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MIDDLE ATMOSPHERIC DYNAMICS AND TRANSPORT: SOME CURRENT CHALLENGES TO OUR UNDERSTANDING

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ABSTRACT. The fluid dynamics of wave propagation, wave breaking, and the resulting turbulence – be it the fully three-dimensional small-scale turbulence due to breaking internal gravity waves, or the layerwise two-dimensional turbulence due to breaking Rossby waves – poses three major challenges to research on middle atmospheric dynamics and chemical transport. These are, first, the unjustifiability of the eddy-diffusivity concept, under conditions often met with in the atmosphere, second, the ill-understood nature of the Rossby-wave-associated dynamical feedbacks on the global circulation and, third, an acute difficulty in parameterizing vertical mixing by convectively overturning gravity waves in the mesosphere and lower thermosphere.

1. Introduction

The three major challenges I have chosen to discuss are all related to a tendency for naturally-occurring turbulence to be spatially inhomogeneous. This often gives rise to situations very different from the situations assumed in classical turbulence theory.

One of the contributing factors seems to be the importance of various kinds of wave propagation mechanism. Besides leading to the propagation of information, angular momentum, etc., between different parts of the atmosphere, the dynamical restoring mechanisms to which the waves owe their existence can act locally to suppress turbulent motion, often in a spatially very selective way. Indeed one often has the impression of dealing with closely adjacent, strongly interacting regions of wavelike motion and turbulent motion, a kind of highly inhomogeneous 'wave-turbulence jigsaw puzzle' in which the waves strongly modify, indeed often give rise to, the turbulence, and in which the turbulence, in turn, modifies the local spatial distribution of the wave restoring mechanism, and also, after a propagation delay, the wave field at greater distances. The word 'turbulence' is being used here in the broad sense that includes not only three-dimensional turbulence – such as that due to cumulus convection, to boundary-layer friction, to Kelvin-Helmholtz instability or to breaking internal gravity waves – but also layerwise two-dimensional turbulence, such as that due to baroclinic instability or to breaking Rossby waves.

The first of the three challenges to be discussed is that posed by the concept of the 'eddy diffusivity' of materially conserved quantities such as long-lived tracer substances (§3 below). Although that concept correctly expresses the statistical tendency for such tracers to move downgradient, in some long time average sense – and will, inevitably, continue to be used *faute de mieux* as a modelling device for some time to come – we cannot be too careful about the use we make of the concept. Model predictions that depend on it too heavily need to be regarded with suspicion. This is because the conditions under which it can be strictly justified in terms of classical turbulence theories, namely spatial near-homogeneity of the turbulence, seldom appear to be met, for the reasons just mentioned. For some purposes the concept may actually be wrong qualitatively, in the sense that fluxes are not even roughly proportional to mean gradients. The Antarctic ozone hole provides one of the more conspicuous examples of this. Various other paradoxes arise, as will be pointed out. There is also the simple but potentially important fact that current models of chemical evolution assume that chemical constituents interdiffuse and react when, in reality, they may well be separate and non-reacting in a fully-resolved, fine-grain view (e.g. Tuck 1979).

The second challenge is how to parameterize global-scale dynamical feedbacks in simplified general circulation models, particularly the feedbacks associated with the Rossby-wave-associated or layerwise two-dimensional phenomena that appear to dominate events in the lower and middle stratosphere. It is widely recognized that there will be a continuing need for simplified circulation models to aid the assessment of multidecadal ozone–climate scenarios. Furthermore, research on the feedback mechanisms will be an important means, in its own right, of improving our understanding of what is robust, and what is sensitive, in the complicated web of causal links involved. There has been no spectacular progress over the past few years, as far as I know, and so the present discussion (§4 below) will confine itself to a very brief update on the lengthier discussion given in a previous informal review and forward look, written for the proceedings of the Erice Workshop (McIntyre 1987, hereafter E87). Progress on this extremely difficult set of problems, which are not unrelated to some of the problems to be discussed in §3, seems likely to depend on continued efforts to combine theoretical insights with ultra-high-resolution numerical modelling as well as with observational information. On the observational side, the proposed new generation of space-based wind sounders and high-resolution scanning limb sounders should in due course provide a particularly important source of new information.

It seems more certain than ever that the strange quantity known as potential vorticity will play a central role in the quest for an improved understanding of the global-scale dynamical feedbacks, and that it will also be important for future attempts at the simultaneous retrieval of dynamical and chemical information from future observing systems, and in the quality control of observational data processing. As a preliminary to §§3 and 4, therefore, §2 briefly recalls some of the fundamental properties of PV, including its relevance to wave–mean interaction theory and the differences between PV and chemical-tracer behaviour.

The third challenge (§5) concerns what may be an even tougher part of the global circulation and transport problem, albeit that its most critical importance appears likely, on present knowledge, to be confined to mesospheric and higher altitudes. This is the problem of how to parameterize the vertical turbulent mixing by convectively breaking internal gravity waves in the mesosphere and lower thermosphere. Such mixing seems likely to be important in summertime, for instance, in transporting atomic oxygen downward against the mean circulation (e.g. Thomas *et al.* 1984, Garcia and Solomon 1985). The turbulence is, again, highly inhomogeneous, but interestingly enough it seems possible that the notion of eddy diffusivity might be justifiable to some extent in a non-classical way, for this purpose. However, it can also be shown that there is still no such thing as a single eddy diffusivity that is applicable for all purposes, and that the tacit assumption that there is such a thing as 'the' eddy diffusivity, which one often encounters in the literature, is still highly dangerous.

