Turbulence and mixing

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1 Introduction

The atmospheric flow has an important effect on the distribution of chemical species by moving them away from the location of their sources and towards the location of their sinks. This process is *transport*. Unless the flow is uniform in space, it also distorts the geometric structure of chemical concentration fields so as to bring air parcels with different chemical character into closer and closer proximity. This process may be called *stirring*. The stirring processes typically draws out a volume of air (perhaps air with an anomalous chemical concentration) into thin filaments or sheets. Ultimately the distance between air parcels of differing chemical concentration is so small that molecular diffusion may act rapidly to homogenise the chemical concentration fields. This latter process is *mixing*. The three processes of transport, stirring and mixing are depicted schematically in Figure 1.

Without the stirring effect of the flow, timescales for diffusive homogenisation would be extremely long. Consider the advection- diffusion equation for the concentration $\chi(\mathbf{x}, t)$ of some chemical species.

$$\begin{array}{lccc} & \dfrac{D\chi}{Dt} = & \dfrac{\partial \chi}{\partial t} + \mathbf{u}.\nabla\chi = & \kappa\nabla^2\chi \\ \text{Estimated size} & & \dfrac{\chi U}{L} & \dfrac{\kappa\chi}{L^2} \end{array} \tag{1}$$

where $\mathbf{u}(\mathbf{x}, t)$ is the velocity field, with $\mathbf{x}$ a vector representing spatial position and t time, and κ is the molecular diffusivity. Suppose that a characteristic length scalefor the concentration field and the velocity field is L and the characteristic velocity scale is

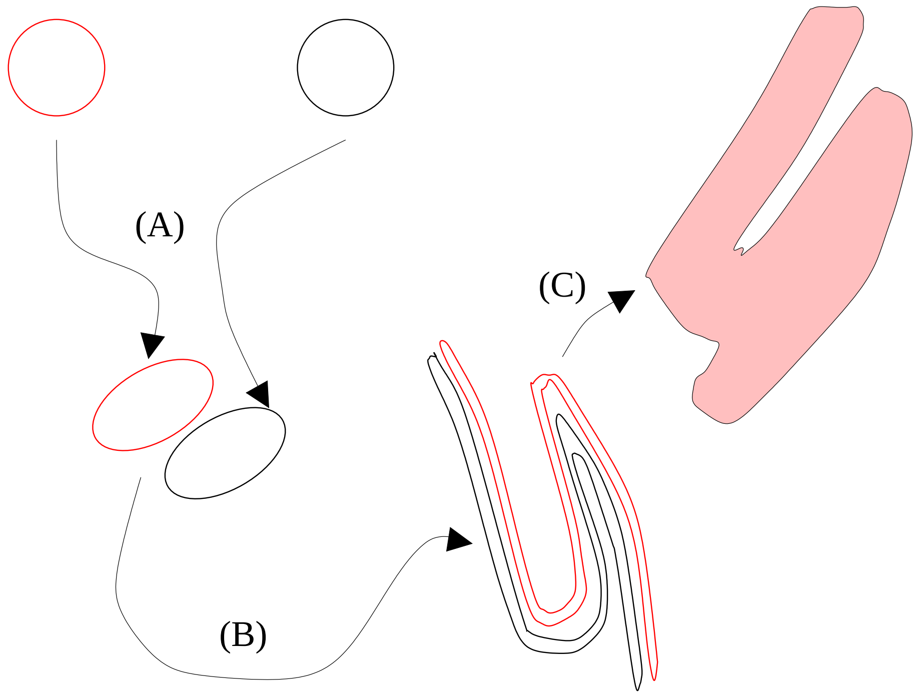

Figure 1: Schematic showing three-stage process leading to mixing. Two air masses containing different chemicals are initially well separated. In stage A *transport* brings the two air masses into the same region. (One might more accurately call this *relative transport*.) However length scales are still relatively large and diffusive timescales are long. In stage B *stirring* distorts the chemical distributions into filaments or sheets, thereby reducing their chararacteristic length scales. As a result diffusive timescales are reduced and in stage C *mixing* between the air masses can occur, leading to homogenization (at the molecular scale) of chemical concentrations. Note that stages A and B have been separated here for clarity, but in many cases it may not be appropriate to distinguish between A and B.

U. These scales might, for example, be imposed by boundary conditions, geometry or forcing, The corresponding estimates for the advection and diffusion terms (respectively the second term on the left-hand side and the term on the right-hand side) in (1) are shown below the equation. Note first that the ratio of the advection term to the diffusion term is UL/κ, generally called the Peclet number (Pe). If this number is large then advection dominates diffusion. If it is small then diffusion dominates advection. It also follows from the above that the timescale for diffusion is given by L^2/κ.

