EAS 471, Atmospheric Modelling

J.D. Wilson

February 25, 2016

Contents

Contents **i**

9 Modelling the Atmospheric Boundary-Layer ("physics") **56**
9.1 Role of the ABL in NWP . . . 57
9.2 Estimating the unresolved fluxes using K-theory . . . 58
9.2.1 Monin-Obukhov Similarity Theory of the ASL (MOST) . . . 59
9.3 A vintage treatment of the ABL (old Canadian Regional Finite Element Model) . . 61

10 Lagrangian approach to dispersion **63**
10.1 Taylor's Lagrangian Theory . . . 64
10.1.1 Comparison with Classical Eddy-Diffusion Solution . . . 66
10.1.2 Asymptotic results . . . 68
10.1.3 What is important about G.I.Taylor's result and when is K-theory valid? . . 68
10.2 Modern single-particle Lagragian stochastic models . . . 69
10.2.1 Zeroth- and first-order LS models . . . 69
10.2.2 Time step for (1st order) Lagrangian stochastic simulations . . . 70
10.2.3 Thomson's well-mixed constraint on first-order LS models . . . 70
10.2.4 Unique 1-d LS Model for Gaussian Inhomogeneous Turbulence . . . 71
10.2.5 Reflection at Boundaries . . . 72
10.2.6 LS models applicable in disturbed flows . . . 73

Bibliography **74**

Chapter 9

Modelling the Atmospheric Boundary-Layer ("physics")

We have seen that it is useful (and proper) to explicitly define, and find evolution equations for, the resolved state of the atmosphere $\overline{u}, \overline{v}, \overline{w}, \overline{p}, \overline{T}, \overline{\rho}_v ...$ In Numerical Weather Prediction, the average can be considered a spatial average over a domain XY of order 10-100 km $\times$ 10-100 km. We saw that the evolution equations $\partial\overline{\rho}_v/\partial t$, etc., contain the divergences of convective fluxes (of heat and vapour and momentum) "carried by" the unresolved motion. Concentrating on the vertical fluxes (which are in any case those we have best prospect of quantifying), the key unresolved fluxes are:

- heat: $\rho c_p \overline{w'T'}$
- vapour: $\overline{w'\rho'_v}$
- momentum: $\overline{w'u'}$, $\overline{w'v'}$, $\overline{w'w'}$

For example, Cumulus convection over a synoptic scale area causes large vertical heat and vapour fluxes at unresolved scales. The effects of such processes (eg. the drying and warming of the atmosphere over a region where precipitation is reaching the ground), then, will need to be "parameterised" and is an aspect of the "model physics" or "grid point computations".

A weather model has, obviously, boundaries in the vertical. Across the lower boundary, there are vertical fluxes into the model domain, and the heat and vapour thus introduced is carried up and redistributed within the atmosphere largely by motions that are unresolved in an NWP model, whose spatial averaging masks the eddies seen near ground. More specifically, the "free atmosphere," the region where the "dynamics" terms in the equations for the resolved variables are considered dominant, is coupled to the ground through the turbulent Atmospheric Boundary Layer (ABL) (or Planetary Boundary Layer (PBL), which feeds up heat and moisture, as well as transferring drag. These influences (friction, surface heating and evaporation) have an importance to a synoptic scale forecast that increases with the range of the forecast. It can readily be shown, for example, that over 24 hours surface evapotranspiration (E, kg m^{-2} s^{-1}) can easily increase the moisture content of the PBL by 25% – and this could be an important moisture supply for (eg.)

development of a tropical cyclone. Not only that: the surface heat flux (over very wet surfaces the virtual heat flux) determines the PBL stability, and thus convection. So surface fluxes are important w.r.t. changes in storage of heat and moisture (significant especially for longer-term forecasts), and w.r.t. stability (significant both in the short and longer range forecasts). It is believed therefore that even short range (12 hr) forecasts will be improved as surface parameterisation improves. When the lowest grid level of a weather model lies within the atmospheric surface layer (ASL), a shallow layer at the base of the PBL having a depth of order 50 m, the surface fluxes can be computed using the "Monin-Obukhov similarity theory" of the ASL. However in many models (especially older ones) the lowest level is far above the surface layer, and to calculate the boundary fluxes the entire PBL must be parameterised.

"Model physics" is the categorical name given to algorithms of a numerical weather model that calculate the above-mentioned and other mechanisms/processes.

9.1 Role of the ABL in NWP

Near ground, essentially all the vertical transport is performed by the unresolved field: there are strong vertical gradients in temperature, etc., and turbulent eddies transport heat (etc.) down these gradients. An NWP model needs to estimate these vertical fluxes and their divergence, or get the part of the tendency in $\overline{T}$ etc. due to ground forcing wrong. I don't want to get into this in detail; the turbulent ABL is the subject of the graduate course EAS 572.

We would like our NWP model to correctly calculate the redistribution of heat and vapour by the unresolved eddies (the turbulence) near ground. The turbulent layer has a diurnally, seasonally, and geographically varying depth $h(t)$. Of course, any model which does not contain grid points at heights below $h(t)$ cannot in any way model the evolution of $h(t)$ and the redistribution of heat and moisture by the turbulence. So it is highly desirable to provide sufficient levels near ground to at least resolve the vertical structure of the PBL in a way that is not incompatible with our very coarse knowledge on the horizontal scale. It is not obvious that anything short of a large number (say 50) of vertical grid points will suffice to model the PBL, in which the flow complexity is such that simple K-theory closure (see below) is not really adequate (there can exist, for example, counter gradient fluxes near the outer edge of the convective PBL or "CBL" – ie. mean heat flux is from heights where it is in the mean cooler to where it is in the mean warmer). Therefore an entire-PBL model will be complex and very time-consuming to compute, and there are competing demands for computer power – eg., to reduce the grid lateral length. In any case (Haltiner & Williams, 1980) for large scale NWP models, the exchange of heat and moisture between the PBL and the free atmosphere above may be more important than details within the PBL. Vertical transfer above the PBL is largely accomplished by cumulus convection and gravity waves (another form of unresolved field), and by the large scale (resolved) vertical velocities.