Another feature of the problem seems to be a pathological sensitivity of the efficiency of vertical mixing to the precise degree of wave supersaturation. In particular, convectively-breaking gravity waves seem likely to be inefficient at vertical mixing unless they break very violently indeed, so as to give a very large supersaturation, or amplitude overshoot. Again, the discussion will be kept very brief since most of the ground has already been covered elsewhere (McIntyre 1989b). Breaking gravity waves provide, also, a particularly striking illustration of the aforementioned differences between PV and chemical-tracer behaviour – differences which can be shown to be of central importance, qualitatively as well as quantitatively, to our understanding of the global circulation.

2. The fundamental properties of potential vorticity

We recall these only briefly since they have been discussed extensively elsewhere (Hoskins *et al.* 1985; Haynes and McIntyre 1987, 1990; McIntyre and Norton, 1990). The most accurate and general version of the potential-vorticity concept, for a continuously stratified fluid, is that associated with the exact set of definitions given by Ertel (1942). A hydrostatic version was given slightly earlier by Rossby (1940). The difference between the exact and hydrostatic versions is usually unimportant in atmospheric dynamics, the main exception being when one seeks to understand in detail how the potential vorticity is affected by three-dimensional turbulent mixing. The exact (Ertel) definition is usually taken for convenience as

$$Q = \rho^{-1}\mathbf{q}_{\mathrm{a}}\cdot\nabla\theta \ , \tag{1}$$

where ρ is the mass density, $\mathbf{q}_{\mathrm{a}}$ the three-dimensional absolute vorticity, including the vorticity of the earth's rotation, ∇ the three-dimensional gradient operator with respect to geometric position $\mathbf{x}$, and θ the potential temperature. As Ertel pointed out, it would be equally valid in principle to adopt any of an infinite number of other definitions in which θ is replaced by some monotonic function of θ. For convenience we shall refer to Q, as defined by (1), as 'the' potential vorticity, hereafter 'PV'. There are three main points about Q.

2.1. MATERIAL TENDENCY, AND VISUALIZABILITY

The first is the well known fact that the PV is *materially conserved* if diabatic heating and nonconservative forces are negligible. This is a particular case of the general result

$$DQ/Dt = -\rho^{-1}\nabla\cdot\mathbf{N}_Q \ , \tag{2}$$

where the material derivative, and the nonadvective flux or transport, are defined respectively by

$$D/Dt = \partial/\partial t + \mathbf{u}\cdot\nabla \ , \qquad \mathbf{N}_Q = -H\mathbf{q}_{\mathrm{a}} - \mathbf{F}\times\nabla\theta \ , \tag{3a, b}$$

$\mathbf{u}$ being the three-dimensional velocity field, $\mathbf{F}$ the viscous or other nonconservative body force per unit mass, and H the diabatic heating rate expressed as the material rate of change of θ. To the extent that the right-hand side of (2) is effectively small, the PV becomes approximately an air-mass marker, making its evolution easy to grasp conceptually, and easy to visualize in terms of isentropic distributions of PV, that is, in terms of layerwise two-dimensional distributions of PV on constant-θ surfaces.

2.2. BALANCE AND INVERTIBILITY

The second main point is the idea, which goes back to Charney (1948) and Kleinschmidt (1950a,b, 1951) – for further historical notes see the review by Hoskins *et al.* (1985) – that, as well as being easy to visualize, isentropic distributions of PV contain nearly all the dynamical information that is relevant to the stratification-constrained, layerwise two-dimensional part of the motion. In other words, isentropic distributions of PV contain nearly all the information about the dynamics of the air motion apart from any inertio-gravity oscillations that may be present. More precisely, there is an 'invertibility principle' saying that if a suitable balance condition is imposed, and a suitable reference state specified – for instance by specifying the mass under each isentropic surface as one does in the theory of available potential energy – then a knowledge of the distribution of PV on each isentropic surface, and of potential temperature at the lower boundary, is sufficient to deduce, diagnostically, all the other dynamical fields such as winds, temperatures, and geopotential heights.

The balance or 'slow-manifold' condition says that inertio-gravity oscillations are either absent, or can be averaged out and ignored. We know that in principle this can be true in general only as an approximation; but the approximation is often amazingly good, far better than might be supposed from the usual theories of balanced motion based on filtered equations (McIntyre and Norton 1990a,b). The succinctness of being able to represent so much dynamical information in the form of isentropic distributions of a single scalar field, the PV, whose evolution is so easy to visualize, is a powerful aid to understanding and quantitatively depicting the layerwise two-dimensional motion. This includes all the usual barotropic and baroclinic instabilities, and other Rossby-wave-associated phenomena. It provides in addition a very succinct way of understanding, and significantly generalizing, the main results of wave–mean interaction theory, and showing how they are relevant to understanding the global atmospheric circulation. For full details, including the relationship between the momentum viewpoint and the viewpoint in terms of isentropic distributions of PV, the reader is referred to a recent paper by McIntyre and Norton (1990b) and to the extensive set of references therein.

2.3. GENERAL CONSERVATION PROPERTIES

The third point has recently been the subject of some controversy. It concerns PV behaviour for general $\mathbf{F}$ and H. The flux form of (2), from which (2) itself can be recovered using the mass-conservation equation $\partial\rho/\partial t + \nabla\cdot\{\rho\mathbf{u}\} = 0$, is exactly

$$\frac{\partial}{\partial t}(\rho Q) + \nabla\cdot\mathbf{J} = 0 \qquad \text{where} \qquad \mathbf{J} = \mathbf{u}\rho Q + \mathbf{N}_Q \ . \qquad (4a,b)$$

This is an equation in what is known as 'conservation form'. Here one does not, of course, mean conservation in the material or Lagrangian sense of §2.1, but in the traditional, general sense used in theoretical chemistry and physics. Material conservation is the special case $\mathbf{N}_Q = 0$. The exact conservation form of (4) is a direct consequence of the mathematical form of (1) and the fact that div curl of any vector field vanishes identically.

