On the Conservation and Impermeability Theorems for Potential Vorticity

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ABSTRACT

If the partial analogy between the behavior of Rossby–Ertel potential vorticity (PV) and the behavior of chemical tracers is to be correctly used in the general case of diabatic, frictional motion, then certain fundamental differences, as well as similarities, between the behavior of PV and that of chemical tracers must be recognized. These differences stem from the well-known kinematical relationship between PV and isentropic circulation (via Stokes' theorem), which has no counterpart for chemical substances.

One way of stating the analogy while recognizing the differences is to say first that PV behaves like the mixing ratio of a peculiar chemical "substance" that has zero source; i.e., is exactly conserved, away from boundaries (conserved not in the material or Lagrangian sense, but in the general sense associated with the idea of an indestructible chemical substance), and second that isentropic surfaces behave exactly as if they were impermeable to this "PV-substance" or "PVS," even when diabatic heating or cooling, including that associated with turbulent mixing, makes them permeable to mass and chemical substances. In this respect isentropic surfaces can be said to act like semipermeable membranes. The PV itself can of course change, as can the mixing ratio of an exactly conserved chemical substance or decay-corrected radioactive tracer. For instance, all these mixing ratios can change by dilution when cumulonimbus clouds penetrate isentropic surfaces in a tropopause fold.

The net flux or transport of PVS along isentropic surfaces can be either up or down any pre-existing isentropic gradient of PV. For instance the typical effect of the small-scale turbulence due to breaking internal gravity waves is to transport PVS along isentropes in a gradient-independent sense, while transporting chemical substances across isentropes in a downgradient sense. It is the turbulent transport of PVS along isentropes that gives rise to the phenomenon of gravity-wave drag. Such a transport is absent from the formulation given in Danielsen (1990), which supposes that PV always behaves like the mixing ratio of a chemical even in three-dimensionally turbulent flow. The latter supposition is demonstrably incorrect.

1. Introduction

The partial analogy between the Rossby–Ertel potential vorticity (PV) and the mixing ratio of a chemical tracer, or long-lived airborne chemical substance, has been recognized and found useful in meteorological research since the 1940s; some historical notes are given in Hoskins et al. (1985). The analogy with chemicals is by no means the only correct way of thinking about PV behavior, but it is exciting renewed interest because it lies at the heart of the complex problems of coupled radiation, chemistry, and dynamics that must be tackled in order to understand our global atmospheric environment. One aspect has been the extensive use of coarse-grain observational PV estimates in the recent airborne polar stratospheric ozone expeditions, both in the flight planning and in the subsequent analysis of chemical data (e.g., Tuck et al. 1989, Hartmann et al. 1989; Lait et al. 1990; McKenna et al. 1989; Proffitt et al. 1989; Schoeberl et al. 1989; Tuck 1989; Yatteau et al. 1990). Important precedents to those expeditions were the beautiful airborne studies of jet structure and tropopause folding by Danielsen and his collaborators (e.g., Danielsen 1968; WMO 1985, sections 5.2.4, 5.2.6; Danielsen et al. 1970, 1987; Danielsen and Hipskind 1980).

The purpose of the present paper is to review some basic aspects of the PV-chemical analogy about which some misunderstanding appears to have arisen. The discussion complements that given in an earlier publication (Haynes and McIntyre 1987, hereafter HM87, q.v. for further history), and in the process corrects some theoretical errors and apparent misapprehensions in the paper by Danielsen (1990, hereafter D) appearing in this issue, which criticizes HM87. Our concern however is not mere correction but rather to set on record, with the Editors' permission, as clear a picture of the PV-chemical analogy as we can. The concern stems from a belief that the analogy is profoundly important, a belief that we clearly share with Dr. Danielsen and with many other colleagues. It therefore seems desirable to have available not only a mathematically correct theory, but also a terminology and set of concepts precisely consistent with that theory, and having the same meaning for PV as for chemicals, however that meaning is expressed. Although we have

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no wish to impose semantic conventions we think it would be valuable, and conducive to progress, if a single convention could be used in a single context, bearing in mind that PV-related dynamics and the resulting chemical transports are likely to be considered together to an increasing extent.

