Diffusion

1 A random walk

Consider a particle that moves randomly along a line in fixed steps Δx that are taken at fixed time intervals, Δt, with an equal probability of moving to the left or right. Averaging over a large number of such particles, what is the probability, $p(m, n)$, that a particle reaches a point m spaces to the right (i.e. $x = m\Delta x$) after n time steps (i.e. at $t = n\Delta t$)? If it takes a steps to the right and b to the left for an individual particle to reach the desired location then the number of possible paths is

$$\frac{n!}{a!b!} = \frac{n!}{\{(n+m)/2\}!\{n-m)/2\}!} \tag{1}$$

(noting that $a - b = m$ and $a + b = n$).

The total number of paths of n steps is 2^n, and thus

$$p(m,n) = \left(\frac{1}{2}\right)^n \frac{n!}{\{(n+m)/2\}!\{n-m)/2\}!} \tag{2}$$

which is the Bernoulli (or binomial) distribution. For large n this distribution converges to the Gaussian distribution, i.e.

$$\lim_{n\to\infty} p(m,n) = \left(\frac{2}{\pi n}\right)^{\frac{1}{2}} \exp\left(\frac{-m^2}{2n}\right) \tag{3}$$

(noting that $n! \sim (2\pi n)^{1/2} n^n e^{-n}$ as $n \to \infty$ – Stirling's formula).

If (x, t), where $x = m\Delta x$ and $t = n\Delta t$, are considered continuous variables, the probability density function of the continuous random walk is

$$p(x,t) = \frac{1}{2(\pi D t)^{1/2}} \exp\left(\frac{-x^2}{4Dt}\right) \tag{4}$$

where D is defined as the *diffusion coefficient* and is given by

$$\lim_{\Delta x, \Delta t \to 0} \frac{(\Delta x)^2}{2\Delta t} \to D \tag{5}$$

The limit of small Δx and Δt is taken such that D is non–zero. (Note D has dimensions L^2/T) The average width of the cluster, σ, grows as $(2Dt)^{1/2}$.

The random walk approach can be related to the diffusion equation by considering the probability $p(x, t)$ in relation to the previous time step. If there is equal probability in moving to the left or right then

$$p(x,t) = \frac{1}{2} p(x - \Delta x, t - \Delta t) + \frac{1}{2} p(x + \Delta x, t - \Delta t) \tag{6}$$

Expanding the right hand side in a Taylor series

$$\frac{\partial p}{\partial t} = \left[\frac{(\Delta x)^2}{2\Delta t}\right] \frac{\partial^2 p}{\partial x^2} + \left[\frac{\Delta t}{2}\right] \frac{\partial^2 p}{\partial t^2} + \dots \tag{7}$$

As before let $\Delta x, \Delta t \to 0$ such that

$$\lim_{\Delta x, \Delta t \to 0} \frac{(\Delta x)^2}{2\Delta t} \to D \tag{8}$$

then

$$\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2} \tag{9}$$

If the total number of particles released is Q then the concentration is given by $c(x,t) = Qp(x,t)$. Extension to more than one dimension is straightforward.

The above approach is somewhat unsatisfactory in that it relies on Δx and Δt tending to zero in a specific way so that D exists. A more rigorous derivation can be done using the Fokker–Plank equation (see Chapter 5, Okubo 1980, for details).

2 The concept of eddy diffusivity

Modelling the effects of random movements by the diffusion equation works well for the macroscopic behaviour produced by molecular, or Brownian, motions. The derivation relies on being able to average over a large number of random events ($n \to \infty$). The apparently random nature of turbulent flow has led to the concept of an eddy diffusivity and the use of the diffusion equation to model the effect of turbulence on the dispersion of tracers (and momentum). [How large 'n' (or the averaging time) has to be for the concept of an eddy diffusivity to be valid for a turbulent flow is discussed in the next section.]

Consider a tracer of concentration, $c(\underline{x}, t)$, in a flow field $\underline{u}(\underline{x}, t)$. Then the evolution of the concentration field is given by

$$\frac{\partial c}{\partial t} + (\underline{u} \cdot \nabla)\, c = D\nabla^2 c \tag{10}$$

where D is the molecular diffusivity of the tracer. Splitting both the concentration field and velocity fields into 'mean' and fluctuating components, and averaging we get an equation for the evolution of the mean concentration field [in Cartesian coordinates (x_1, x_2, x_3)]

$$\frac{\partial < c >}{\partial t} + < u_i > \frac{\partial}{\partial x_i} < c > = D\nabla^2 < c > - \frac{\partial}{\partial x_i} < u_i' c' > \tag{11}$$

(sometimes referred to as the Reynolds averaged equation). The mean concentration field is therefore affected by the correlation between fluctuations in velocity and concentration producing an eddy flux of tracer. Assuming the eddy flux is related to the gradient of the mean field (analogous to the molecular flux) we can write

$$\frac{\partial < c >}{\partial t} + (< \underline{u} > \cdot \nabla) < c > = D\nabla^2 < c > + \frac{\partial}{\partial x_i} K_i \frac{\partial}{\partial x_i} < c > \tag{12}$$

where K_i is the *eddy* diffusivity of the tracer in the i^{th} direction. We may expect the eddy diffusivity to scale as $u^* \mathcal{L}$, where u^* and $\mathcal{L}$ are typical velocity and length scales of the turbulence. We therefore expect the value of the eddy viscosity to be dependent on the type of flow we are considering and that the horizontal diffusivity, K_h, may be different to the vertical, K_v, because of the anisotropy of many environmental flows .

Within the boundary layers of the atmosphere and ocean the turbulence is three dimensional and $K_h \simeq K_v$. Typical values for the atmospheric b.l. ~ 10 m^{2}s^{-1} For the oceanic b.l. $\sim 10^{-2}$ m^{2}s^{-1}.

Outside the b.l. the flow is much more anisotropic. For the ocean $K_v \sim 10^{-5} - 10^{-3}$ m^{2}s^{-1} (the higher values being in regions of rough topography, Polzin et al, 1997), whilst if we include mesoscale eddies in our definition of the turbulence $K_h \sim 10^2 - 10^4$ m^{2}s^{-1}.