In the atmosphere the molecular diffusivity of most gaseous chemical species varies from about 10^{-5} $\mathrm{m^2s^{-1}}$in the troposphere to 10^{-3} $\mathrm{m^2s^{-1}}$in the upper stratosphere to higher values still in the mesosphere and thermosphere. The corresponding estimate for the time needed for molecular diffusion to homogenise chemical concentrations in the troposphere and lower stratosphere over a distance of, say, 100m would therefore be more than 10^8 seconds, i.e. a few years. In reality the effect of molecular diffusion is considerably enhanced by the stirring effect of the flow, which reduces the length scale of the concentration field, thereby increasing the size of the diffusive term on the right-hand side of (1), which has magnitude $\kappa\chi/l^2$ when the length scale of the concentration field is l. The diffusive term therefore becomes comparable to the advective term when $\kappa/l^2 \sim U/L$, i.e. when $l \sim L(\kappa/UL)^{1/2} = LPe^{-1/2}$.

2 Stretching, relative dispersion and mixing

The stirring process involves the geometrical deformation of material lines and surfaces. One useful measure of the stirring effect of the flow is the rate at which material lines or surfaces are stretched. For example, the equation for a material line element $\mathbf{l}(t)$ ($\mathbf{l}$ represents the difference in position between two nearby marked fluid particles is

$$\frac{d\mathbf{l}}{dt} = \mathbf{l}.(\nabla\mathbf{u}) \tag{2}$$

This equation is valid providing that the separation distance $|\mathbf{l}|$ is smaller than the length scale on which the flow varies. If there is a systematic tendency for nearby particles to separate then, for any pair of particles with finite initial separation, (2) will eventually become invalid. Note that velocity gradient tensor on the right-hand side of this equation must be evaluated following one of the fluid particles defining the line element. It is therefore the time history of this tensor following the flow that determines the stretching.

A very simple example is that where the flow is two dimensional and the velocity gradient tensor is steady, taking the form

$$(\nabla\mathbf{u})_{ij} = \left(\frac{\partial u_i}{\partial x_j}\right) = \begin{pmatrix} a & b-c \\ b+c & -a \end{pmatrix} \tag{3}$$

(chosen to match the requirement that the flow is incompressible, i.e. $\partial u_1/\partial x_1 + \partial u_2/\partial x_2 = 0$). Then it is straightforward to solve (2) to show that if $a^2+b^2 > c^2$ the solution is $\mathbf{l}(t) = l_+\mathbf{e}_+ \exp(\sqrt{a^2+b^2-c^2}t) + l_-\mathbf{e}_- \exp(-\sqrt{a^2+b^2-c^2}t)$, where l_+ and l_- are constants and $\mathbf{e}_+$ and $\mathbf{e}_-$ are constant vectors. The first term dominates at large time implying that the length of line elements increases exponentially with time and hence that there is effective relative dispersion of nearby fluid particles. On the other hand, if $a^2+b^2 < c^2$, then the solutions of (2) are oscillatory, i.e. there is no systematic increase with time.

The model above in which the velocity gradient tensor is constant in time is not very relevant to real atmospheric flows. (Note the model corresponds to the tensor being constant following an air parcel, not simply constant at fixed points in space.) In many realistic flows, particularly turbulent flows, the velocity gradient tensor experienced by an air parcel has a complex time variation and might be represented as a random function of time. A model where the velocity gradient tensor is represented as a random function, with certain specified statistical properties, is called a random-straining model. Such models predict that the exponential stretching is robust, although there is an important dependence of the rate of increase on the correlation time for the random variation of the velocity gradient tensor. More detailed investigation of more realistic models for a wide variety of atmospheric flows shown that there is very often exponential stretching of line elements at a rate that roughly corresponds to the size of the components of the velocity gradient tensor. Exceptions might be in interior of long-lived eddies, where the regime for oscillatory solutions of (2) might be relevant, and in cases where the correlation time for the velocity gradient tensor is very short, when the stretching rate will be reduced.