9.2 Estimating the unresolved fluxes using K-theory

Although there are synoptic scale horizontal gradients in our resolved meteorological fields $\overline{u}, \overline{T}$, etc., we might postulate some sort of "locally-uniformity" within the boundary-layer, such that the resolved vertical structure implies some "equilibrium" pattern to the vertical unresolved fluxes, and the horizontal unresolved fluxes are negligible. This permits a 1-dimensional (vertical variation only) treatment of the ABL.

Suppose, then, we concentrate on estimating only the vertical unresolved fluxes,

$$\left(\frac{\partial \overline{T}}{\partial t}\right)_{phys} = -\frac{\partial \overline{w'T'}}{\partial z} \tag{9.1}$$

(etc). The vertical eddy heat flux $Q_H = \rho c_p \overline{w'T'}$ is unknown[1]. If we attempt to derive a rigorous equation for it from the Navier-Stokes equations and the thermodynamic equation, the outcome is

$$\begin{aligned} \frac{\partial \overline{w'T'}}{\partial t} = 0 \quad &= \quad -\overline{w'^2}\,\frac{\partial \overline{T}}{\partial z} - \frac{\partial \overline{w'w'T'}}{\partial z} - \frac{1}{\rho_0}\,\overline{T'\frac{\partial p'}{\partial z}} + \frac{g}{T_0}\,\overline{T'^2} \\ &+ \quad \nu\,\overline{T'\nabla^2 w'} + \kappa\,\overline{w'\nabla^2 T'} \end{aligned} \tag{9.2}$$

The terms ρ_0, T_0 are reference density and temperature, and may be considered to be mean values across the ABL. It is important to note that all terms involving horizontal hetereogeneity have been neglected, ie. eqn (9.2) assumes $\partial \overline{w'T'}/\partial x = \partial \overline{w'T'}/\partial y = 0$; the proper interpretation here is that we are assuming the time tendency in statistics of the unresolved flow, and all terms involving horizontal derivatives, are small compared to other terms.

This is a complicated equation which has only deepened our problem, for now we have further unknown terms (the "closure problem"). However the equation at least offers us some insight, and can certainly be used diagnostically in the context of measurements. The first term on the r.h.s. is a production term: if there is unresolved motion then (by definition) $\overline{w'^2} \neq 0$, and if there is also a temperature gradient, then the motion acts to create a (mean) unresolved flow of heat - the sign of the flux depending on the sign of the temperature gradient. However the fourth term on the r.h.s. shows that the mere existence of temperature variance, in the presence of a gravity field, *always* acts to result in upward transport of heat (temperature variance vanishes only in a neutral atmosphere).

There is no rigorous way around the closure problem. Ultimately an assumption must be made. Here I will describe only the most basic closure assumption, namely the assumption of a linear flux-gradient relationship (most commonly called K-theory or first-order closure or gradient-diffusion closure). The model is certainly wrong in general, but one must go to much trouble to improve upon it.

In K-theory it is assumed that the mean gradient in a given "driving force" (such as temperature or humidity) drives a corresponding turbulent (more generally, unresolved) flux (of heat or

[1]Note: $\overline{w'T'}$ is called the "kinematic heat flux", or more precisely "kinematic heat flux density."

moisture). The K-theory closure for the vertical sensible (as distinct from latent; defined below) heat flux density is

$$Q_H = -\rho c_p \, K_H(z) \left(\frac{\partial \overline{T}}{\partial z} - \gamma_d \right) \tag{9.3}$$

where $K_H(z)$, $\mathrm{m}^2\ \mathrm{s}^{-1}$ is the "eddy diffusivity for heat" and the subtraction of the adiabatic lapse rate $\gamma_d = -g/c_p$ ensures zero heat flux in the neutral (adiabatically mixed) state of stratification. Similarly the moisture flux is

$$E(z) = \overline{w'\rho_v'} = -K_v \frac{\partial \overline{\rho}_v}{\partial z} \tag{9.4}$$

where K_v, $\mathrm{m}^2\ \mathrm{s}^{-1}$ is the eddy diffusivity for water vapour.

Note that these flux models are simply an analogy to molecular diffusion (conduction), but with vastly greater diffusivities which are properties of the turbulent flow rather than of the fluid. Experiments have approximately determined the values of the K's very near ground over the range in atmospheric stratification; those values are themselves affected by stratification, windspeed, and the depth of the PBL.

9.2.1 Monin-Obukhov Similarity Theory of the ASL (MOST)

The Atmospheric Surface Layer (ASL) is the lowest 50 m (or so) of the ABL, where proximity to ground limits vertical motion and mixing, and so vertical gradients in mean windspeed, temperature, humidity (etc.) are very large. This is an important layer of the atmosphere - we live in it! Let us call its depth h_{ASL} and accept that the precise definition of this depth is vague.

Monin and Obuknov provided an empirical theory of the ASL in its simplest, horizontally-uniform state, by hypothesizing that that state is determined by the (roughly, height-independent[2]) turbulent fluxes of momentum and heat across it. Specifically Monin and Obukhov postulated that the most important "global" (or "external" or "governing") scales are the friction velocity $u_* = \sqrt{-\overline{u'w'}}$ and the kinematic heat flux $Q_H/\rho c_p = \overline{w'T'}$ (from the latter a turbulent temperature scale $T^* = -\overline{w'T'}/u_*$ is derived). Monin-Obukhov similarity theory ('MOST') specifically pertains to the hh_ASL at heights far enough above the surface that no length scales pertaining to the surface are relevant, thus only height z enters the picture; and since buoyancy effects hinge on existence of gravity, let's just say that a scale g/T_0 is also needed.