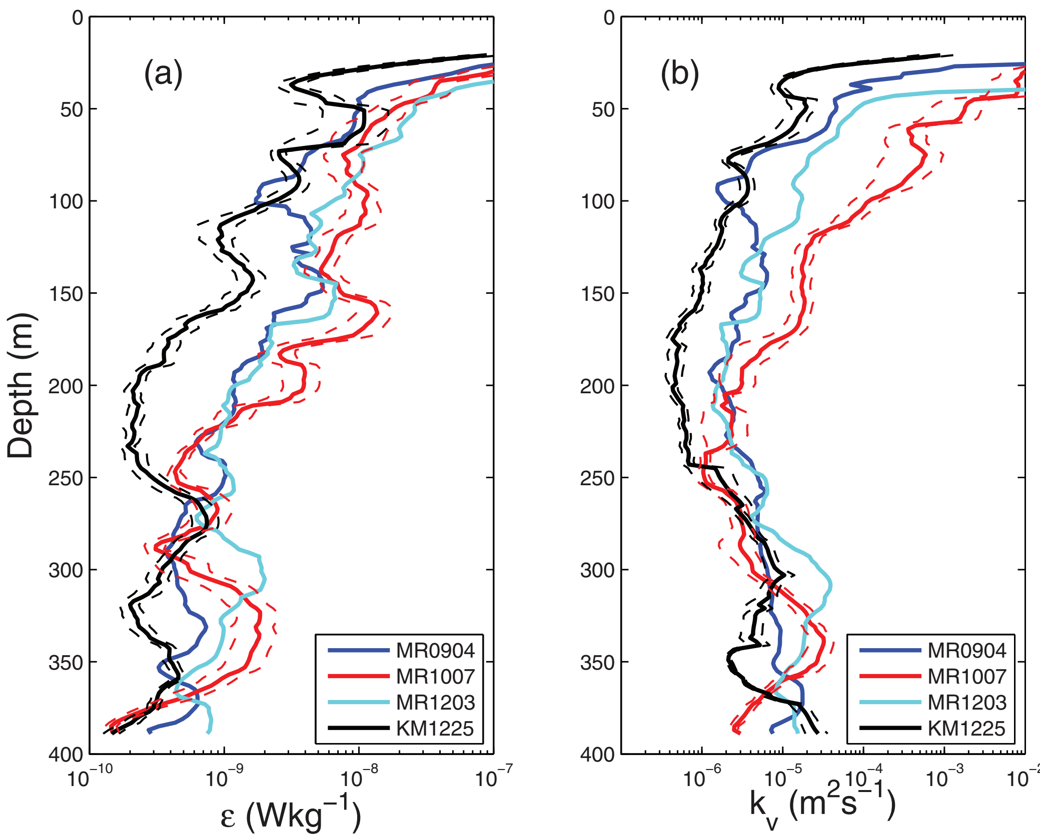


Figure 2. Cruise average vertical profiles of (a) turbulent kinetic energy dissipation rate, ϵ, and (b) vertical diffusion coefficient, κ_v. A 10 m running mean has been applied to individual profiles before averaging. Dashed lines indicate the standard error of the mean based on the variation of individual profiles for cruises MR1007 and KM1225.

Increased mixing at the equator (figure from Richards et al, 2015)

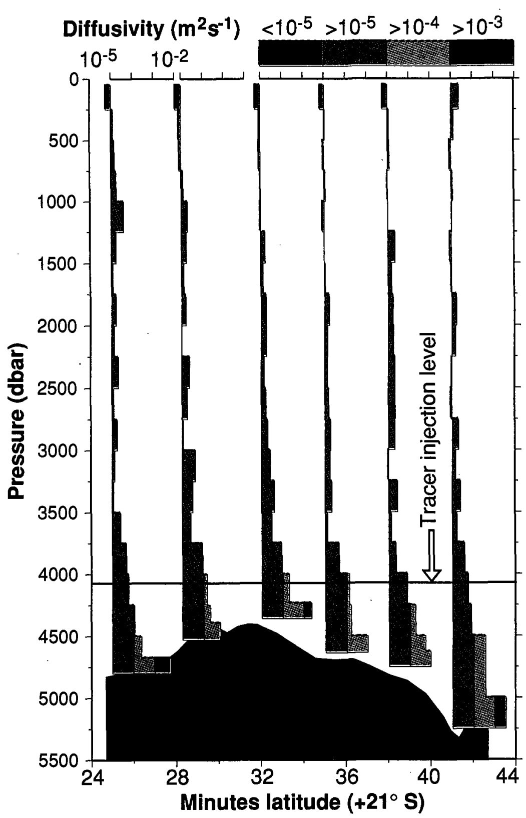
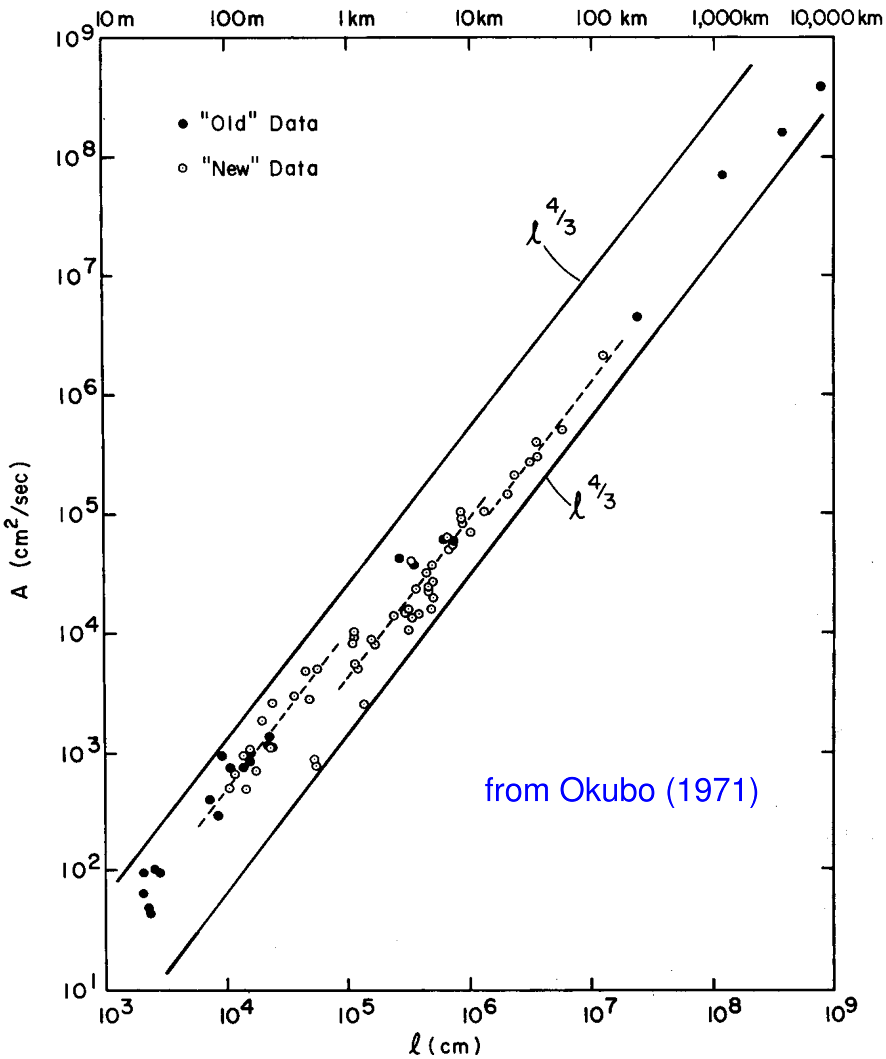