It would be even more valuable, we believe, if the particular semantic convention already accepted for airborne chemicals, and for conservable physical quantities in general [such as energy; e.g., Feynman et al. (1964), Vol. II, p. 27-1], were to be accepted also as a possible way of discussing PV behavior, thus minimizing the proliferation of terminology. The most pointed criticisms of HM87 in D arise mainly from disagreement over the definitions of basic concepts like flux, transport, source, sink, creation, destruction, etc. These are tacitly defined in D to have meanings that differ from the meanings traditionally used in connection with conservation relations and conservable quantities in chemistry and physics. Statements (i) and (ii) of HM87, quoted out of context in D, depend for their correctness on using the latter, traditional meanings. That is why we warned the reader that the statements hold "in a sense to be explained carefully in section 2" of HM87. We were at fault, however, in not emphasizing this crucial point even more strongly, and in not spelling out earlier and more explicitly that in statements (i) and (ii) the term "PV" was intended to refer to the PV regarded as a conservable, in fact conserved, quantity, in the general sense. Perhaps indeed we were quite wrong, as suggested by a reviewer of this paper, to have risked using the term "PV" at all in this way, even though no other accepted term is available. Sections 2 and 3 of the present paper review the basic concepts, and try very carefully to make clear the distinction between the conventions used in D, on the one hand, and the conventions used in HM87 and in connection with the general notions of conservation relation and conservable quantity, on the other [Eqs. (3.8)–(3.10) below]. To be sure of clarity we have taken another risk, that of introducing one new term, "PV-substance," to denote the conserved quantity whose mixing ratio is the PV.

There is, however, still more at issue than basic concepts, definitions, and semantics. The viewpoint presented in D is not, in its own terms, fully self-consistent. For instance if the suppositions in D about PV behavior in three-dimensionally turbulent flow were correct, then all the accepted theories and parameterizations of the drag due to breaking internal gravity waves would have to be abandoned. That would be contrary to the implications of a large body of laboratory, field-observational, and theoretical evidence. We return to this point (sections 6 and 7 below), and to some other points raised in D (section 8 below), after recalling the relevant fundamentals as briefly as possible consistent with clarity, in sections 2–4, and discussing a basic example in section 5. The reader already familiar with the fundamentals, and with a sufficient set of examples,

may wish to jump straight to section 8 and then to the brief concluding remarks in section 9. Readers who require, instead, the quickest possible appreciation of the most basic point at issue may prefer to jump to section 5, where the point is demonstrated from first principles in two self-contained lines of mathematical manipulation.

2. The analogy

The basis of the PV-chemical analogy is, of course, Ertel's theorem that the PV is materially conserved in the absence of diabatic heating and frictional or other nonconservative forces, plus the fact that the mixing ratio of a chemical substance is materially conserved in the absence of chemical sources and sinks and in the absence of diffusion, sedimentation, etc. The analogy, if it is to be pursued, therefore requires us—and it seems that there is no escape from this requirement— to regard the PV as the mixing ratio of a notional "substance," a case of the generalized tracer referred to in HM87, section 2. This notion of "tracer" was crucial to the thinking that we tried to express in HM87; and it will be equally crucial here. To avoid further confusion, we introduce one new piece of terminology to make explicit the distinction between the notional tracer substance on the one hand, and its mixing ratio on the other. The notional substance, which lacks an accepted name, will here be called the "PV-substance" or "PVS." In thus naming it we need to recognize that the amount of this "substance" contained in a given region is a signed quantity constructed by algebraic summation, unlike the amount of a real chemical substance, which is always nonnegative.