From the available parameters, one may form a new length scale, the Obukhov length

$$L = \frac{-u_*^3}{k_v \, \frac{g}{T_0} \, \frac{Q_H}{\rho_0 c_p}} \tag{9.5}$$

where the von-Karman constant $k_v = 0.4$ is included purely by convention. If the ASL is neutral, by definition $|L| = \infty$, while if the ASL is unstable then $L < 0$ (and vice versa). If $|L| \lesssim 2$ m, we have such light winds and/or strong heat fluxes that the state of the ASL is ill-defined

[2]In the sense that, say, $|\overline{w'T'}(h_{ASL}) - \overline{w'T'}(0)| \leq 0.1\ |\overline{w'T'}(0)|$, etc. Thus we may call the hhASL the "constant flux layer".

(and difficult to even measure). Otherwise, MOST has been found to give a good description. Its specific predictions are (for example)

$$\begin{aligned}
\frac{k_v z}{u_*}\frac{\partial \overline{u}}{\partial z} &= \phi_m\left(\frac{z}{L}\right)\\
\frac{k_{vh} z}{T_*}\frac{\partial \overline{T}}{\partial z} &= \phi_h\left(\frac{z}{L}\right)\\
\frac{k_{vw} z}{r_*}\frac{\partial \overline{\rho}_v}{\partial z} &= \phi_w\left(\frac{z}{L}\right)\\
\frac{k_{vc} z}{c_*}\frac{\partial \overline{c}}{\partial z} &= \phi_c\left(\frac{z}{L}\right)
\end{aligned} \tag{9.6}$$

where the functions on the r.h.s. are universal empirical Monin-Obukhov ("MO") functions[3] and the k_v's are defined such that in each case $\phi(0) = 1$ (the normalizing lengthscales on the l.h.s. could equally have been L, but then different functions would result on the rhs). The scales for water vapour and for a generic gas (concentration $\overline{c}$) have been formed from their respective fluxes, viz. $r_* = -\overline{w'\rho_v'}/u_*$, $c_* = -\overline{w'c'}/u_*$.

The consensus view at present from the available experiments is that $k_{vw} = k_{vh} = k_v = 0.4$, while the best atmospheric dispersion experiments indicate $k_{vc} > k_v$, ie. $S_c = k_v/k_{vc} < 1$. Taking the stable case, experiments show $\phi_m \approx \phi_h \approx \phi_v \approx 1 + \beta\ z/L$ with $\beta \approx 5$. The corresponding wind profile is the "log-linear" profile

$$\overline{u} = \frac{u_*}{k_v}\left[\ln\frac{z}{z_0} + \beta\,\frac{z - z_0}{L}\right] \tag{9.7}$$

where z_0 is a constant of integration, defined to be the location on the z-axis where mean windspeed (apparently) vanishes... the "surface roughness length". While MO theory does not hold down as low as $z \sim z_0$, in practise we apply it unless we want to go to the trouble of exploiting a more detailed theory.

Now the MOST does not explicitly hinge on introducing the flux-gradient closure, but we can readily see that it provides us formulae for the diffusivities. By re-arranging eqns(9.8) it is easy to show that the K's for momentum, heat, water vapour and a (general) gaseous additive are

$$K_m = \frac{k_v u_* z}{\phi_m}$$

$$K_h = \frac{k_v u_* z}{\phi_h} \tag{9.8}$$

$$K_w = \frac{k_v u_* z}{\phi_w} \tag{9.9}$$

$$K_c = \frac{k_{vc} u_* z}{\phi_c} \tag{9.10}$$

where we shall often denote the eddy viscosity more simply as K.

[3]The ratio z/L approximately equals the ratio of the rates of buoyant and shear production of turbulent kinetic energy (more on this below).

9.3 A vintage treatment of the ABL (old Canadian Regional Finite Element Model)

The K's were specified as multiples of an eddy viscosity formulated as

$$K = a\ \lambda\ \sqrt{k} \tag{9.11}$$

where a is a constant (near 1), λ is a height-dependent "mixing length" that relates to the size of the unresolved eddies, and k is the kinetic energy (per unit mass) in the unresolved motion, defined by

$$k = \frac{1}{2}\left(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}\right) \tag{9.12}$$

Since $\sqrt{k}$ is a velocity, we can regard it as a measure of the strength of the unresolved (turbulent) velocities, and λ as a measure of the distance along which an eddy persists. The "exchange coefficient" K, measuring the efficiency of transport by the unresolved motions, depends on both these factors.

An exact evolution equation for k can be derived from the Navier-Stokes equations, by steps we will not cover. In a simplified form in which advective terms have been dropped (which is appropriate in the context of "grid point computations") the k-equation is:

$$\frac{\partial k(z,t)}{\partial t} = P_S + P_B + T_k - \epsilon \tag{9.13}$$

Here $P = P_S + P_B$ is the rate of production of unresolved kinetic energy (KE), and

$$T_k = -\frac{\partial}{\partial z}\,\overline{w'\,\frac{1}{2}\left(u'^2 + v'^2 + w'^2\right)} = \frac{\partial}{\partial z}\left(K_k\,\frac{\partial k}{\partial z}\right) \tag{9.14}$$

is the "turbulent transport" term, modelled (in the closed form on the right) as a gradient-diffusion process with diffusivity $K_k \propto K$. The the KE production rates may be written

$$P_S = -\overline{u'w'}\,\frac{\partial \overline{u}}{\partial z} - \overline{v'w'}\,\frac{\partial \overline{v}}{\partial z} = K\left[\left(\frac{\partial \overline{u}}{\partial z}\right)^2 + \left(\frac{\partial \overline{v}}{\partial z}\right)^2\right] \tag{9.15}$$

$$P_B = \frac{g}{T_0}\,\overline{w'T'} = -\frac{g}{T_0}\,\frac{K}{P_r}\left(\frac{\partial \overline{T}}{\partial z} - \gamma_d\right) \equiv -\frac{g}{T_0}\,\frac{K}{P_r}\,\frac{\partial \overline{\theta}}{\partial z} \tag{9.16}$$

where (again) the closed form exploits the gradient-diffusion approximation for the unresolved fluxes (the turbulent Prandtl number $P_r = K/K_h$ is the ratio of the eddy diffusivities for momentum and heat, so $K_h = K/P_r$). Note that the buoyancy part can be a source or a sink for KE in the unresolved scales, according to the sign of the unresolved heat flux. In unstable stratification the heat flux is positive and buoyant production is a source for KE. The opposite is true at night, explaining why the surface layer may become very quiescent at night, unless shear production is

maintained large by a large free-atmosphere wind at the top of the ABL. It is helpful to note that in the surface layer (say, $z \lesssim 50 - 100$ m) to within a good approximation

$$\frac{P_B}{P_S} = \frac{z}{L} , \tag{9.17}$$

which gives us a useful interpretation of the MO length (depth of the layer of shear-dominated turbulence).