One way of talking about the general meaning of (2) and (4) that I find vivid and useful is to state it in terms of the analogy between PV and chemical mixing ratios. This is because the general notion of conservation can be put into correspondence with the notion of an indestructible chemical substance, or decay-corrected radioactive tracer, that is to say a chemical constituent that has zero source. Equations (2) and (4) can be interpreted as saying that the PV behaves like the mixing ratio of a peculiar chemical 'substance', or generalized tracer, that has zero source away from boundaries. The word 'source' is being used here in its standard chemical sense. A chemical substance with zero source means a chemical substance whose molecules are neither created nor destroyed. The *mixing ratio* of such a substance can of course change – for instance by dilution – and so, likewise, of course, can the PV.

One of the peculiarities of the generalized tracer substance whose mixing ratio is the PV is that one can have both positive and negative amounts of it, like electric charge. Another peculiarity is what might be called the 'impermeability property'. This expresses a strikingly simple fact about the flux or transport $\mathbf{J}$ relative to isentropic surfaces that promises useful simplifications in our thinking about the global circulation. It seems likely, in any case, that we shall tend more and more to think about everything relative to isentropic surfaces, both for dynamical (recall §2.2) and chemical reasons (e.g. Yang and Tung 1990, this Proceedings), taking advantage of the fact that radiative transfer tends to keep the middle atmosphere stably stratified.

The impermeability property is another direct consequence of the mathematical form of the definition (1). One can show quite straightforwardly, by manipulating the expressions (3*b*) and (4*b*) giving the total (advective plus nonadvective) flux or transport $\mathbf{J}$, that

A point moving with velocity $\mathbf{J}/(\rho Q)$ always remains on exactly the same isentropic surface.

Various alternative proofs are given in Haynes and McIntyre (1987, 1990) and in McIntyre and Norton (1990a). This result says that isentropic surfaces behave exactly as if they were impermeable to the generalized tracer substance whose mixing ratio is the PV. This is true not just for adiabatic motion, but also when diabatic heating or cooling ($H \neq 0$) makes isentropic surfaces permeable to mass and chemical substances. In this respect isentropic surfaces can be said to act like semi-permeable membranes. These statements, being completely general, apply to the real global atmospheric 'wave-turbulence jigsaw puzzle' in all its enormous complexity.

The general conservation property is mathematically equivalent to an integral relation pointed out by Thorpe and Emanuel (1985), and the impermeability property was, as far as I know, first pointed out by Haynes and myself (1987, *q.v.* for further history). In publishing the latter paper we inadvertently got ourselves into some controversy over both properties. Part of the reason was insufficient care on our part over the wording of the introduction to that paper. (The interested reader is recommended to start at §2!) This was compounded by an interdisciplinary language-barrier problem of which we were unaware at the time. [It appears that, despite the analogy between PV and chemical mixing ratios, a separate convention has grown up in which PV behaviour is thought of in a manner not directly related to the traditional, general notions of conservation relation and conservable quantity, and that along with this has grown up a separate usage of words like flux, transport, creation, destruction, etc., when used in connection with the PV. I have not seen a systematic account of this separate convention, nor a set of explicit definitions of the associated vocabulary, but the convention appears to define the words 'flux' and 'transport' to mean the quantity $\mathbf{u}\rho Q$, in traditional language the *advective contribution* to the total transport $\mathbf{J}$. There appears also, although I am not sure of this, to be a third convention in which the word 'transport' is used to mean the quantity $\mathbf{u}\cdot\nabla Q$, in traditional language the *advection.* It should be noted that each of the latter two conventions prohibit the use of a traditional physico-chemical idea such as 'molecular-diffusive transport' since they render such an idea self-contradictory.]

The other reason for the controversy is more substantial. There appears to be a genuine mistake in the literature, to the effect that PV behaves like a chemical mixing ratio in all essential respects, even when three-dimensionally turbulent mixing is taking place. The impermeability theorem makes it particularly clear, however, that no such behaviour is possible, inasmuch as there is nothing to stop chemicals being turbulently mixed across isentropic surfaces. The same conclusion can be drawn, albeit less directly, from other well known principles like the Kelvin-Bjerknes circulation theorem.

The origin of the mistake appears to be a tacit neglect of the strong diabatic heating or cooling that occurs on the Kolmogorov microscale during turbulent mixing. This is crucially important first for seeing how air and trace chemicals can cross isentropic surfaces, and second for seeing how (2) and (4) are satisfied in the presence of three-dimensional turbulence. The point is relevant irrespective of whether one is thinking of the ρ, θ, $\mathbf{u}$ and $\mathbf{q}_\mathrm{a}$ fields as explicitly representing the detailed, fine-grain reality including the Kolomogorov microscales, so that the diabatic heating field H represents the effects of molecular conduction only, or whether one is taking the coarse-grain view necessary in practical observational work, in which the ρ, θ, $\mathbf{u}$ and $\mathbf{q}_\mathrm{a}$ fields are considered to be coarse-grain approximations to reality, with corresponding adjustments to the fields H and $\mathbf{F}$ to include the eddy flux convergences from unresolved scales. The interested reader may consult our (1990) paper for further discussion, along with a forthcoming paper by Keyser and Rotunno (1990). An example that is relevant to the global circulation problem, and in which the fundamental difference between PV and chemical behaviour shows up especially strikingly, will be noted in §5.