If one wishes to pursue the analogy further, it is necessary to consider what other properties the notional PVS might have in the presence of diabatic heating and nonconservative forces. The general theorems discussed in HM87, and summarized in the Abstract of the present paper, provide one among several ways of seeing that in certain respects the PV behaves very differently, in a fundamental sense, from the mixing ratio of a chemical substance, quite apart from its signedness and its special significance for the dynamics. The differences can also be seen from the well-known relationship of the PV with Rossby's isentropic vorticity and hence, via Stokes' theorem, with the Kelvin–Bjerknes circulation around a closed isentropic contour (e.g., Hoskins et al. 1985). The latter relationship has no counterpart for chemicals. As any of these considerations show, the differences between PV and chemical behavior are not artifacts of any choice of semantics, formulation or coordinate system, but are real, and inescapable, differences. For instance they are (i) independent of whether one adopts an Eulerian, a Lagrangian, or an isentropic viewpoint, (ii) independent of whether or not one is using a coarse-grain approximation to the velocity and thermodynamic fields (HM87, Abstract), (iii) independent of whether one

considers local densities and fluxes on the one hand, or integrated quantities on the other, and (iv) independent, in the latter case, of the choice of volume of integration.

It should be said immediately that there is nothing about these differences that conflicts with the striking correlations between PV and chemical mixing ratios, including the mixing ratios of ozone and decay-corrected radioactive tracers, that have been seen in many of the aircraft observations already cited. But it is no surprise, on the other hand, to find cases where such correlations are imperfect (e.g., Keyser and Shapiro 1986, Fig. 11; WMO 1985, §5.2.4). These points will be dealt with in section 8. There is no conflict, either, with the illustrative examples presented in D. These do not disprove any result or statement in HM87—indeed D (4.17) confirms HM87 (2.15)—they disprove only D's reading of statements (i) and (ii) of HM87 with the different meanings of the terms transport, etc., used in D.

It should also be said that HM87 did not mean to give an impression that all alternative viewpoints on the PV-chemical analogy are untenable. On the contrary, there are an infinite number of self-consistent alternative viewpoints, if only because of the well-known ambiguities inherent in the fluxes and densities appearing in conservation relations (e.g., Feynman et al. 1964, Vol.II, p. 27-6; HM87, p. 830). One example of this is the fact that one can add the curl of an arbitrary vector field to the flux whose divergence appears in a scalar conservation relation. This does not invalidate the equation, since div curl of any vector field vanishes identically. The curl of any vector is a "do-nothing" flux. For that matter one can add anything at all to both sides of an equation. Such diagnostic ambiguities are inescapable in the case of PV, since PV is a derived entity whose total flux or transport—in the traditional sense, advective plus nonadvective, see (3.9) below—has no unique, independent, local physical meaning. The traditionally defined total flux or transport of a chemical, by contrast, has such a meaning, in terms of the number of molecules of the chemical substance crossing unit area per unit time. This holds regardless of what particular transport mechanism or mechanisms are in operation, and of whether or not mixing-ratio isopleths are moving with the bulk air motion, as happens in the case of purely advective transport, but not, for example, in the case of transport by molecular diffusion or by particle sedimentation.

A better form of words to summarize the viewpoint adopted in HM87, without seeming to claim its uniqueness, is that given in the statements about "conservation" and "impermeability" in the Abstract of the present paper. The wording also takes care, this time, to make explicit the requirement to think in terms of a generalized tracer "substance," despite the lack of an accepted name for that entity. We still think that this viewpoint is not only correct and self-consistent but