To emphasise the implications of material line lengthening and relative dispersion for stirring and mixing, it is useful to consider the evolution of a small material surface (assumed smaller than the length scale on which the velocity field varies) that is initially a sphere (or, in two-dimensions, a small material contour that is initially a circle). The tendency of line elements to stretch, as described by (2), implies that the sphere is deformed into an ellipsoid, at least one axis of which systematically increases in time. In an incompressible flow the volume of the sphere remains constant with time, therefore the systematic increase in length of one axis is inevitably accompanied by the systematic decrease in

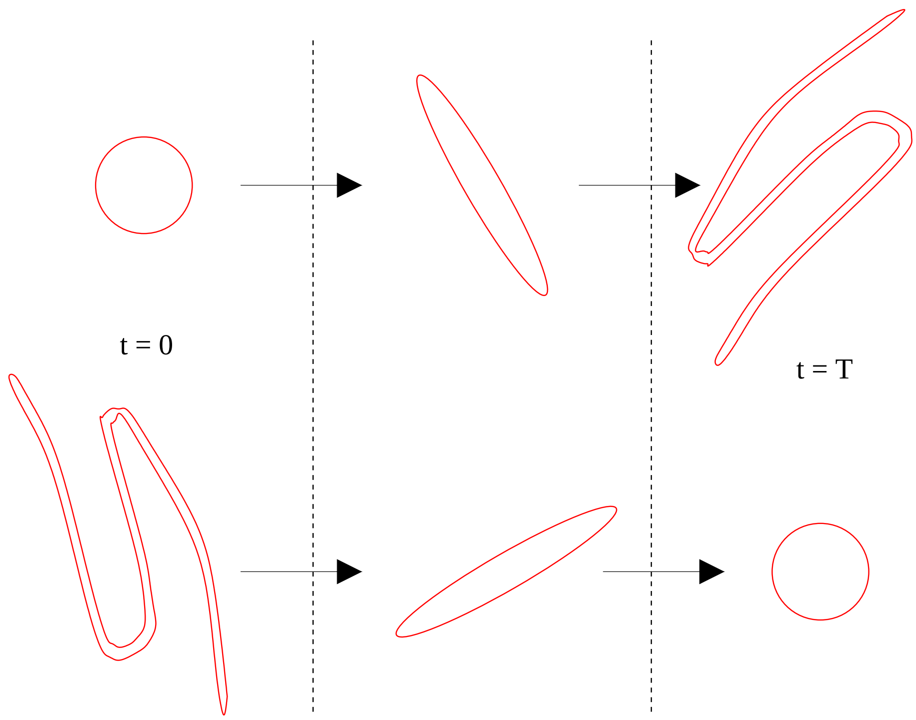

Figure 2: Schematic of the deformation of two material curves/surfaces. The top panel shows a small circle at time $t = 0$, which is then deformed into an ellipse (while its maximum dimension is less than the characteristic scale of the flow) and then into a more complex structure (as different parts of the curve experience very different velocity fields). The bottom panel shows a small circle at time $t = T$, which originated from a complex filamental structure at $t = 0$. This structure may be obtained by deforming the circle in backward time. The values of chemical concentration inside the circle at $t = T$ are just those sampled by the filamental structure at time $t = 0$. (Note that the two panels do not imply any kind of reversibility – the lower panel corresponds to a particular choice of initial condition that involves into a circle at time T. If the evolution was continued after time T the circle would stretch and eventually become geometrically complex, much as in the top panel.)

length of another axis. This is a manifestation of the scale reduction that leads to mixing. In a compressible flow there is no absolute constraint on the volume of the sphere, but nonetheless it is the case that in almost all flows the density will not systematically reduce, implying again that one axis must systematically reduce in length. The geometry of the ellipsoidal material surface becomes more complicated when its maximum dimension becomes as large as the length scale on which the velocity field varies. The surface is then strongly distorted and folded as different parts of the surface sample very different velocity gradients.

The relevance of deformation of material surfaces or curves to the evolution of the concentration of a chemical species is emphasised by noting that a similar picture holds in backward time. Neglecting the effects of diffusivity for the present, the values of concentration in a small spherical region will be the values that were present in the same material region at the initial time. If that material region is stretched (in backward time) to length scales greater than those on which the concentration varies in the initial condition, then the small spherical region will contain a wide range of different concentration values and it can be safely assumed that the effect of diffusivity will eventually be to homogenize those values over the region. The intimate relation between relative dispersion, i.e. the separation of nearby particles, and mixing has been exploited in many theoretical studies of the mixing problem.

The stirring and mixing process has so far been described as completely generic. One could equally well be considering the mixing of a smoke plume from a factory into the surrounding boundary layer air, or the mixing into the upper troposphere of boundary layer air that has been lofted in a convective cloud or a convective complex, or the mixing of stratospheric ozone-depleted Antarctic air into mid-latitudes as the polar vortex breaks up in the late spring. These examples range in scales from a hundred metres or so to several thousand kilometres. But the flows that are responsible for stirring and mixing in each of the cases are very different and that has important implications for the stirring and mixing process.