The fact that the notional tracer substance whose mixing ratio is the PV is, in some ways, more like electric charge, ties in with the notion of PV invertibility. In the Boussinesq, quasi-geostrophic approximation, for a fluid of constant static stability, the mathematical process of PV inversion is the same as the mathematical process of finding the electrostatic potential from a given charge distribution (Obukhov 1962; Hoskins *et al.* 1965, §5).

3. Some remarks on the eddy diffusivity concept

One often reads about 'the' eddy diffusivity of the atmosphere, or 'the' small-scale mixing, as if it were something ubiquitous whose prior existence can be taken for granted, and which always acts to smooth out small-scale variations in any quantity in which we might be interested. Some models of atmospheric motion have even been criticized from time to time as 'unrealistic' for the *lack* of a powerful eddy smoothing term.

I have been worried about our dependence on the eddy-diffusivity concept for a long time, without knowing quite what to do about it. We depend on numerical models to help us grasp the complexities of atmospheric motion, and its implications for chemical evolution. We hope to develop them to the point where they can be useful predictors of, among other things, global environmental change. But nearly all our atmospheric numerical modelling, be it one, two, or three dimensional, depends on the notion of eddy diffusivity, in one version or another. To what extent does that notion ever make sense, except possibly as an artifice that we have been compelled to adopt *faute de mieux* in order to keep our numerical models stable, and as a very rough way of expressing the observed tendency of materially conserved tracer quantities to be transported down their gradients, in some average sense?

3.1. THE INHOMOGENEITY OF SMALL-SCALE TURBULENCE

Anyone who has observed what can be seen out of aeroplane windows must feel uncomfortable with the idea – which seems to be widely held – that the atmosphere *above* the planetary boundary layer is permeated by quasi-uniform, small-scale, three-dimensional turbulence giving rise to a ubiquitous, pre-existing small-scale eddy diffusivity. Looking at the variety of cloud forms, all the way from turbulently-convecting cumulus and Kelvin-Helmholtz billows to silky-smooth, laminar-looking wave clouds revealing thin layers in the humidity field, one gets the impression, rather, of extreme spatial inhomogeneity. For what it is worth, this impression is reinforced by the amazing smoothness of passenger-jet flight in the upper troposphere or lower stratosphere, interrupted only now and then by the more obvious encounters with clear-air turbulence. The sample may be biased but the point seems significant nonetheless. The impression one gets, in this and in other ways, is that very large portions of the atmosphere are actually in laminar motion, in the sense that small-scale, truly three-dimensional turbulence is altogether absent. This hypothesis is consistent with the fact that Richardson numbers are usually observed to be considerably larger than unity.

3.2. SMALL-SCALE INHOMOGENEITY, LARGE-SCALE INHOMOGENEITY AND WAVE BREAKING

One can make sense of the extreme spatial and temporal intermittency of small-scale turbulence in the real atmosphere, outside convective clouds and the planetary boundary layer, by adopting the time-honoured hypothesis that clear-air turbulence is often due to breaking waves of one kind or another. This notion can actually be generalized in a significant way, adumbrated long ago by Deem and Zabusky (1978). When suitably formulated (a careful discussion is given in McIntyre and Palmer 1985), it applies in various forms over a vast range of scales, from ordinary small-scale gravity waves up to planetary-scale Rossby waves.

Just as breaking gravity waves produce three-dimensional turbulence and mix potential temperature vertically, so do breaking Rossby waves produce layerwise two-dimensional 'turbulence' and mix PV isentropically, that is to say along isentropic surfaces. Recent satellite data studies and high-resolution numerical simulations have vividly revealed just how spatially inhomogeneous is the resulting wave-turbulence jigsaw puzzle when viewed on a global scale (Juckes and McIntyre 1987, hereafter JM, Haynes and Norton 1989, Salby *et al.* 1989, Juckes 1989, Juckes *et al.* 1989). Animated grayscale PV maps were shown at the workshop, vividly conveying this inhomogeneity in a numerical model of the wintertime stratosphere; see also figure 1 below.

3.3. THE ANTARCTIC OZONE HOLE, AND SUBPOLAR PV BARRIERS

A striking feature seen again and again in the high-resolution simulations is made clear by looking at the motion of a band of PV values embedded in the region of very steep PV gradients that mark the edge of the main polar vortex. Such a band of values was highlighted in one of the animated sequences shown at the workshop, and a frame from that sequence is shown here in figure 1 below. The band exhibits a peculiar resilience or elasticity that, in the case shown, altogether prevents it from being entrained into the more turbulent-looking regions on either side of it, especially on the tropical side, where the motion is arguably two-dimensionally turbulent by most accepted criteria and where it seems appropriate to speak of a Rossby-wave 'surf zone'. It is clear from the animated version of figure 1 that, by contrast, the band undulates reversibly: its motion is wavelike rather than turbulent. To very good approximation it is a material contour; and this means that *all the material it encloses is chemically isolated from its surroundings.* This vortex isolation phenomenon – JM called the polar vortex a 'containment vessel' – seems to be a crucial factor in the genesis of the Antarctic ozone hole, possibly just as crucial as the non-standard chemistry involved† (e.g. Tuck *et al.* 1989, and other papers appearing in the two special JGR issues on the Airborne Antarctic Ozone Experiment). As is well known, neither factor was represented in the models on which the Montreal Protocol on chlorofluorocarbons was based.