that it will also prove to be a useful viewpoint, in a wholly practical sense. It is not meant to exclude other, complementary viewpoints but it is arguably the simplest way, in the long run, of understanding, quantifying, and parameterizing the behavior of isentropic distributions of PV, in a way that is universally valid and gives both a local and a global perspective. The form of the flux expressing the impermeability property (section 4) is a numerically well-conditioned quantity, in all the many examples we know of for stably stratified atmospheres in a practical, coarse-grain description (see section 6). These include examples of the kind discussed in D, as well as more complicated examples encountered in atmospheric modeling work, some of which are discussed in a recent paper by McIntyre and Norton (1990). The validity encompasses the real atmospheric circulation with its crucial dependence on nonlinear eddy effects, such as the breaking of Rossby and gravity waves (e.g., WMO 1985), and the consequent "PV barrier" effects upon chemical transport, whose reality and importance, for the formation of the Antarctic ozone hole for example, are now well recognized. The impermeability theorem makes explicit a strikingly simple fact about PV transport, implicit in the circulation theorem, that is relevant even in these enormously complicated circumstances. Purely advective transport is incorporated quite naturally as a special case.

The next two sections provide a brief but systematic theoretical review, before proceeding to the basic example of section 5.

3. Basic equations and concepts, including the concept of "transport"

How, it might be asked, can we claim that the diabatic behavior of PV is in some respects fundamentally different from that of a chemical substance, when both the PV and the chemical mixing ratio satisfy an equation of the form

$$DX/Dt = \text{right-hand side}, \qquad (3.1)$$

where D/Dt is the material derivative? One answer is that the form of the right-hand side is all-important, including, of course, any interdependence with the left-hand side. The point can be seen at once from the fact that Eq. (3.1) is satisfied by any field X whatever, with some expression or other on the right-hand side. An arbitrary field X does not necessarily behave in any way like a chemical mixing ratio.

In the case where X is the PV, the equation for its material tendency is usually written as

$$DQ/Dt = \rho^{-1}\mathbf{q}_a \cdot \nabla H + \rho^{-1}(\nabla \times \mathbf{F}) \cdot \nabla\theta \quad (3.2)$$

in geometric coordinates, which as noted for instance by Obukhov (1962) is equivalent to

$$DQ/Dt = -\rho^{-1}\nabla \cdot \mathbf{N}_Q \qquad (3.3)$$

where

$$N_Q = -H\mathbf{q}_a - \mathbf{F} \times \nabla\theta. \qquad (3.4)$$

Here ρ is the mass density, $\mathbf{q}_a$ the three-dimensional absolute vorticity, equal to the curl of the absolute velocity, $\mathbf{F}$ the viscous or other nonconservative body force per unit mass, ∇ the three-dimensional gradient operator with respect to geometric position $\mathbf{x}$, and H the diabatic heating rate expressed as the material tendency of potential temperature θ, so that the thermal energy equation is

$$D\theta/Dt = H. \qquad (3.5)$$

The PV is defined here, as it often is, in terms of θ, that is to say

$$Q = \rho^{-1}\mathbf{q}_a \cdot \nabla\theta \qquad (3.6)$$

[cf. (8.1) below]. The material derivative (corresponding to d/dt in the equations presented in D) is defined in the usual way,

$$D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla, \qquad (3.7)$$

where $\mathbf{u}$ is the three-dimensional velocity field. We postpone until section 6 the question of whether to use the exact $\mathbf{u}$, θ and ρ fields or smoothed, coarse-grain, "observable" approximations to them, since as was pointed out in HM87 the basic theory applies equally well to either case (with appropriate adjustments to the meanings of H and $\mathbf{F}$ to include eddy contributions from finer-grain motions where necessary).

The equivalence of (3.2) and (3.3) depends on the fact that $\nabla \cdot \mathbf{q}_a = 0$, a consequence of the vanishing of div curl and of the fact that $\mathbf{q}_a = 2\Omega + \nabla \times \mathbf{u}$, where Ω is the Earth's angular velocity. Equations (3.2), (3.3) or elements of them were derived for instance in the papers by Truesdell (1951), Staley (1960) as noted in D, Obukhov (1962), and Pedlosky (1979) among others; the derivation given in D yields the form (3.2) provided that the force-curl, $\nabla \times \mathbf{F}$ (not torque!), is added to the right of the vorticity equation.