Fig. 3. Profiles of average cross-isopycnal diffusivity versus depth as a function of position relative to a spur of the MAR (whose bathymetry is shown versus latitude). Diffusivity profiles have been offset horizontally to roughly correspond to their physical position relative to the spur and are plotted on a logarithmic axis. The tick marks and color scheme denote decadal intervals, and the vertical reference lines denote $K = 10^{-5}\ \mathrm{m^2\,s^{-1}}$. The 95% confidence intervals are roughly ±50% of the depicted estimates. The horizontal line marks the average depth at which the SF_6 tracer was injected. Polzin et al (1997)

Increased mixing above topography (figure from Polzin et al, 1997)

Attempts have been made to provide a 'universal' scaling for the eddy diffusivity. Most notable are those of Richardson(1926) and Okubo(1971) who proposed a $l^{4/3}$ scaling.



2.1 Example 1: Gaussian plume

A classic problem is the distribution of a tracer downstream from a source emitting the tracer at a constant rate, Q. The simplest case is to consider a constant flow, U, past the source, and the turbulence modelled by a constant eddy diffusivity, K. Then the concentration downstream is given by

$$< c > (x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{1}{2}(y^2/\sigma_y^2 + z^2/\sigma_z^2)\right). \tag{13}$$

where $\sigma_y^2 = \sigma_z^2 = 2Kx/U$. Equation (13) can be used reasonably successfully for more complicated flows where the turbulence is modelled by a variable eddy diffusion coefficient, and σ_y, σ_z calculated accordingly.

2.2 Example 2: Shear enhanced dispersion

Consider now a tracer cloud released in a laminar flow in a pipe. The velocity distribution is then given by $U(r) = U_0(1 - r^2/a^2)$, where a is the radius of the pipe. The cross-sectional average concentration $\overline{c}$ will spread in the along pipe direction at a rate $d\sigma_x/dt = \sqrt{2K_d}\, t^{-\frac{1}{2}}/2$. The effective along pipe diffusion coefficient is given by

$$K_d = a^2 U_0^2 / 192D \tag{14}$$

where D is the molecular diffusion coefficient of the tracer. Note that K_d is inversely proportional to D. Taking $D = 10^{-5}$ cm^2/s, $U_0 = 1$ cm/s and $a = 2$ mm, then $K_d = 20$ cm^2/s ($>> D$). The same concepts can be used for turbulent shear flows. Much of the early work is reviewed by Fisher (1973). Note that (14) is only valid after a sufficiently long time after the release.

3 Diffusion by continuous movements

In his seminal paper Taylor (1921) recognized that in a turbulent flow for finite times the velocity of a particle is correlated, and introduced the use of the Lagrangian autocorrelation function. Here we work in a Lagrangian framework. Consider the position, x_n and velocity u_n of the n_{th} particle of an ensemble of particles, starting at $x = 0$ (we will consider only one space dimension and assume the mean velocity is zero). Then

$$\frac{dx_n}{dt} = u_n(t), \;\; \Rightarrow \;\; x_n(t) = \int_0^t u_n(t')dt'. \tag{15}$$

and

$$\frac{dx_n^2}{dt} = 2x_n u_n(t), \;\; \Rightarrow \;\; \frac{dx_n^2}{dt} = 2\int_0^t u_n(t)u_n(t')dt'. \tag{16}$$

Taking an ensemble mean we find the rate at which the mean square displacement, $< x^2 >$, of the cloud of particles about its centre of mass increases at the rate

$$\frac{d < x^2 >}{dt} = 2\int_0^t < u(t)u(t') > dt'. \tag{17}$$

The rate of separation of particles is therefore dependent on the correlation between the velocity at times separated by t'. For sufficiently small t' we expect the correlation to be close to one, whilst for large times the correlation will go to zero. If the correlation goes to zero sufficiently fast as $t' \to \infty$ that the integral (17) converges then we can write

$$D = \int_0^\infty < u(t)u(t') > dt', \tag{18}$$

and $< x^2 > \sim 2Dt$, where D is the diffusivity (sometimes referred to as *Fickian* diffusion).

Note for small times $< x^2 > \sim < u^2 > t^2$ (*ballistic* diffusion).