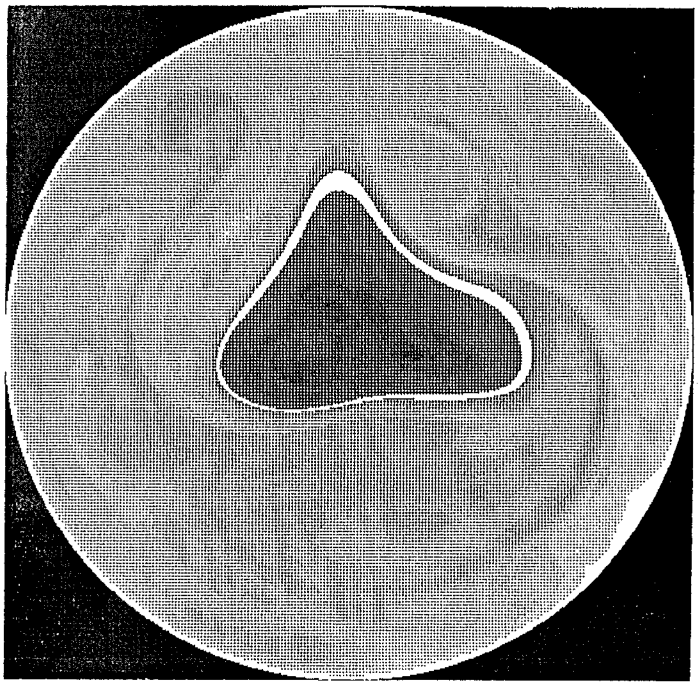

Figure 1. Grayscale representation of the PV in a hemispheric single-layer model of the stratosphere (shallow water equations with mean equivalent depth 4 km), shown in a polar stereographic projection. The grayscale mapping is monotonic (dark cyclonic and light anticyclonic) *except* that a substantial band of PV values embedded in the main polar vortex edge is also made light, in order to make the edge, or region of steep PV gradients, more easily visible. In an animated version of this display shown at the Workshop, this white band was seen to undulate as if made of elastic, making the PV barrier effect due to the concentrated Rossby-wave restoring mechanism visually evident.

Part of the explanation for the contour's effectiveness as a dynamical barrier is that its undular motion is a case of Rossby-wave motion. As with other wavemotions there is a *restoring mechanism*, in this case a sideways restoring mechanism due to the large PV gradient concentrated in the vortex edge – somewhat analogous to the vertical, gravity-wave restoring mechanism due to the potential temperature gradient concentrated in a strong temperature-inversion layer. But that is only part of the story. The problem of why the contour presents such an effective barrier to material incursions even on the very smallest

† Also Solomon, S., this Proceedings.

resolved scales, on which the Rossby restoring mechanism is relatively weak (Hoskins *et al.*, 1985, p.920), is in reality a highly nonlinear, highly scale-interactive problem – hence the need for very accurate, fine-resolution simulations (see JM and Juckes *et al.* 1990 for a demonstration of their numerical integrity) before claiming that this 'PV barrier' effect has really been shown to be implied by the dynamics. As already emphasized elsewhere (McIntyre 1989a), "It is possible, for all we can tell from linearized Rossby-wave theory, that material might be able to cross the putative PV barrier like water through a sieve". But in nonlinear reality this is not so: careful numerical simulations like those cited consistently show that the barrier is effective. Some very recent, multi-layer high resolution numerical experiments that add to this evidence will be described in a forthcoming paper by Haynes and Norton (1990). An independent laboratory demonstration of a PV barrier (in a single-layer system), confirming that it is a robust consequence of the fluid dynamics, has been given by Sommeria *et al.* (1989).

It hardly needs saying that the nonlinear PV barrier dynamics just described contradicts the eddy-diffusivity assumption, as it is usually applied. The transport of PV and long-lived chemical tracers is least, not greatest, where PV and chemical gradients are greatest. Of course one can to some extent mimic polar vortex isolation in a model based on the eddy-diffusivity assumption, by forcing the assumed eddy diffusivity, K_{yy} say, to be highly structured in space and time (e.g. Plumb and Mahlman 1987, Juckes 1989, Yang and Tung 1989), and in particular by forcing it to a very small value at some subpolar location (M.P. Chipperfield, J.A. Pyle, personal communication). Such devices will continue to be used until improved modelling concepts are developed. Yang and Tung (1990, this proceedings) have taken the use of spatially variable K_{yy} in height-latitude global chemical models to a considerable degree of sophistication; and this may well lead to a line of work that represents the best we can do with the K_{yy} concept. The approach depends crucially on the isentropic distributions of all the chemicals concerned being well correlated with the isentropic distributions of PV (in reality, as well as in the small-displacement *theory* used to motivate the modelling approach – which, incidentally, is the origin of the scale separation in that approach). It is clear that for the real atmosphere this does not add up to a fully justifiable procedure, and it remains to be seen how well it does in practice.

3.4. QBO DYNAMICS SUGGESTS THE EXISTENCE OF SUBTROPICAL PV BARRIERS

The observed quasi-biennial oscillation of the zonal winds in the equatorial lower stratosphere (QBO) implies the existence of subtropical PV barriers that must, to a considerable extent, isolate the tropical region from the mid-latitude planetary wave activity of the winter hemisphere. These, too, will need to be taken into account in future chemical modelling.