3 Mixing in three-dimensional turbulence

One important category of flow that gives rise to effective mixing is three-dimensional turbulence that occurs, for example, in the boundary layer and in convective clouds and also in intermittent internal mixing events in the troposphere and the stratosphere.

The dynamics of three-dimensional turbulence is characterised by energy input at some large scale, L. If velocities at the large scale are of typical size U, then the energy input rate ϵ satisfies $\epsilon \sim U^3/L$. The dynamics of the turbulent eddies transfer energy from the input scale to smaller and smaller scales through a so-called 'inertial range'. The classical Kolmogorov scaling predicts that in the inertial range the velocity fluctuations at length scale l vary as $\epsilon^{1/3}l^{1/3} = U(l/L)^{1/3}$ and therefore that the typical size of components of the velocity gradient tensor is $(U/L)(L/l)^{2/3}$. The energy transfer is terminated at the dissipation scale l_ν, often called the Kolmogorov scale, where molecular diffusion of momentum becomes competitive with other flow processes. l_ν may be estimated by assuming that stretching and diffusion timescales are equal, implying that $l_\nu \sim \nu^{3/4}\epsilon^{-1/4}$, where ν is the momentum diffusivity. The rate of energy dissipation at the Kolmogorov scale must, in a steady state, equal ϵ, the rate of energy input at the large scale.

It follows that the largest contributions to the stretching come from the velocity field at the dissipation scale and furthermore the stretching rate at those scales is considerably larger (by a factor of $(UL/\nu)^{1/2}$) than that estimated using velocity and length scales at the energy input scale. (Note the velocity gradient is a good estimate for the inverse of the timescale for line stretching since, for three-dimensional turbulence, the time series of velocity gradient experienced by an air parcel is essentially random and, furthermore, the correlation time is of order the inverse of the velocity gradient at the dissipation scale.)

If the diffusivity κ for the chemical species is much less than ν, then the Peclet number at the Kolmogorov scale may be large and the eddies at this scale must stir the chemical concentration field to smaller scales for diffusive homogenization to occur. However, for most chemical species of interest in the atmosphere we may assume $\kappa \sim \nu$ and therefore diffusive homogenisation occurs at the Kolmogorov scale. The time scale required for a chemical concentration field that is initially on the energy input scale, i.e. large scale, to be geometrically deformed until molecular diffusion is important may be estimated by assuming that $(L/U)(l/L)^{2/3}$ is roughly the time required to reduce the scale from l to $l/2$. Summing the times needed to reduce the scale from L to l_ν gives a convergent geometric series whose sum is estimated by L/U multiplied by some moderate factor which is independent of ν and hence κ, if these are small. The time scale required for homogenization on the molecular scale is therefore the same order of magnitude as the time required for advection around the turbulent region on the large scale. Thus the timescale for mixing within a region containing three-dimensionally turbulent flow is the same order of magnitude as the timescale for transport across that region. The implication is that three-dimensional turbulence is very effective at mixing and that, to some reasonable approximation, if there is time for transport of air parcels across a turbulent region then there is also time for mixing within that region.

Mixing in three-dimensionally turbulent flows has been much studied in the laboratory and is of great practical significance because of its relation to the dispersion of pollutants in the atmospheric boundary layer. Research has focussed on considering the mixing problem via the problem of relative dispersion and stochastic models have carefully been formulated and refined to describe this relative dispersion process.

4 Large-scale flows: quasi-two-dimensional turbulence and chaotic advection

Rotation and buoyancy stratification both tend to inhibit three-dimensional turbulence on sufficiently large scales. On scales larger than a few tens of kilometers transport is accomplished by frontal systems, cyclones and anticyclones and, in the stratosphere, propagating and breaking planetary-scale Rossby waves. The stable stratification and geometric constraints ensure that air parcel trajectories are along weakly sloping surfaces, so that horizontal displacement are generally much larger than vertical displacements.

These flows have a dual character, with some aspects of their behaviour appearing organised and wave-like and other aspects exhibiting considerable nonlinearity and randomness. In the latter respect these flows might therefore be regarded as a kind of turbulence, analogous to the two-dimensional turbulence studied in idealised numerical simulations and laboratory experiments. However, the strong difference of these flows from three-dimensional turbulence is that strong vortex stretching is inhibited and therefore the cascade of energy to small scales is inhibited. The velocity field has a finite spatial scale and hence there is no strong increase of velocity gradients as scale shrinks.