Now in the case where the field X in (3.1) equals the mixing ratio χ of an exactly conserved chemical substance, considered for definiteness to be a decay-corrected radioactive tracer, we have

$$D\chi/Dt = -\rho^{-1}\nabla \cdot \mathbf{N}_\chi, \qquad (3.8)$$

which may be compared to (3.3). Here $\mathbf{N}_\chi$ is the non-advective flux or transport of tracer substance, describing transport processes like molecular diffusion, scavenging and sedimentation.

Equation (3.8) contains no source or sink term, in the traditional chemical sense. The form of the right-hand side, specific volume times a divergence, expresses the physical fact that the total number of heavy atomic nuclei involved, counting daughter as well as parent nuclei but discounting alpha particles, is exactly conserved. That is, the heavy nuclei in question are neither created nor destroyed, the most that can happen to them being changes in atomic weight and atomic number. This means, in particular, that any changes in their spatial distribution, as described by the function $\chi(\mathbf{x}, t)$ or in any other way, are due solely to their transport from place to place or to their introduction or removal at a boundary.

If the tracer substance happens to be in the form of particles that can sediment at a significant rate, then it is necessary to include in $\mathbf{N}_\chi$ a contribution proportional to the local mean fall speed of the particles in still air. The fact that upgradient transport is physically possible should be noted. If χ has a maximum at some altitude z_m, but faster-falling particles are located at higher altitudes, then particles may subsequently concentrate near z_m causing the maximum value of χ to increase with time. Note also that isopleths of χ can move upward even when the transport is downward, reminding us, as does simple diffusion also, that the motion of mixing-ratio isopleths is not generally indicative of the direction in which a chemical substance is being transported, unless the transport happens to be purely advective ($\mathbf{N}_\chi = 0$ everywhere).

Now as mentioned in section 1, words like flux, transport, source, sink, create, destroy, production, destruction, etc., are used throughout most of D in a different sense incompatible with the foregoing. For instance flux and transport are implicitly defined to mean advective transport only (so that a traditional phrase like "molecular-diffusive transport" becomes a contradiction in terms). Source and sink are defined to mean the material or Lagrangian tendency. That is, a "source" is defined to mean whatever expression appears on the right-hand side of an equation of the form (3.1), regardless, for instance, of whether or not the right-hand side has the special divergence form illustrated by (3.3) and (3.8). Again, words like "creation," "production," "destruction," etc., are used in D to mean the nonvanishing of the material tendency.

Material tendencies, or air-mass transformation rates, are of course useful and interesting quantities and have long been recognized as such in meteorology. If, however, the convention of calling them "sources" were to be applied to chemicals as well as to PV, then a radical, and presumably unacceptable, revision of chemical terminology would be required. When considering, for example, the molecular diffusion of a gaseous tracer substance like radon from one place to another, one would have to call the right-hand side of (3.8) a "source" or "sink," and to consider that the radon and its heavy daughter nuclei are destroyed in the first location and recreated in the second. Similarly, when ice crystals fall out from a cloud and evaporate in some lower layer of the atmosphere one would have to say that the water substance, along with any other substance that is carried down in the ice crystals, is

destroyed at the original location of the cloud and re-created lower down. Indeed, below D Eq. (4.12), exactly this suggestion seems to be made. It seems to be suggested that the right-hand side of an equation of the type (3.3) or (3.8) should be thought of as a "self-cancelling source and sink." In fact there is nothing strictly illogical about such a convention, if applied self-consistently. But we think that most readers would agree with us that it is conceptually simpler (and still consistent, of course, with the idea of air-mass transformation) to retain the conventional physico-chemical terminology and speak of the flux or transport of the substance in question from one three-dimensional location to another, rather than its destruction and recreation.