The point is better appreciated by contrasting the real tropics with the tropics in the one-layer numerical experiments already cited. An *unrealistic* feature of these experiments, seen for instance in figure 1 above, is a tendency for the planetary-scale Rossby waves to break all the way to the equator. This produces unrealistically strong easterly accelerations in the tropics, about an order of magnitude greater than those observed in the easterly acceleration phase of the QBO in the real atmosphere. We are forced to the conclusion that the planetary-scale Rossby wave 'breakers' in the real atmosphere usually reach no further than the subtropics, and that the deep tropics is to a large extent isolated laterally from middle latitudes, albeit possibly not completely. Satellite observations of volcanic aerosols lend independent support to this idea (G.S. Kent, M.P. McCormick, personal communication).

Now published in Norton (1994), JAS 51, 654–673 "Breaking Rossby waves in a model stratosphere diagnosed by a vortex-following coordinate and a technique for advecting material contours". See also Waugh & Plumb 51, 530

Stop press: Drs P.H. Haynes and W.A. Norton (personal communication) have very recently taken single-layer modelling to a higher level of sophistication, including a promising way of relating single-layer model runs more closely to multi-layer model runs and, it is hoped, ultimately to observational data. One result has been the discovery of single-layer cases (not shown here) that appear to have a more realistic tropics. This has opened the way to some key experiments on the interaction between nonlinear eddy transport with photochemically different types of chemical constituent, which we believe will have a bearing on recent arguments about extravortical ozone depletion (Proffitt *et al.* 1989).

3.5. WHEN CAN ONE JUSTIFY THE NOTION OF EDDY DIFFUSIVITY?

Why does the classical justification of the eddy-diffusive or flux-gradient hypothesis involve assuming that the turbulence is nearly homogeneous? The reason is that there has to be a separation of spatial scales: it has to be assumed *inter alia* that the mean gradients are characterized by much larger spatial scales than the largest turbulent eddies (e.g. Batchelor and Townsend, 1956). Many examples, including the foregoing, suggest that this scale-separation assumption may often be one of the worst modeling assumptions one can make. The real atmosphere often seems to prefer a diametrically opposite state of affairs in which 'mean gradients' develop scales as small as the definition of 'mean' allows them to be. The dynamical PV barrier that permits the Antarctic ozone hole to form provides merely the most conspicuous example.

It is not just a question of fluxes generally failing to be proportional to gradients, as the existence of PV barriers shows. It is also a question of non-localness. The flux-gradient hypothesis, as usually applied in practice, carries not only the assumption that fluxes are at least roughly proportional to gradients, with a proportionality 'constant' K say (scalar or tensor), but also the assumption that K can be preassigned or computed *locally*, e.g. from some measure of local turbulent intensity. This is another way of seeing that a separation of scales is required. (In the case of molecular diffusion, molecular mean free paths or interaction distances provide the inner scale, and temperatures provide the preassigned intensity).

I do not want to overdo my critique of the eddy-diffusivity concept; and the concluding §6 will mention two naturally occurring cases where the concept does appear, in fact, to have some partial *prima facie* justifiability.

3.6. A 'HOMOGENEOUS TURBULENCE' PARADOX

It is interesting to recall how drastically the eddy-diffusivity idea can fail even for passive-tracer dispersion in a classical homogeneous-turbulence model, if the scale-separation assumption is violated by the *tracer* distribution. One might be tempted for instance to take the classical enstrophy-cascading inertial subrange model of 2D turbulence (k^{-3} energy spectrum) as a model of a stratospheric Rossby-wave 'surf zone'. A well known property of this model is the scale-independence of eddy turnaround times (e.g. the enstrophy or mean-square vorticity in an octave from wavenumber k_0 to $2k_0$ is proportional to $\int_{k_0}^{2k_0} k^2 k^{-3} dk = \ln 2$, independent of k_0). Take a tracer blob whose initial spatial distribution has characteristic scale L. The ensemble-mean concentration can certainly be expected to spread out as time goes on, the tracer in other words being turbulently transported down its gradient. But can we characterize this process by an eddy diffusivity K homogeneous in space? Certainly not, since if we could, then the time for the mean tracer distribution to double its spatial scale would $\propto K^{-1}L^2$. But this immediately contradicts the basic property of the homogeneous turbulence model, that characteristic eddy times are independent of spatial scale. The model clearly predicts, therefore, that if we repeated the thought-experiment with L half as big, then the size-doubling time would be the same as before, not four times faster.

Some other, very intriguing, paradoxes associated with the idea of eddy diffusivity are described by Kraichnan (1976; see also Corrsin 1974). I am indebted to T.G. Shepherd for drawing my attention to these two references.

4. Dynamical feedbacks on the global circulation: Rossby-wave aspects

Besides those just discussed, another basic difficulty is that Rossby-wave propagation is not easily quantified. Wavelengths are comparable to basic-state variations, phase speeds are comparable to mean flow speeds, and amplitudes are typically large, in the appropriate dimensionless sense, this of course being the reason for the relevance of the generalized 'wave breaking' concept. Unresolved questions include the longstanding question of how to quantify the forcing of stratospheric planetary-scale Rossby waves by their putative tropospheric sources. Another – an inhomogeneous-turbulence question par excellence – concerns the (perhaps highly variable) reflectivity of Rossby-wave surf zones. Such questions were aired extensively in E87 (*q.v.*, & references therein), and still need to be answered before final warmings, QBO modulations, and other possible manifestations of planetary-wave coupling can be said to be fully understood.