The quantity

$$R_L(t') = \frac{1}{< u^2 >} < u(t)u(t') > \tag{19}$$

is known as the Lagrangian velocity autocorrelation function. We can define a timescale

$$T_L = \int_0^\infty R_L(t)dt \tag{20}$$

known as the Lagrangian integral timescale. See Swenson and Niiler (1996) for an example of a autocorrelation function calculated from drifter data and Lumpkin *et al* (2002) for practical ways of estimating T_L. See also the analysis of atmospheric dispersion by Huber *et al* (2001)

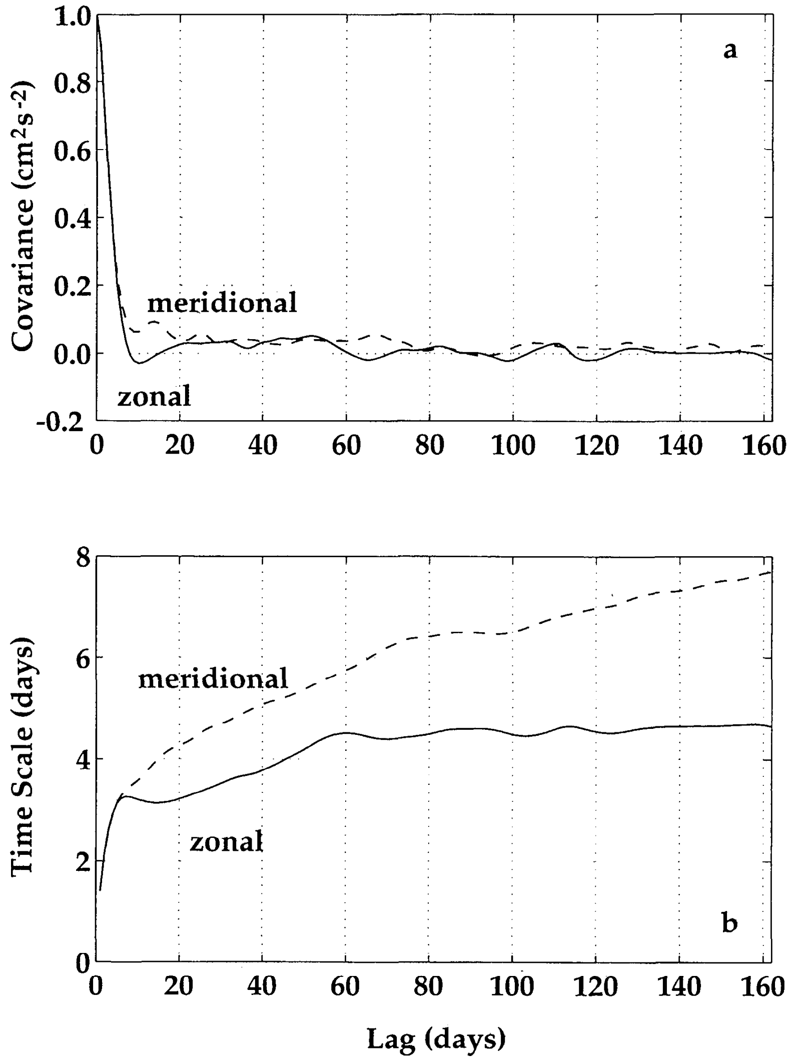


Figure 6. (a) Normalized mean time-lagged departure velocity products based on the full data set and (b) estimates of integral timescales as a function of integration range.

Swenson and Niiler (1996)

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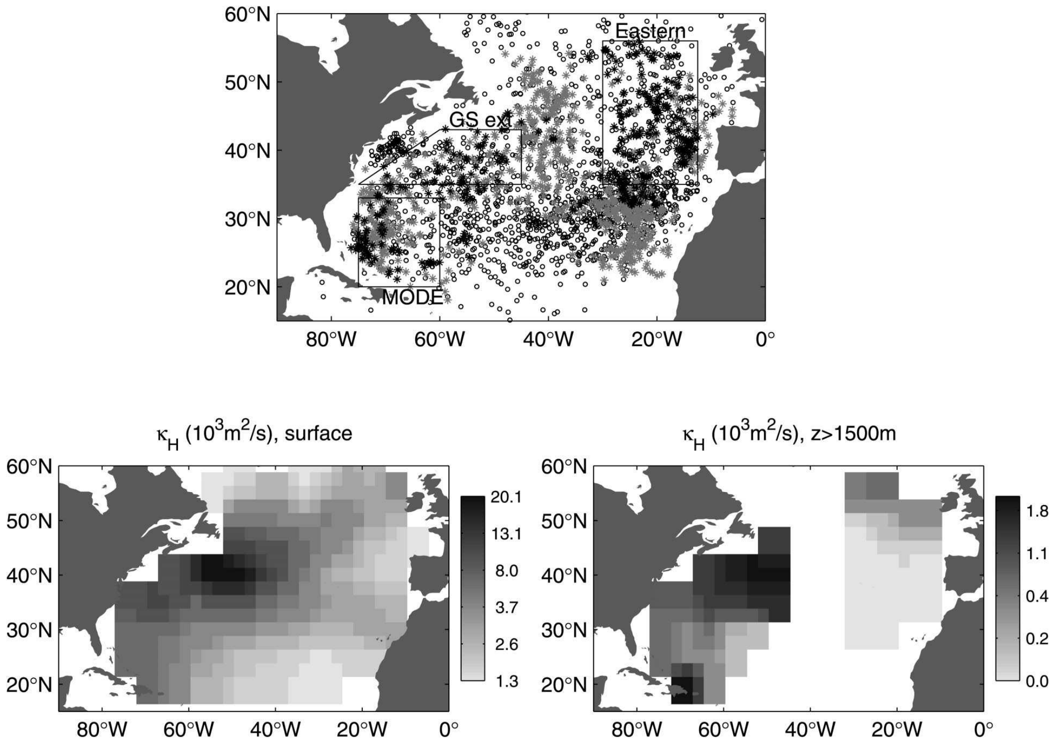


FIG. 1. (Top) median positions for 120-day segments of drifter and float trajectories at the surface (open circles), subsurface to depth 1500 m (gray stars), and deeper than 1500 m (black stars). Boxes indicate regions isolated in Fig. 3. Bottom: apparent eddy diffusivity from surface drifters (left) and floats below 1500 m (right).