It is now realised that flows such as these, with a relatively simple structure in space and time, may be highly effective at stirring and mixing through a phenomenon known as 'chaotic advection'. The idea here is that velocity fields with a very simple structure in space and time may lead to complex and irregular, i.e. chaotic, particle trajectories, with, for example, the distance between initially nearby particles, increasing exponentially in time. As explained above, this separation of nearby particles implies that chemical concentration fields rapidly become complex, with variations on scales much smaller than that of the advecting flow.

In large-scale chaotic-advection type flows the magnitude of velocity gradients is constant with scale and may be estimated as L/U, where L is a typical length scale and U a typical velocity magnitude of the large scale flow. In this case diffusive mixing takes place on a length scale of $(\kappa L/U)^{1/2}$. The time to reach this scale from the large scale is $(L/U)\log(UL/\kappa)^{1/2}$, i.e. considerably larger than the timescale for transport by the large-scale flow. The implication is that in these flows advected chemical species may be spread across the flow domain on the large scale, but for a substantial time may remain unmixed on the small-scale (in contrast to the case in three-dimensional turbulence). Furthermore the fact that the velocity field itself varies only weakly on the scale $(\kappa L/U)^{1/2}$ suggests that the chemical concentration fields tends to be aligned in smooth (but thin) filaments or sheets. Such filaments or sheets of anomalous chemical species, that have not yet been mixed with their environment, are widely observed in the atmosphere.

5 Mixing processes in the real atmosphere

In the real atmosphere three-dimensional turbulence is inevitably affected by the presence of stable density stratification which implies that energy input is needed to move fluid particles in the vertical. Broadly speaking the effect of the stratification is to limit the vertical length scales of the turbulence and hence the vertical length scales over which mixing can occur. The dynamics of the mixing also tends to lead to the formation of interfaces at the upper or lower limits of the turbulent regions across which there are strong density gradients. The stability of these interfaces implies that mixing across them occurs relatively infrequently, often through complex phenomena such as the breaking of waves propagating on the interfaces themselves.

For the planetary boundary layer, the role of stable stratification is to limit the height of the turbulent layer. The strong stable stratification often found at the top of the boundary layer has an important effect on exchange between the turbulent boundary layer and the free atmosphere above it. But when considering transport within the boundary layer stratification may often be neglected.

In the 'free' atmosphere above the boundary layer there is certainly no permanent 'background' field of three-dimensional turbulence. In the troposphere convection gives rise to turbulence, but the fraction of the atmosphere that is actively convecting at any instant is relatively small. In the upper troposphere and stratosphere there is little or no convection, but localised regions of turbulence arise through shear instability or through breaking of inertia-gravity waves. These turbulent regions form sporadically, mix in a localised region and then decay. Thus, outside the planetary boundary layer, turbulent mixing occurs through the net effect of localised, intermittent turbulent events.

The route by which air masses with different chemical characteristics are mixed in the free atmosphere is therefore as follows. Long-range transport and stirring on the large scale is accomplished by quasi-horizontal motion which draws chemical fields out into filaments or sheets. If there was no three-dimensional turbulence, then mixing would eventually be achieved by molecular diffusion alone, but this mixing would occur at very small scales. In practice the effects of molecular diffusion are likely to be enhanced through intermittent encounters of air parcels with three-dimensional turbulence. This enhancement might be substantial in the troposphere, where convection is common, is likely to be much weaker in the lower stratosphere and then to increase again in the upper stratosphere and mesosphere, where three-dimensional turbulence associated with the breaking of gravity waves is more widespread.

See also: Boundary Layers, Clear Air Turbulence, Kelvin-Helmholtz Instability, Lee Waves and Mountain Waves, Parametrization of Physical Processes, Stratospheric Chemistry and Composition, Tropospheric Chemistry and Composition, Two-dimensional Turbulence, Turbulent Diffusion.

Further Reading

Fernando, H. J. S., 1991: Turbulent mixing in stratified fluids. Ann. Rev. Fluid Mech., 23, 455–493.

Ottino, J. M., 1990: Mixing, chaotic advection, and turbulence. Ann. Rev. Fluid Mech., 22, 207–253.

Pierrehumbert, R. T., Yang, H., 1993: Global chaotic mixing on isentropic surfaces. J Atmos Sci, 50, 2462–2480.

Sawford, B., 2001: Turbulent Relative Dispersion. Ann. Rev. Fluid Mech., 33, 289–318.

Shraiman, B. I., Siggia, E. D., 2000: Scalar turbulence. Nature, 405, 639–646.