Returning to eqn (9.13), ϵ is called the turbulent kinetic energy (TKE) dissipation rate, and quantifies the rate of conversion of KE to heat due to working by viscous forces. It was modelled in the RFE model (in accordance with widespread custom) as

$$\epsilon = \frac{k^{3/2}}{\lambda_e} \tag{9.18}$$

where λ_e is called the equilibrium length scale (discussed below). This formula can be seen to be dimensionally correct, and says that the more energy present, the faster its rate of conversion to heat. The other term in the evolution equation for k is called "turbulent transport," and actually the diffusion form shown for it is just a model, but a nice model because it results in the k-eqn containing a diffusion operator - and consequently nice numerical behaviour, filtering of short waves, etc.

The mixing lengths were related by

$$\frac{d\lambda}{dt} = \frac{\lambda_e - \lambda}{\tau} \tag{9.19}$$

where τ is some timescale. This simply says that the lengthscale λ is always evolving towards an equilibrium value, λ_e, the latter being a specified continuous function of height (measured relative to ABL depth, ie. z/h) and a discontinuous (categorical) function of stratification (unstable or stable).

Chapter 10

Lagrangian modelling of dispersion due to unresolved velocity field

What is often called "eddy diffusion", and modelled as such, is in reality a convection process, better called "turbulent convection" or "convection by the unresolved flow". The word "dispersion" is preferable to "diffusion", for it encodes one's recognition that the process is not a diffusion process. We will consider the dispersion of a non-buoyant and non-reactive species whose instantaneous concentration is c. It is evident that in the context of turbulent or unresolved flow, there is prospect of success only for a theory of concentration *statistics*. So we shall be focused on modelling the mean concentration (C or equivalently $\overline{c}$).

The mass conservation equation is:

$$\frac{\partial c}{\partial t} = -\nabla \cdot (\vec{u}\, c \; - \; D\, \nabla c) \; + Q \tag{10.1}$$

and we already know that if we perform a Reynolds decomposition $c = C + c'$ (etc.) then we will find

$$\frac{\partial C}{\partial t} = - \frac{\partial}{\partial x_i} \left(\overline{u}_i \, C \; + \overline{u_i' c'} \right) \tag{10.2}$$

(where I have dropped the molecular diffusion term, and assumed there is no in-situ production). The term $\partial \overline{u_i' c'} / \partial x_i$ is the flux of c carried by the unresolved motion (turbulent or unresolved flux), and its divergence impacts the evolution of the mean (resolved) concentration. The eddy diffusion model introduces a closure assumption, viz.

$$\overline{u_i' c'} = \; - K_{ij} \, \frac{\partial C}{\partial x_j} \tag{10.3}$$

There is no a priori reason not to regard the eddy diffusivity as a tensor; however this is rarely found to be necessary, and more typically the eddy-diffusion model (K-theory) is expressed

$$\begin{aligned} \overline{u'c'} &= -K_x \, \frac{\partial C}{\partial x} \\ \overline{v'c'} &= -K_y \, \frac{\partial C}{\partial y} \\ \overline{w'c'} &= -K_z \, \frac{\partial C}{\partial z} \end{aligned} \tag{10.4}$$

where these K's are scalar eddy diffusivities ([m^2 s^{-1}]), allowed to be different for different directions of motion.

But the mass conservation equation can also be written

$$\frac{dc}{dt} = D\,\nabla^2 c + Q \tag{10.5}$$

In general, transport by (true, ie. molecular) diffusion can be neglected relative to convection provided the Peclet number $P_e = \frac{U\,L}{D} \gg 1$ where U, L are velocity and length scales of the turbulence. Therefore, provided there are no in-situ sources or sinks of c,

$$\frac{dc}{dt} = 0 \tag{10.6}$$

This is the basis for the Lagrangian approach to turbulent dispersion. It says that away from any source, concentration is constant along trajectories. If a fluid element is at $t = 0$ "tagged" with concentration C_0, its concentration will remain constant at $c = C_0$ - or almost so, except for a slow "leakage" through the diffusion term on the rhs.

Consider a point source emitting N particles (or kilograms) per second, and a volume V downstream. Any given particle, say particle-i, may or may not pass through volume V. Let t_i be the time it spends in V (perhaps composed of many intervals of occupancy separated by periods of absence from V). Then if $\bar{t}$ is the average time a particle spends in V, the mean concentration therein is simply:

$$C = \frac{N\,\bar{t}}{V} \tag{10.7}$$

Thus if we can calculate trajectories, we can calculate mean concentrations.

Notation for Lagrangian variables

In the preceding work we had sometimes used upper case symbols to distinguish averages, e.g. the mean velocity along the x-axis was sometimes labelled $\overline{u}$ and sometimes U.

In the context of Lagrangian methods we shall reserve upper case symbols to designate the position and velocity of a particle[1], viz. the height and the vertical velocity of a particle are (Z, W).

10.1 Taylor's Lagrangian Theory

Taylor's (1921) analytical theory for dispersion in homogeneous turbulence shows up the weakness in the Eulerian approach, and suggests the important factors in constructing a Lagrangian model.

[1]We shall restrict our attention to the motion of "particles" of passive tracer, i.e. particles that are non-buoyant. We can think of these particles as being "marked" fluid elements, where a "fluid element" is a tiny finite volume of the fluid whose characteristic dimension is very large compared to the mean free path, yet very small compared to the smallest scales of convective motion (i.e. fluid element dimension is much smaller than the diameter of the smallest eddies).