4 Anomalous diffusion and Lévy flights

The convergence of the integral (18) is not guaranteed. As an example the integral diverges if $\mathcal{C}(t') =< u(t)u(t+t') >\sim t'^{-\eta}$ with $0 < \eta < 1$, as $t \to \infty$. However the rate of spread of particles may still be well defined. Integrating (17) then we obtain an expression for $< x^2 >$, namely

$$< x^2 >= 2\int_0^t (t-t')\mathcal{C}(t')dt' \tag{21}$$

Even though the diffusivity does not exist with the conditions above, the variance of particle position about the mean follows the power law

$$< x^2 >\sim t^{2-\eta} \tag{22}$$

which is greater than Fickian (but less than ballistic) diffusion. This type of diffusion is known as *superdiffusion*. Examples of such superdiffusion observed in a laboratory experiment are given by Soloman *et al* (1994) and Weeks and Swinney (1998). The particle displacement is characterized by trappings by a vortex followed by prolonged *flights* (referred to as *Lévy flights*).

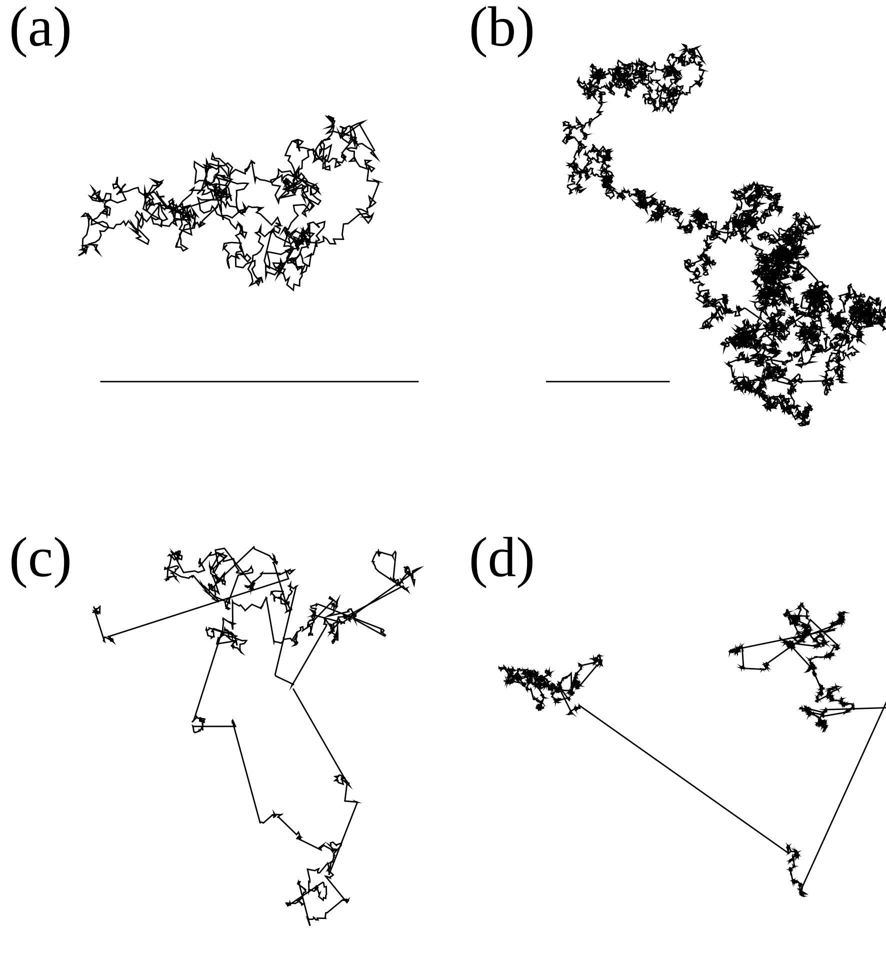
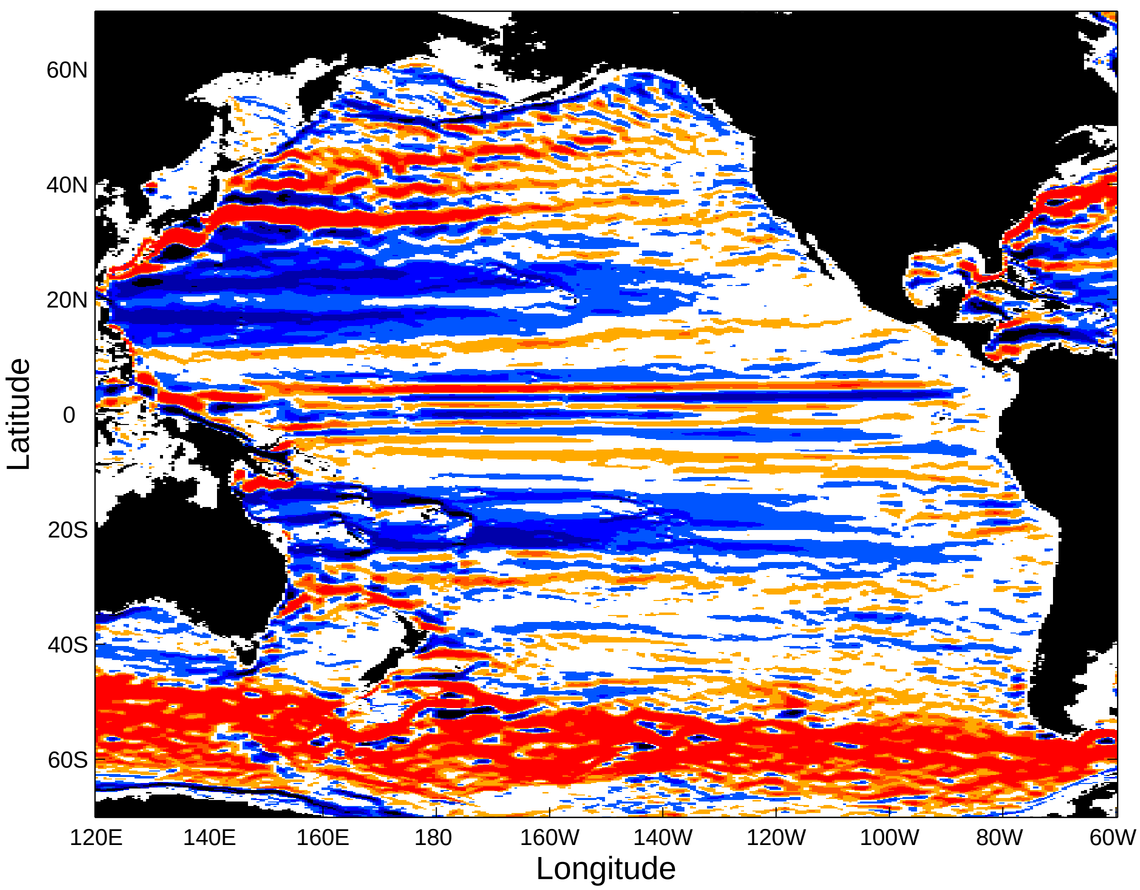