The flux forms of (3.3) and (3.8) are

$$\frac{\partial}{\partial t}(\rho Q) + \nabla \cdot \{\mathbf{u}\rho Q + \mathbf{N}_Q\} = 0 \qquad (3.9)$$

and

$$\frac{\partial}{\partial t}(\rho X) + \nabla \cdot \{\mathbf{u}\rho X + \mathbf{N}_X\} = 0. \qquad (3.10)$$

The expressions within parentheses are the densities, or amounts per unit volume: just as the decay-corrected tracer has amount per unit mass X and amount per unit volume ρX, the PVS has amount per unit mass Q and amount per unit volume ρQ. The expressions within braces are the total, advective plus nonadvective, fluxes or transports, in the language used here, and also used in HM87, and traditionally in the literature of physics and chemistry.

Equations in this form are the most general possible way, consistent with fundamental principles (e.g., Feynman et al. 1964), of expressing exact conservation of the additive, extensive quantity of which the amount per unit volume appears in parentheses. In this form the conservation relations are sufficiently general to be indifferent to whether the system is also mass-conserving. This latter point is just as true of X as it is of Q. That is, (3.10) as well as (3.9) is actually true whether or not the air molecules themselves are conserved; (3.10) depends only on conservation of the totality of radioactive parent and heavy daughter nuclei. The point is an academic one for meteorological purposes, but is noted here because of the emphasis placed on it in D in the case of (3.9). Since in the meteorological context mass is in fact conserved, we have

$$\partial \rho / \partial t + \nabla \cdot \{\rho \mathbf{u}\} = 0, \qquad (3.11)$$

from which the material or Lagrangian forms (3.3), (3.8) can be recovered from the flux forms (3.9), (3.10) in a line or two of manipulation in the usual way, paralleling D (2.1). That is, since (3.11) always holds in practice, (3.9) and (3.10) are exactly equivalent to (3.3) and (3.8). The different forms may be convenient for

different purposes, but the underlying physical reality, and the associated set of concepts, is the same.

If X were a reactive chemical then the right-hand side of (3.10) would be replaced by a nonvanishing source-sink or creation-destruction term. Apart from a factor ρ^{-1} this would correspond to an *additional* term on the right of (3.8), not of divergence form when written in terms of locally measurable quantities. By contrast, the right-hand side of (3.9) always vanishes, no matter what diabatic heating field H and force field $\mathbf{F}$ are acting, and so there is never a corresponding additional term on the right of (3.3).

To summarize, then, if one accepts the standard, traditional set of physical and chemical concepts associated with the idea that a decay-corrected radioactive tracer is exactly conserved—i.e., that the tracer substance is neither created nor destroyed away from boundaries, and its mixing ratio X consequently satisfies (3.8) or (3.10)—then, if the analogy between PV and chemicals is to be pursued, using the same set of concepts, PVS, too, must be considered to be an exactly conserved quantity, incapable of being created or destroyed away from boundaries, since its mixing ratio Q always satisfies the analogous equations (3.3), (3.9). In other words, PVS has zero source in a sense precisely analogous to the sense in which a decay-corrected radioactive tracer has zero source, which is the standard chemical sense. A local maximum in X or Q that increases with time does not necessitate the existence of a source, in this standard sense, but can arise purely from upgradient transport. The sedimentation example illustrates this possibility in the case of a decay-corrected radioactive tracer.

4. The impermeability theorem

If the traditional concepts just outlined are accepted, then the differences between the behavior of PVS and that of an exactly conserved tracer substance can be described completely in terms of the differences between their transport properties. One general difference is that expressed by the impermeability theorem pointed out in HM87. An alternative to the several derivations indicated there is to note that, in a stably stratified atmosphere, the net flux or transport of PVS, $\mathbf{J}$ say, appearing in (3.9), can be rewritten as