Consider the vertical motion (there is nothing special about our choice of the vertical axis) of a fluid element which is marked purple and released at $z = t = 0$ into an infinite domain of homogeneous and stationary turbulence[2]. At subsequent times (t) its vertical coordinate is:

$$Z = \int_0^{t'=t} W(t')\, dt' \tag{10.8}$$

where $W(t')$ is the particle velocity. This vertical velocity is by definition

$$W(t') = \left(\frac{dZ}{dt}\right)_{t=t'} \tag{10.9}$$

Now we may write

$$\frac{dZ^2}{dt} = 2\, Z(t)\, \frac{dZ}{dt} \tag{10.10}$$

If we consider the release of many particles in such a way that they sample many realisations of the transporting velocity field, we may define an ensemble average value for any property of these fluid elements at any time t since release. For example, $\overline{Z^2}$, "mean square Z," denotes the mean value (in an ensemble average sense) of the square of the particle displacement along the z-axis at time t since release. Obviously this somehow relates to spread, and we will define the "spread" as:

$$\sigma_z = \sqrt{\overline{Z^2}} \tag{10.11}$$

In fact σ_z is the standard deviation of the concentration distribution along z. The particle position (transition) probability density function $p(z, t|0, 0), [m^{-1}]$ is defined such that $p(z_1, t|0, 0)dz$ is the probability that the particle released at $z = t = 0$ is at later time t between $z_1 - dz/2$ and $z_1 + dz/2$. Often this (transition) probability density will be called simply the concentration (but note again that it is a density on a line, rather than in a volume). Clearly it must satisfy

$$\int_{-\infty}^{\infty} p(z, t|0, 0)\, dz = 1 \tag{10.12}$$

since the particle must lie *somewhere* on the z-axis. Now by the usual rules of probability, the mean square particle displacement is

$$\overline{Z^2}(t) = \int_{-\infty}^{\infty} z^2\, p(z, t|0, 0)\, dz \tag{10.13}$$

and σ_z is just the standard deviation of the concentration distribution.

Now we return to derivation of a prediction for σ_z. The ensemble-averaging operation we

[2]In an alternative and broader terminology, the prescription is that *velocity statistics* of the unresolved motion do not vary in space or time.

assume as usual to commute with differentiation or integration. Then

$$\begin{aligned}
\frac{d\overline{Z^2}}{dt} &= \overline{\frac{dZ^2}{dt}} \\
&= 2\,\overline{Z\,\frac{dZ}{dt}} \\
&= 2\,\overline{W(t)\int_0^{t'=t} W(t')\,dt'} \\
&= 2\int_0^{t'=t} \overline{W(t)\,W(t')}\,dt' \qquad (10.14)
\end{aligned}$$

Now define a Lagrangian velocity autocorrelation coefficient

$$R(t,t') = \frac{\overline{W(t)\,W(t')}}{{\sigma_w}^2} \qquad (10.15)$$

which, defining $\tau = t - t'$, may be re-written:

$$R(t',\tau) = \frac{\overline{W(t')\,W(t'+\tau)}}{{\sigma_w}^2} \qquad (10.16)$$

But statistics of stationary turbulence are independent of any particular "starting time" t', so that $R(t',\tau) = R(\tau)$ (and in fact it is also true that $R(-\tau) = R(\tau)$. Therefore, noting $d\tau = -dt'$ and $\tau = 0$ when $t' = t$ and $\tau = t$ when $t' = 0$, we have:

$$\frac{d\overline{Z^2}}{dt} = 2\,{\sigma_w}^2 \int_0^{\tau=t} R(\tau)\,d\tau \qquad (10.17)$$

This is Sir Geoffrey Ingram Taylor's famous result for the rate of increase of mean square particle displacement, which is revealed to depend on the Lagrangian velocity autocorrelation function. Taylor's solution does not tell us the form of the concentration distribution, but gives us the second moment of that unknown distribution.

Note that we can define a Lagrangian integral time scale from $R(\tau)$ as

$$T_L = \int_0^{\tau=\infty} R(\tau)\,d\tau\ , \qquad (10.18)$$

i.e. as the area underneath the curve $R(\tau)$.

10.1.1 Comparison with Classical Eddy-Diffusion Solution

Remember we are considering the time-dependent evolution of the vertical position of a particle released at $z = t = 0$, and we aim to determine ensemble mean statistics (average over many trial releases). Now with the eddy diffusion closure the governing mass conservation equation reduces to[3]

$$\frac{\partial C}{\partial t} + \overline{u}\,\frac{\partial \overline{c}}{\partial x} = \frac{\partial}{\partial x}\left(K_x\,\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\,\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\,\frac{\partial C}{\partial z}\right) \qquad (10.19)$$

[3]I have assumed the resolved velocity field to be uni-directional and aligned with the x-axis, i.e. $\overline{u}_i = (\overline{u}, 0, 0)$.

where (of course) we have assumed there is no in-situ production or destruction ($Q = 0$), and neglected molecular transport. Now let us set the mean velocity to zero, and assume the K's are independent of position - homogeneous turbulence. Furthermore, since we don't care where in x, y the particle is, we can define a new concentration $C_*[\mathrm{m}^{-1}]$

$$C_*(z,t) = \int_{-\infty}^{x=\infty} \int_{-\infty}^{y=\infty} C(x,y,z)\, dx\, dy \tag{10.20}$$

Thus C_* is the earlier-mentioned probability density $p(z,t|0,0)$ for particle position, in the sense that $C_*(z_1,t)dz$ is the probability that a particle released at $z = t = 0$ is at time t lying in the range $z_1 - dz/2$ to $z_1 + dz/2$. By performing the double integral in x, y on the mass conservation equation we find C_* satisfies:

$$\frac{\partial C_*}{\partial t} = K_z \frac{\partial^2 C_*}{\partial z^2} \tag{10.21}$$

It is easy to show that the solution to this equation that satisfies

$$C_*(z,0) = \delta(z-0) \tag{10.22}$$

(unit release at $t = z = 0$) is the Gaussian (ie. Normal) distribution

$$C_*(z,t) = \frac{1}{\sqrt{2\pi}\ \sigma_z}\ e^{-\frac{z^2}{2{\sigma_z}^2}} \tag{10.23}$$

with standard deviation $\sigma_z(t) = \sqrt{2\ K_z\ t}$.