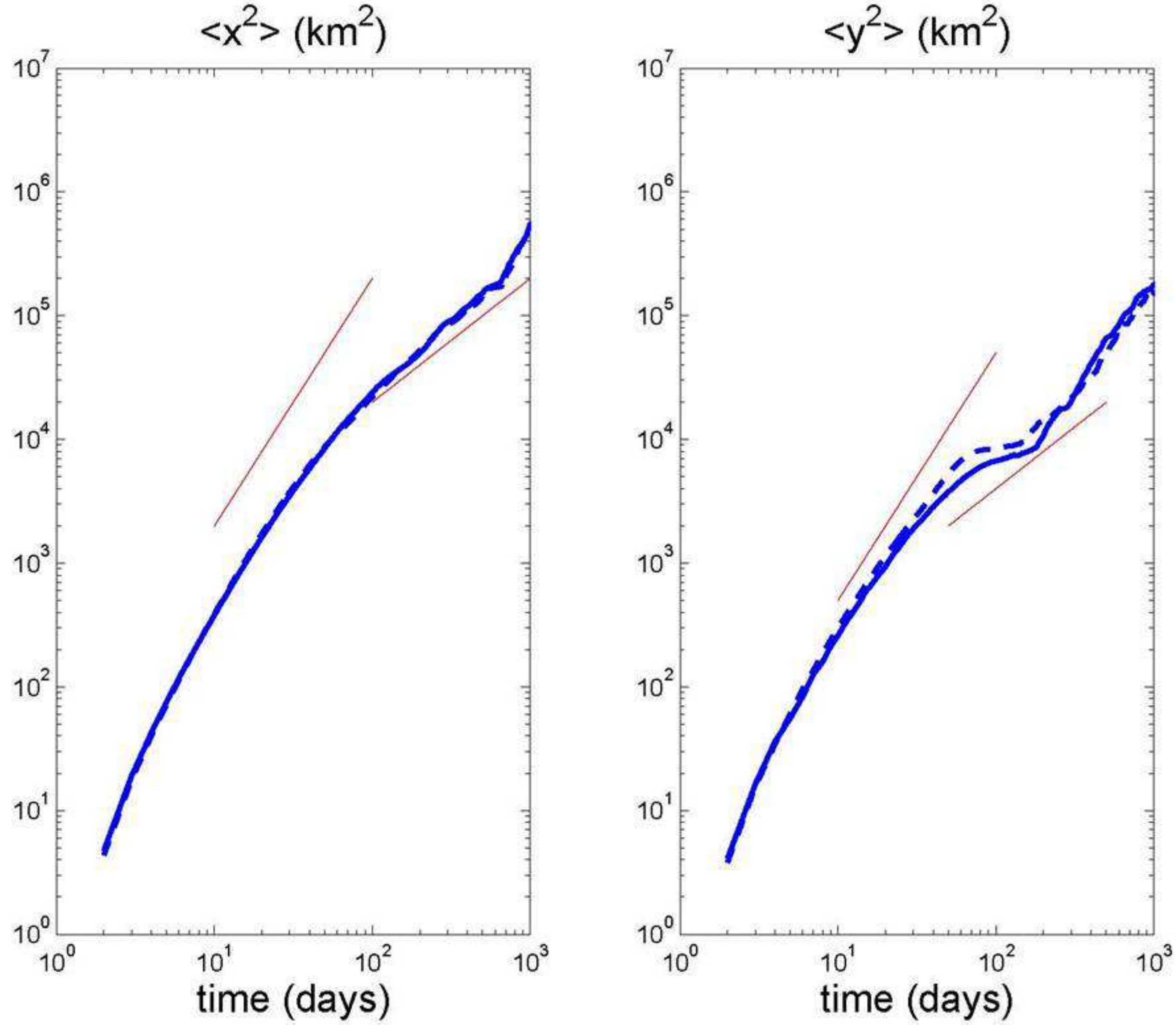
FIG. 1. Random walk leading to normal diffusion (a) after 1000 steps; (b) after 10000 steps; random walk (Lévy flight) leading to superdiffusion (c) after 1000 steps; (d) after 10000 steps.

Another class of diffusion (known as *subdiffusion*) can occur when D is zero, but the integral (21) diverges, which can occur if $\mathcal{C}(t') \sim t'^{-\eta}$ with $1 < \eta < 2$.

Numerical experiments (Elhmaidi *et al*, 1993) and analysis of float data (Rupolo *et al*, 1996) suggest that geophysical flows tend to display superdiffusive characteristics (see Provenzale, 1999, Chapter 5, for a review of estimates of dispersion by flows dominated by vortices).