One of the key challenges here will, I think, be that of understanding the Antarctic final warming. Not only is this of great potential interest in its own right, as suggested recently by Farman *et al.* (1988), for understanding the interannual variability being observed in ozone-hole chemistry; it also seems to me to be one of the litmus tests of our understanding of the range of purely dynamical questions just mentioned. I can do no better than to quote from an earlier paper (McIntyre 1989a), regarding scientific opportunities arising from the recently increased supply of observational information about the Antarctic:

"One of these [opportunities] might be the long-awaited chance to test theoretical ideas on vortex erosion as a self-tuning Rossby-wave resonance mechanism (Haynes 1985). Self-tuning resonance, albeit with a different tuning mechanism, was originally suggested by Plumb (1981) as a contributing factor in the dynamics of northern hemispheric stratospheric warmings. There are good theoretical grounds (Haynes, *op. cit.*) for believing that the poleward-downward vortex erosion suggested by Antarctic observational data for late winter and early spring (e.g. Farrara and Mechoso 1986, Shiotani and Gille 1987) will tune the vortex in such a way that the speed of long Rossby waves systematically becomes less retrograde. Diabatic heating as well as erosion is involved, of course, especially at the higher stratospheric altitudes, and so it would be more accurate to think in terms of a highly interactive *combination* of self-tuning and externally imposed tuning.

"Suppose, for instance, that the gravest wave-1 free mode of the vortex were to become stationary as a result of the poleward-downward attrition of the vortex. The physical implication is that the vortex would become easy to push off the pole. Any forcing mechanism tied to geography, such as tropospheric storm-track activity or blocking, could do the pushing. Numerical experiments are being planned to test this idea. [I can add that these are now under way (P.D. Clark, personal communication).] They not only promise to give us a better understanding of Antarctic final warmings but, because stratospheric warmings in the northern hemisphere pose a far more complicated modelling problem, which has yet to be surmounted, the Antarctic might also turn out to give us the first convincing test of the relevance of Rossby-wave resonance in the real atmosphere."

Other updates to the discussion of E87 are:

1. Progress has been made on the fundamental theory of wave-activity conservation relations (Haynes 1988). As a result, we now know not only how quantities like the Eliassen-Palm flux are related to the underlying Hamiltonian dynamics, but also how to fit it into a coherent wave-mean interaction theory, taking account of wave dissipation. However, the details are dauntingly complicated, and there is a deeper problem of knowing what choice to make to define the basic state. It is not clear to me that any analytically simple averaging operator gives a good way of doing this; the concept of PV rearrangement, subject to the fundamental conservation properties summarized in §2.3, seems likely to be more fruitful, but there is still an enormous range of apparently arbitrary choices to be made.

2. I now think that spontaneous inertio-gravity-wave emission is not very likely to be a powerful contributor, at least not directly, to the middle-atmospheric angular momentum balance. Kelvin-Helmholtz envelope radiation (Fritts 1984) still seems to be a strong contender.

3. Signficant progress on assessing the mathematical status, and ultimate accuracy, of the PV inversion and balance concepts has been made (Egger 1990; McIntyre and Norton 1990b).

5. Further remarks on breaking gravity waves

The observed structure of breaking gravity waves both in the laboratory (e.g. Koop and McGee 1986) and in the atmosphere (e.g. Kopp *et al.* 1985) provides a small-scale three-dimensional example of the extreme spatial inhomogeneity that seems to characterize many naturally-occurring turbulent fluid flows. There are further small-scale examples in the book by Turner (1973). In the case of breaking gravity waves, an important consequence is that vertical mixing of tracers is often far less efficient than one might guess from the requirements of wave dissipation, or from observed turbulent dissipation rates (Chao and Schoeberl 1984, Fritts and Dunkerton 1985, Coy and Fritts 1988, McIntyre 1989b, Walterscheid and Schubert 1989). This seems true at any rate unless the waves break extremely suddenly and violently, as may occur in the winter mesosphere and the summer lower thermosphere. The latest conclusions on this problem seem to be:

1. Vertical mixing seems likely to be even more sensitive to the wave supersaturation $(a-1)$ than was deduced in earlier work; and
2. There is no such thing as 'the' eddy diffusivity for all purposes. For instance, values required to account for wave dissipation can be quite different from values that might be relevant to the vertical transport of chemical constituents. In particular, the idea of 'the' turbulent Prandtl number does not appear to be well defined.

In the gravity-wave case, it is worth noting that breaking not only mixes entropy and chemicals vertically, but also transports PV sideways, and often upgradient; a detailed analysis is given in the paper by McIntyre and Norton (1990a). This is consistent with the basic theorems of §2.3: the notional tracer substance whose mixing ratio is the PV can be, and in this case is, transported exactly along isentropic surfaces, no approximations being involved. In both the gravity and the Rossby case, and for more complicated wave types such as the various equatorial waveguide modes, the irreversible effect of breaking or otherwise-dissipating waves on PV and vorticity distributions is perhaps the most general way of describing the wave-induced mean effects associated with breakdown of the nonacceleration theorem of wave-mean interaction theory; again, the reader may consult the recent paper by McIntyre and Norton (1990a) for a detailed discussion. The high-resolution Rossby wave-breaking simulations cited in §3 provide one very clear illustration of these wave-induced mean flows.

6. Concluding remarks

Every time one looks at the evidence about real fluid motion, or pushes up the resolution in one's numerical experiments, one sees an increasingly striking departure from the conditions of near-homogeneous turbulence that comprise the classical justification of the eddy-diffusivity concept. There is also the problem of finite chemical 'mixdown time' discussed in JM, stemming from the remarks in Tuck (1979). It is difficult to escape the conclusion that we should be looking for radically new modelling concepts in order to represent correctly both the dynamics, and the interactions between dynamics and chemistry.