Observations show that the concentration distribution is more or less Gaussian, for all distances from the source (but remember: this is an unbounded domain of homogeneous turbulence). But the really important point is that this result states that

$$\frac{\partial {\sigma_z}^2}{\partial t} = 2\ K_z \tag{10.24}$$

while G. I. Taylor's result, which is exact, says

$$\frac{d\overline{Z^2}}{dt} = 2\ {\sigma_w}^2 \int_0^{\tau=t} R(\tau)\, d\tau\ . \tag{10.25}$$

To reconcile these results we must have:

$$K_z = {\sigma_w}^2 \int_0^{\tau=t} R(\tau)\, d\tau \tag{10.26}$$

The eddy diffusivity, which we would have liked to be a property of the turbulence, turns out to be a function of the time since the particle was released: and only when $t \gg T_L$ (in the "far field") does the eddy diffusivity assume a value independent of t, namely the "far field limit" $K_\infty = {\sigma_w}^2\ T_L$.

Thus we conclude the classical diffusion theory, which predicts a plume width σ_z increasing as $\sqrt{t}$ for all t is wrong at short travel times. In truth, σ_z goes linearly with t in the "near field"

(when $t \ll T_L$). In the near field, travel time is so short that the particle flies with an essentially constant velocity - that it assumed upon release.

Taylor's result for the time-derivative of $\overline{Z^2}$ may be further integrated to obtain:

$$\overline{z^2} = 2\ {\sigma_w}^2 \int_0^t (t-\tau)\ R(\tau)\ d\tau\ . \tag{10.27}$$

If, as is often assumed, the autocorrelation function is exponential with timescale T_L, ie.

$$R(\tau) = e^{-\frac{\tau}{T_L}} \tag{10.28}$$

the result for the spread specialises to:

$$\frac{\overline{z^2}}{2{\sigma_w}^2} = t\ T_L - \ T_L^2\ \left[1 - \ e^{-\frac{t}{T_L}}\ \right]\ . \tag{10.29}$$

10.1.2 Asymptotic results

The following results are valid for a general autocorrelation function.

Small time limit (near field): If $t \ll T_L$ then $R(\tau) = 1$ throughout the required integral. It follows that:

$$\overline{z^2} = {\sigma_w}^2\ t^2 \tag{10.30}$$

or $\sigma_z = \sigma_w\ t$. The plume spreads linearly in time for short times after release: that is because for short times the spread is not a diffusion process, but simply an advection at a constant random starting velocity.

Large time limit (far field): If $t \gg T_L$ then $\sigma_z = \sqrt{2{\sigma_w}^2 T_L}\ \sqrt{t}$.

10.1.3 What is important about G.I.Taylor's result and when is K-theory valid?

- If we insist on using an eddy diffusivity K to close the mass conservation equation, we have to accept that, of the totality of particles seen at a point z, a sub-ensemble of particles having been released at time t_1 may have a different diffusivity from a sub-ensemble of particles that were released at t_2. This is logically absurd, the result of K-theory being fundamentally wrong.

- The statistical evolution of concentration in this simple turbulence is completely governed by two statistical properties of the turbulence: σ_w, T_L.

- The "far field" diffusivity is $K_\infty = {\sigma_w}^2\ T_L$.

We expect K-theory to be useful when the turbulence is "fine-grained" relative to the length scale over which there is curvature in the concentration distribution (Corrsin, 1974).

10.2 Modern single-particle Lagragian stochastic models

Taylor's analytical solution is highly restricted in its validity. With the arrival of computers came the possibility of "Monte-Carlo" type Lagrangian simulations that treat dispersion by literally computing the paths of computational particles. The name "Lagrangian stochastic model" has emerged as the most common term for what is also known as the trajectory-simulation, random-flight, random-walk, or (occasionally) Markov-chain method.

We shall consider the modelling of dispersion in a flow whose velocity statistics are known, and horizontally-uniform. For the time being we will concentrate on motion along a single dimension (z). Evidently if we can generate a sequence for the vertical velocity W of a "particle" we can generate a set of trajectories.

These are not real trajectories. Then we must ask, what properties of real trajectories, ie. what statistical properties of the Lagrangian velocity W, is it necessary to mimic correctly? Surely, from previous considerations, σ_w and T_L. The first LS models were heuristic, but due to the contribution of Thomson (1987) we now have rigorous criteria.

10.2.1 Zeroth- and first-order LS models

The "zeroth-order" LS model for motion along a single axis (say z, the vertical), is a random walk in position (the drunkard's walk, or Random Displacement Model, RDM). Over each time increment dt the increment dZ in particle position is given by:

$$dZ = a\ dt + \ b\ d\xi \tag{10.31}$$

where a, b are deterministic coefficients, and $d\xi$ is drawn randomly from a Gaussian distribution with mean zero, and (by convention) variance dt. This model is easily shown to be equivalent to the treatment of turbulent convection as a diffusion process, and for stationary turbulence

$$\begin{aligned} a &= \frac{\partial K}{\partial z} \\ b^2 &= 2\ K \end{aligned} \tag{10.32}$$

The RDM model is fundamentally wrong, and manifests as such close to a source. (For a recent study of the RDM model see Wilson and Yee 2007).