What about this flow?





Single particle statistics for particles released on a density surface in the North Pacific of a high resolution Ocean General Circulation Model. The red lines have slope t^2 and t reflecting ballistic and Fickian behaviour.

5 Relative dispersion

More information about the dispersion characteristics of a flow can be gained by considering the dispersion of a pair of particles, i.e. the statistics of the average distance between two particles that were a given distance at t_o. This is usually referred to as *relative* dispersion.

5.1 Theoretical expectations

Taken from LaCasce and Bower (2000) (see their paper for references). See also LaCasce, 2008, for a review of Lagrangian observations in the ocean.

The relative diffusivity can be defined as

$$K^{(2)} \equiv \frac{1}{2}\frac{d}{dt}\langle D^2\rangle \tag{23}$$

where the superscript (2) is used to distinguish the diffusivity from its single particle counterpart, $\langle D^2\rangle$ is the mean square particle separation over an ensemble of pairs, and t is the time since pair deployment with an initial separation D_o. In an energy cascade regime (either to small scales for 3D turbulence, or to large scales for 2D turbulence), then for isotropic, homogeneous turbulence, on dimensional grounds

$$K^{(2)} = \epsilon t^2 f\left(\frac{D_o}{\epsilon^{1/2}t^{3/2}}, \frac{t\epsilon^{1/2}}{\nu^{1/2}}\right) \tag{24}$$

where ϵ is the rate of energy dissipation and ν a viscosity. In the inertial range we expect the diffusion to be independent of ν and so $f = f(D_o/\epsilon^{1/2}t^{3/2})$.

As with single particle diffusion for small times we expect $K^{(2)} \sim t$ and so

$$K^{(2)} \propto t(\epsilon D_o)^{2/3} \tag{25}$$

After sufficient time we expect the dependence on D_o to be lost and so $f =$ constant. Thus $K^{(2)} \sim \epsilon t^2$, or

$$K^{(2)} \propto \epsilon^{1/3}(\langle D^2\rangle)^{2/3} \tag{26}$$

the well known "4/3" law.

In the enstrophy cascade regime of 2D turbulence then for small times we expect

$$K^{(2)} \propto \eta^{2/3} t\langle D_o^2\rangle \tag{27}$$

and

$$K^{(2)} \propto \eta^{1/3}\langle D^2\rangle \tag{28}$$

once the dependence on initial separation has been lost. Here η is the enstrophy dissipation rate, which has dimensions $1/T^3$. The fact that η is independent of the length scale produces the difference in the longer time limit behaviour with the energy cascade regime.

Using the definition (23) then (28) implies particle separations grow exponentially in the enstropy cascade regime, i.e.

$$\langle D^2\rangle \propto \exp\,(\eta^{1/3}t) \tag{29}$$

For very long times when the separations get to the scale of the energy containing eddies then the velocities of individual particles become uncorrelated and we may expect