As already mentioned, I don't want to overdo my criticism of the eddy diffusivity concept. It may somehow manage to be qualitatively correct in some instances where it is not justifiable. There are even a few cases in which a partial justification seems possible – mainly concerning situations where it makes sense to consider only fluxes and mean states averaged over long times, and where problems like mixdown are not important. For instance Holton (1986) gives an interesting argument as to why globally averaged one-dimensional models might actually make sense as along as attention is confined to very long-lived tracers, and to global-average mixing ratios on isentropic surfaces. The requirement of very long chemical timescales (much longer than global circulation turnover times, i.e. several years) is stringent. Also, PV barriers might vitiate the argument!

There are two other naturally occurring turbulent cases I know of at present where the eddy-diffusivity concept appears to have some chance of a *prima facie* justifiability. One is the ocean gyre case, where the Rossby length is small in comparison with gyre scales and gives at least the possibility of a scale separation (Rhines 1977). But in this case it is still difficult to believe in the relevance of preassigning the eddy intensity.

The other case was recently pointed out to me by T. VanZandt, who drew my attention to an interesting paper by Woodman and Rastogi (1984) on the thin turbulent layers observed by the Arecibo radar in the tropical lower stratosphere. They argue cogently that, according to the radar evidence, there is some degree of statistical homogeneity in the altitude distribution of the occurrence of these layers. In that case one *can* get a scale separation, and hence eddy-diffusive behaviour, for long-lived tracers with smooth vertical profiles, despite the undoubtedly extreme inhomogeneity of the turbulence within each turbulent layer. The scale separation is based on the thinness of the complete turbulent layers relative to the scale height of the tracer.*

In this last case, the idea of a preassigned eddy intensity might make sense also, up to a point. If one assumes that the turbulence is due to an input of inertio-gravity waves generated by topography, or for instance by spontaneous wave emission from jet streaks, with the waves subsequently breaking via Kelvin-Helmholtz instability as can be expected for such waves, then one can imagine sensible modelling experiments in which the wave input is preassigned. Such a scenario seems self-consistent in that waves that propagate vertically while breaking could well give approximately homogeneous statistics of turbulent layer occurrence, after averaging over many breaking events and detailed profile changes. It would probably be pushing the idea too far, however, to suppose that the resulting eddy diffusivity is a true diffusivity that acts most strongly to smooth the *smaller* vertical

* It has come to my attention that the essential idea was previously published by E.M. Dewan in Science 211, 1041-2 (1981).

scales, since the problem of statistical inhomogeneity will reappear at such scales, This is presumably why balloon and aircraft data (e.g. Proffitt and McLaughlin 1983; Danielsen *et al.* 1987, Tuck *et al.* 1989) often show fine vertical scale features, much as one might also expect from casual observations of lenticular clouds.

Modelling studies to examine such situations more closely might well be of great interest, aiming for an improved understanding of the breaking of lower-stratospheric inertio-gravity waves and the detailed way in which this interacts with the vertical profile changes due to individual breaking events, perhaps leading to a more accurate model to which to fit the radar results. Such studies might also throw some light on an unresolved disagreement between radar results like those of Woodman and Rastogi (also references therein) and an interpretation of aircraft data by Lilly *et al.* (1974). The radar results give values of the order of 0.2 to $0.3\mathrm{m}^2\mathrm{s}^{-1}$, but the aircraft data an order of magnitude less, at $0.012\mathrm{m}^2\mathrm{s}^{-1}$. Of course the measurements were made at different times and places, and might merely be reminding us that we should never fall into the trap of thinking in terms of 'the' eddy diffusivity.

Corresponding results might well hold also for the mesosphere, apart from the different predominant mode of wave breaking (and also, it must be presumed, in the ocean thermocline), although in the case of the mesosphere this will not take away the problem of sensitivity to supersaturation noted in §5. In the mesosphere it is interesting to note that the inefficiency of vertical mixing, which is associated with the fact that we expect these waves to be breaking more by convective overturning than by Kelvin-Helmholtz instability, can be shown to mean that the effective thickness of the turbulent layers is likely to be a great deal less than their instantaneous thickness as seen in rocket profiles such as those presented in Kopp *et al.* (1985). This is because of the geometrical nature of the distortion of the isentropic surfaces by the convectively overturning gravity waves, in relation to the phase of the waves.

Thus, in the upper mesosphere and lower thermosphere, there might also be some justification to the notion that vertical mixing of long-lived tracers could be described by an eddy diffusivity. The difficulty remains that, even if so, its value appears certain to be highly sensitive to wave parameters, particularly wave intermittency. This again has been discussed at greater length elsewhere (McIntyre 1989b). In particular, a given long-time-mean momentum flux, such as would be required to account for a given global mean circulation strength, could well be associated with very different intensities of vertical mixing, being smaller or greater, in fact, according to whether the wave flux is more steady or more intermittent.

The foregoing implies a correction to the mixdown-time estimate given in JM (penultimate section). If the suggestion of a vertical eddy diffusivity of the order of 0.2 to $0.3\mathrm{m}^2\mathrm{s}^{-1}$is correct, then the mixdown time of a month becomes more like a week, and the corresponding vertical scale a few hundred rather than a few tens of metres. In this connection an examination of the aircraft data from the recent airborne polar stratospheric ozone expeditions would be of the greatest interest, and comprises yet another interesting challenge, in which I should like to get involved very soon.

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