In the Random Displacement model, X_i is treated as Markovian, ie. correlation of particle velocity from one timestep to the next is ignored: thus the problem that the model is invalid for travel times short compared to the typical velocity correlation timescale. This deficiency is remedied in the "first-order" LS model, wherein the Markovian state variable is (X_i, U_i), and the velocity evolves in time according to a "generalised Langevin equation" (Thomson, 1987),

$$dU_i = a_i\ dt + \ \sqrt{C_0\ \epsilon}\ d\xi_i \tag{10.33}$$

where dU_i are the increments over timestep dt in the three components of Lagrangian velocity, ϵ is the rate of dissipation of the kinetic energy of the unresolved flow (TKE), and C_0 is a dimensionless and (supposedly) universal constant (prescription of the universal constant C_0 in an LS model is equivalent to the prescription of the turbulent Schmidt number S_c in a K-theory model). The 1^{st}-order LS model correctly predicts the rate of dispersion even in the near field of a source, where travel time t is not large w.r.t. T_L, in contradistinction to the RDM and to Eulerian models. (For a review of Lagrangian models, see Wilson and Sawford 1996).

10.2.2 Time step for (1st order) Lagrangian stochastic simulations

Integral (outer) scales measure typical spatial and temporal persistence of the unresolved (turbulent) velocity. In stationary, homogeneous turbulence, the Lagrangian integral timescale can be determined from the velocity variance (${\sigma_w}^2$) and the TKE dissipation rate (ϵ) as (Tennekes, 1979)

$$T_L = \frac{2\ {\sigma_w}^2}{C_0\ \epsilon} \tag{10.34}$$

In a simulation we should ensure the timestep $dt << T_L$

10.2.3 Thomson's well-mixed constraint on first-order LS models

Suppose we would like to determine the coefficient a in the generalized Langevin equation for vertical motion

$$dW = a\ dt + \ b\ d\xi \tag{10.35}$$

where the coefficient b is known ($b = \sqrt{C_0\ \epsilon}$).

Let us define $p(z, w, t)$ as the density function (in $z - w$ space) for particle location. For example, for release at $z = t = 0$ with a random velocity from the Eulerian pdf $g_a(w)$,

$$p(z, w, 0) = \delta(z - 0)\ g_a(w) \tag{10.36}$$

Now, being a statistic, $p(z, w, t)$ undergoes a deterministic evolution. Over discrete intervals Δt, it evolves according to the "Chapman-Kolmogorov" equation

$$p(z, w, t + \Delta t) = \int_{z_0} \int_{w_0} p\left(z, w, t + \Delta t | z_0, w_0, t\right)\ p\left(z_0, w_0, t\right)\ dz_0\ dw_0 \tag{10.37}$$

which expresses conservation of probability (at any time after release, the particle must exist somewhere with some velocity). It is possible to derive from the CK equation a differential equation for the evolution of the density function. Provided the random forcing ($d\xi$) is Gaussian (which it must be, on other grounds), the differential equation corresponding to the stochastic model (eqn 10.35) is the "Fokker-Plank equation,"

$$\frac{\partial p(z, w, t)}{\partial t} = -\ \frac{\partial}{\partial z}\ (w\ p) - \ \frac{\partial}{\partial w}\ (a\ p) + \ \frac{1}{2}\ \frac{\partial^2}{\partial w^2}\ \left(b^2\ p\right) \tag{10.38}$$

The rhs is the divergence of a probability flux (in $z - w$ space): $w\ p$ is the flux along the z-axis, while $a\ p - \frac{1}{2}\ \partial(b^2\ p)/\partial w$ is the flux along the w-axis.

Now, we can apply our LS model to any initial distribution of tracer. Suppose we apply it to the particular case where the tracer is initially well-mixed in the flow,

$$p(z, w, 0) \propto \rho(z)\ g_a(z, w) \tag{10.39}$$

where I have implicitly assumed stationarity of the flow, since the Eulerian velocity pdf g_a lacks time-dependence. Assume the fluid density ρ is constant. Then, $p(z, w, 0) \propto g_a(z, w)$ and, since the particles are initially well-mixed, they must remain so, ie. $p(z, w, t) \propto g_a(z, w)$. Hence, g_a must be a stationary solution to the FP equation,

$$\frac{\partial}{\partial w}\ (a\ g_a) = -\ \frac{\partial(w\ g_a)}{\partial z} + \frac{1}{2}\ \frac{\partial^2\ (b^2\ g_a)}{\partial w^2} \tag{10.40}$$

Since b is known (see above), this result determines the conditional mean acceleration a, for a specified Eulerian velocity pdf! This is a very powerful result, constraining the Lagrangian stochastic model.

10.2.4 Unique 1-d LS Model for Gaussian Inhomogeneous Turbulence

It is usual to treat surface-layer turbulence in the atmosphere as Gaussian, but vertically-inhomogeneous. And except very close to ground (or within a canopy; a case we exclude here), the mean velocity is large w.r.t. the typical fluctuations (u'): thus dispersion in the streamwise direction is frequently ignored, or at least, u' is treated as independent of w. This leads to a focus on 1-component models, for the particle's vertical velocity, W.

The Eulerian velocity pdf, if assumed Gaussian (with zero mean), is

$$g_a(z, w) = \frac{1}{\sqrt{2\pi}\ \sigma_w(z)}\ \exp\left(-\ \frac{w^2}{2{\sigma_w}^2}\right) \tag{10.41}$$

It follows that the (unique) well-mixed, 1-component (here W) model for stationary Gaussian turbulence (Thomson, 1987) is

$$\begin{aligned} a &= -\ \frac{C_0\ \epsilon(z)}{2{\sigma_w}^2(z)}\ W + \frac{1}{2}\frac{\partial {\sigma_w}^2}{\partial z}\ \left(\frac{w^2}{{\sigma_w}^2} + \ 1\right) \\ b &= \sqrt{C_0\ \epsilon(z)} \end{aligned} \tag{10.42}$$

The influence of atmospheric stratification enters through the turbulence parameters and the mean velocity profile $\overline{u}(z)$.

In inhomogeneous turbulence a Lagrangian timescale $T_L(z)$ can still be defined through eqn (10.34), but can no longer be interpreted as an integral time scale. In the neutral surface layer, where $\sigma_w \approx 1.3\ u_*$, inhomogeneity arises solely through the TKE dissipation rate.