$$K^{(2)} = 2K^{(1)} \tag{30}$$

5.2 Observations

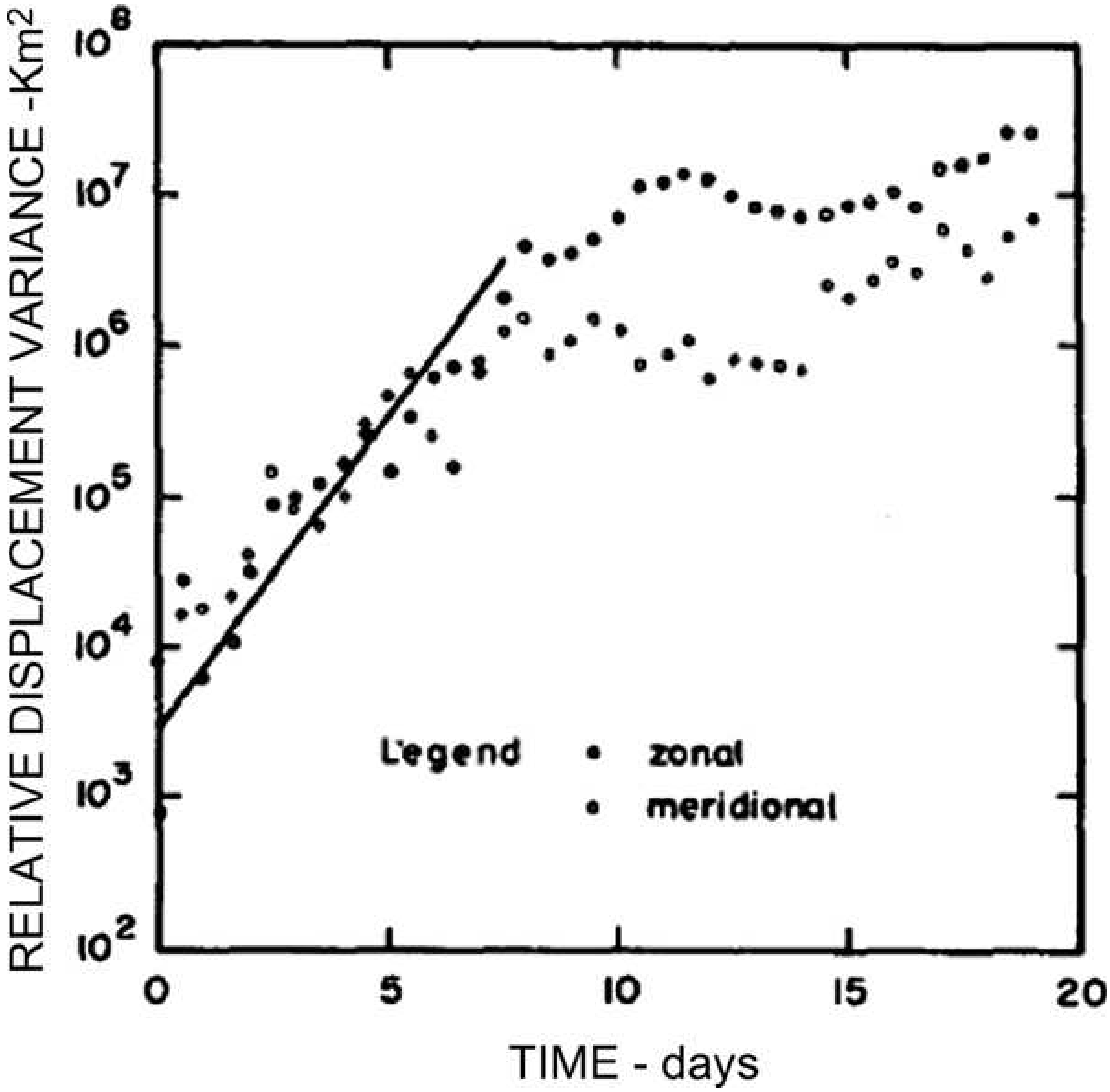


Figure 1: Relative dispersion vs. time for the TWERLE balloons (from Er-el and Peskin, 1981)

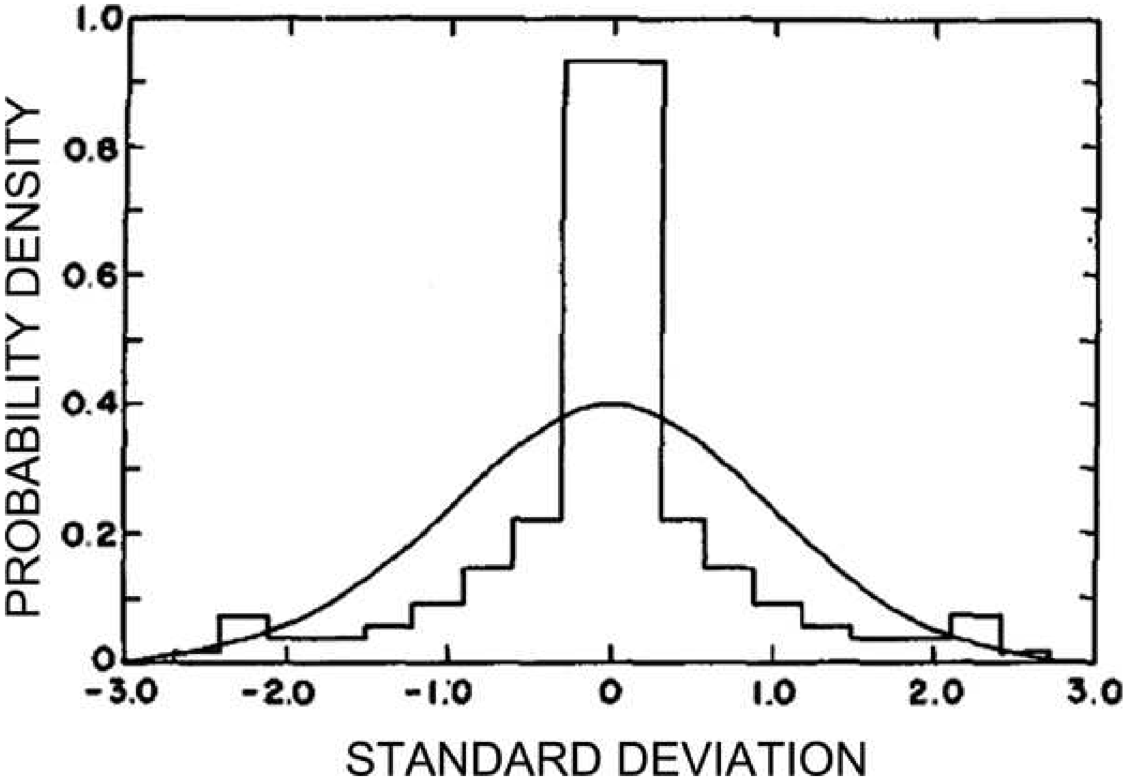


Figure 2: PDF of relative zonal displacements 5 days after deployment from the TWERLE balloons (from Er-el and Peskin, 1981). Note the non-Gaussian behaviour.

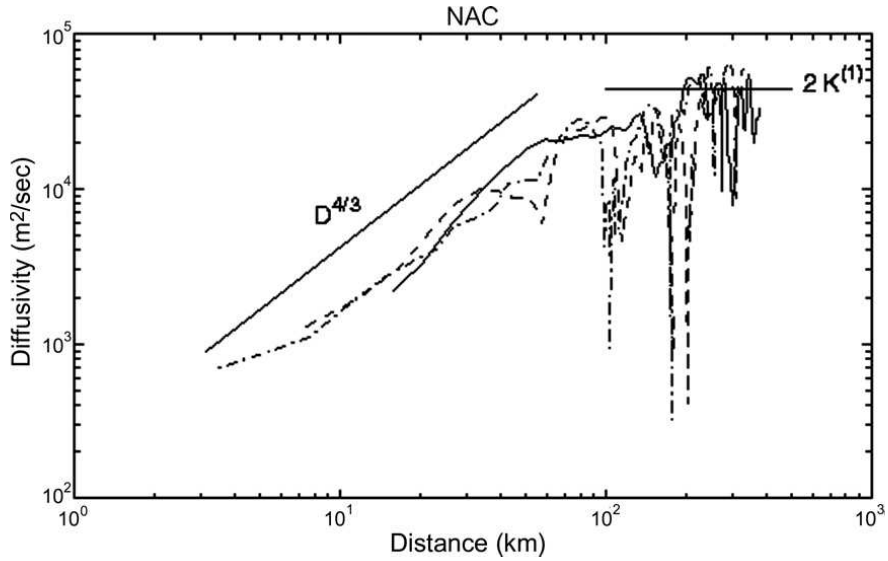


Figure 3: Relative diffusivity vs. distance for floats in the western N Atlantic (from LaCasce and Bower, 2000). The 4/3 behaviour is consistent with an energy cascade regime, although the shear of the Gulf Stream will also influence the dispersion rate

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