brost (1986). To simulate the decay of convective turbulence the surface heat flux is switched instantaneously from its daytime CBL value of 100 Wm^{-2}, to zero. The effect the resulting transition has on dispersion is investigated through the release of particles at various times relative to this switch-off.

Figure 5 shows the vertical particle concentration over 6000 seconds from their time of release. The left hand plot represents particles released before the switch-off of surface heat flux into a CBL with strong vertical mixing. The particle concentration decreases rapidly after release as the material is mixed over the entire boundary layer. After a peak aloft at approximately 1200 s the particles reach a well-mixed state over the depth of the BL. In the right hand plot we have the behaviour of particles released 1200 s after the switch-off of surface heat flux. We see that in this case vertical mixing is significantly less, with particles remaining in high concentrations near the source height.

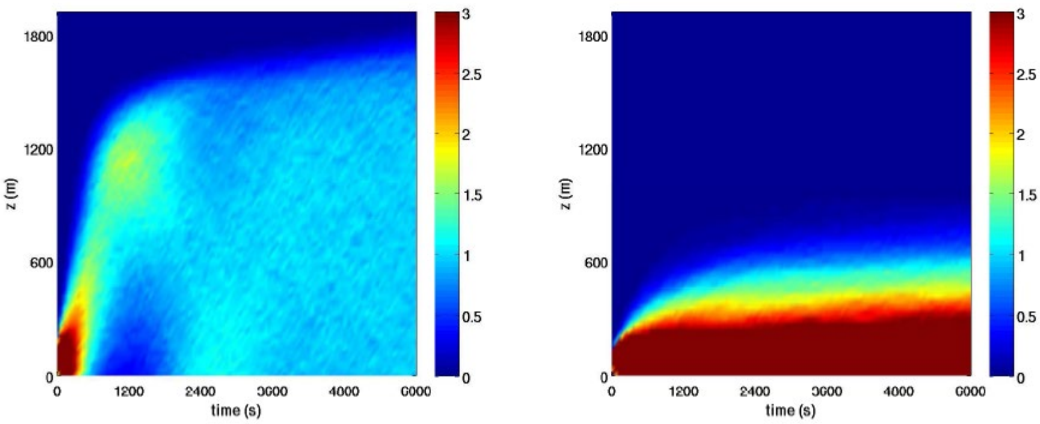

Figure 5: Particle concentration from a near surface release 1200 seconds before the switch-off of surface heat flux (left) and 1200 seconds after (right). Particle released at height $z = 100$ m and paths produced using large-eddy simulation.

When using LS methods (red) to simulate particles released after the transition we find that the mean plume height (solid) plus and minus one standard deviation (dashed) are not in agreement with LES (blue) (figure 6). The LS model has a tendency to over-estimate mixing in the transition phase. We theorise that this is due to stratification in the flow suppressing vertical motions, an effect not represented in the LS model. By modifying the profile of σ_w^2 according to the strength of the stratification, significantly better agreement to LES can be obtained (green).

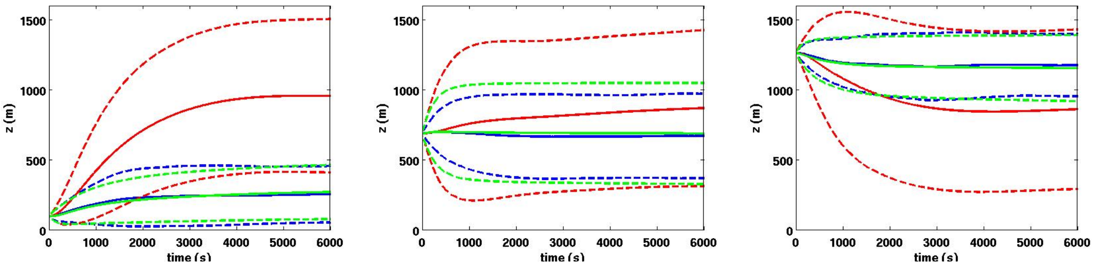

Figure 6: Plume mean height (solid) plus and minus one standard deviation (dashed) for particles released 1200 seconds after the switch-off of surface heat flux. Simulated using LES (blue), LS model with skewness (red), and LS model with modified σ_w^2 (green).

SUMMARY

We have outlined two methods of modelling dispersion: A Lagrangian stochastic model re-formulated to represent skewness of vertical velocities; and large-eddy simulation using resolved eddy motions combined with a random displacement model to produce particle paths.

In statistically stationary convective turbulence we have shown that representing skewness of vertical velocities in Lagrangian stochastic models gives better mean plume height agreement to dispersion results of large-eddy simulation.

In an idealised evening transition, we have shown that the time of particle release is important in predicting the vertical concentration over the depth of the decaying CBL. We have also shown that modifying the σ_w^2 profile driving our Lagrangian stochastic model significantly improves agreement of mean plume heights and spread with LES for a post-transition particle release.

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