It can be shown that the model compared in detail with the Project Prairie Grass field observations by Wilson et al. (1981; WTK) is the discrete-time version of eqn (10.42). Using a time scale parameterisation equivalent to $C_0 = 3.1$, which value accords with latest estimates from simpler flows, WTK showed this LS model to be in excellent agreement with the observations. They also obtained good agreement with unstable and stable PPG runs, using the parameterisations (which are consistent with $C_0 = 3.1$ in neutral conditions):

$$\begin{aligned} \frac{2\ {\sigma_w}^2}{C_0\ \epsilon} &= T_L(z) = \frac{0.5\ z}{\sigma_w}\left(1 - \ 6\frac{z}{L}\right)^{\frac{1}{4}},\ L < 0 \\ \frac{2\ {\sigma_w}^2}{C_0\ \epsilon} &= T_L(z) = \frac{0.5\ z}{\sigma_w}\left(1 + \ 5\frac{z}{L}\right)^{-1},\ L > 0 \end{aligned} \tag{10.43}$$

where L is the Monin-Obukhov length. These formulae can be used to parameterise the compound variable $C_0\epsilon$ in (modern) LS models of the equilibrium atmospheric surface layer.

We have focused here on vertical dispersion, and ignored the important question of the impact of the fluctuating alongwind component u', which is correlated with the vertical velocity, and of the lateral turbulence component. The inclusion of u' and/or v' presents a difficult problem. There is firstly the difficulty that as yet we do not have a unique well-mixed 2- or 3-dimensional LS model, even if we are prepared to accept Gaussian velocity pdfs.

The second difficulty of including U, V, a difficulty not peculiar to LS modelling, is that u' and v' contain energy at much lower frequencies than w - wind direction and strength change on a continuous range of scales, from the almost-microscopic (Kolmogorov) scale, up through scales of order 10 min (cloud/meso scale), to hourly and daily scales (changing large scale pressure patterns). Therefore no matter what our choice of averaging time, there is always the likelihood of an irregular and possibly multi-modal distribution of material along the horizontal direction(s). In general the (mean) mass distribution in x, y cannot be sharply predicted unless we can forecast the mesoscale fluctuations in wind direction. Practical means of accomplishing this involve prediction of the mesoscale wind variations with a prognostic mesoscale wind-field model and coupling these to a LS model for the turbulence.

10.2.5 Reflection at Boundaries

Except in cases that permit analytic solution, an LS model will be implemented with finite timestep Δt, and it may be necessary to tack onto the model an algorithm that assures particles remain in the computational domain (not necessarily only because the timestep is finite). The best available criterion remains the w.m.c., whose satisfaction may be checked simply by calculating (numerically) the evolution of an initially well-mixed tracer distribution.

For example for surface-layer simulations we may choose to reflect trajectories at height $z_{refl} \geq z_0$, where typically there is little loss of accuracy with $z_{refl} \sim 10z_0$. Suppose that at the end of a timestep a particle has moved to a position $Z < z_{refl}$. The reflection strategy is simply to correct

the position and velocity as if the particle, like a billiard ball, had bounced off an apparent wall at z_{refl}, viz.

$$\begin{aligned} Z &\leftarrow 2z_{refl} - Z \\ W &\leftarrow -W \end{aligned} \tag{10.44}$$

10.2.6 LS models applicable in disturbed flows

Throughout this section we have assumed the flow and turbulence to be horizontally-uniform, so that the joint pdf for the Eulerian velocity fluctuations $g_a(u', v', w'; z)$ is a function only of the height z. In a disturbed flow, $g_a = g_a(\vec{u}', \vec{x})$.

Provided an analytical description of g_a is given, it remains possible to derive a well-mixed LS model for the disturbed flow - and this is a *huge* advance over the Eulerian description, where any such attempt would be desperately heuristic.

Suppose that g_a remained Gaussian. Then the turbulence would be described by the velocity standard deviations ($\sigma_u = \sigma_u(x, y, z)$, etc.) and covariances like ($\overline{u'w'} = \overline{u'w'}(x, y, z)$). The LS model will involve not only vertical derivatives of flow statistics, but also the horizontal derivatives, such as $\partial\sigma_u/\partial x$, $\partial\overline{u'w'}/\partial y$ and so on.

Of course, such an LS model demands that all these flow statistics be provided - it must be "fed" this information. It is no mean feat to supply such data. Measurements are out of the question. The only possibility, if it must be done, is a judicious combination of a sufficient number of measurements in the disturbed flow that one can prove (establish the correctness of) a disturbed flow model, which can then be used interpolatively and extrapolatively to "procure" all the needed derivatives, specifically, in the case where g_a is presumed Gaussian, all components of $\partial\overline{u}_i/\partial x_j$ and $\partial/\partial x_k\overline{u_i'\, u_j'}$.

Bibliography

Corrsin, S. 1974. Limitations of Gradient Transport Models. *Adv. Geophys.*, **18A**, 25–60.

Haltiner, G.J., & Williams, R.T. 1980. *Numerical Prediction and Dynamic Meteorology*. J. Wiley.

Taylor, G.I. 1921. Diffusion by Continuous Movements. *Proc. London Math. Soc., Ser. 2*, **A20**, 196–211.

Tennekes, H. 1979. The Exponential Lagrangian Correlation Function and Turbulent Diffusion in the Inertial Subrange. *Atmos. Env.*, **13**, 1565–1567.

Thomson, D.J. 1987. Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid Mech.*, **180**, 529–556.

Wilson, J.D., & Sawford, B.L. 1996. Review of Lagrangian stochastic models for trajectories in the turbulent atmosphere. *Boundary-Layer Meteorol*, **78**, 191–210.

Wilson, J.D., & Yee, E. 2007. A Critical Examination of the Random Displacement Model of Turbulent Dispersion. *Boundary-Layer Meteorol*, **125**, 399–416.

Wilson, J.D., Thurtell, G.W., & Kidd, G.E. 1981. Numerical Simulation of Particle Trajectories in Inhomogeneous Turbulence. III. Comparison of Predictions with Experimental Data for the Atmospheric Surface-Layer. *Boundary-Layer Meteorol.*, **21**, 443–463.