$$\mathbf{J} = \mathbf{u}\rho Q + \mathbf{N}_Q = \rho \mathbf{u}_{\theta\perp}Q + \rho \mathbf{u}_{\|}Q - H\mathbf{q}_{a\|} - \mathbf{F} \times \nabla\theta, \qquad (4.1)$$

where the subscript "$\|$" denotes projections parallel to the local isentropic surface:

$$\mathbf{u}_{\|} = \mathbf{u} - \frac{\mathbf{u} \cdot \nabla\theta}{|\nabla\theta|^2}\nabla\theta, \qquad \mathbf{q}_{a\|} = \mathbf{q}_a - \frac{\mathbf{q}_a \cdot \nabla\theta}{|\nabla\theta|^2}\nabla\theta,$$

$$(4.2a,b)$$

and where

$$\mathbf{u}_{\theta\perp} = - \frac{\partial\theta/\partial t}{|\nabla\theta|^2} \nabla\theta, \qquad (4.2c)$$

which is just the velocity of the isentropic surface normal to itself. The exact result (4.1) is straightforward to verify from (3.4), (3.5), (3.6), (3.7) and (4.2) in one or two lines of manipulation.

Since the last three terms in (4.1) all represent vectors lying parallel to the local isentropic surface, while the first is just ρQ times the normal velocity $\mathbf{u}_{\theta\perp}$ of that surface, it follows that a point moving with velocity $\mathbf{J}/(\rho Q)$ always remains on exactly the same isentropic surface. This is true even when the air is moving across that surface, as occurs when the diabatic heating $H \neq 0$. The velocity $\mathbf{J}/(\rho Q)$ can be pictured as the velocity with which PVS molecules would move if the notional substance PVS were made of molecules, discounting thermal motions. Therefore (4.1) says that such notional molecules move through space in just such a way as never to cross any isentropic surface. That is, in this version of the basic analogy (which is the version put forward in HM87), isentropic surfaces behave like semipermeable membranes. Even when the diabatic heating H makes them permeable to mass and chemical substances, they always behave as if they were completely impermeable to PVS.

Putting this together with the traditional concepts outlined in section 3, we may conclude furthermore that, in a stably stratified atmosphere, PVS can be created or destroyed only where isentropic surfaces intersect boundaries such as the earth's surface. It follows also that the stratospheric reservoir of PVS does not need maintaining by any "source," a point now demonstrated directly.

5. Some easily provable facts about stratospheric PV

The mathematical facts just summarized provide one way of understanding many aspects of PV behavior that might otherwise, to borrow a phrase from D, appear to be "major, unexplained, mysterious coincidences." The example now to be described is a case in point and is rederived independently from first principles.

Consider any layer of the stratosphere between two isentropes—say, for definiteness, the layer L between the 400 K isentropic surface and the 2000 K isentropic surface. Any other pair of isentropes that do not intersect the ground would do equally well. Let us compare PV behavior with the behavior of a decay-corrected radioactive tracer whose mixing ratio χ is assumed, for definiteness, to be much larger above the 400 K surface than below it.

Denote the volume element by dV, so that the mass element is ρdV. The total amounts of PVS and radioactive tracer within L are, respectively,

$$A_L(Q) = \iiint_L Q\rho dV \qquad (5.1)$$

and

$$A_L(\chi) = \iiint_L \chi\rho dV. \qquad (5.2)$$

The factor ρ is required in both integrands, because it is the tracer mixing ratio χ to which Q is analogous.

Now $A_L(\chi)$ can change in all kinds of ways—for instance by sedimentation, by diffusion, or by diabatic advection. But $A_L(Q)$ cannot change! It is always exactly constant. It happens moreover that this constant is equal to zero. The amount of positive PVS in the layer L, $A_{L_N}(Q)$ say (mostly located in the Northern Hemispheric part of L) is always exactly equal, in absolute value, to the amount of negative PVS in L, $A_{L_S}(Q)$ say (mostly located in the Southern Hemispheric part of L):

$$A_{L_N}(Q) = -A_{L_S}(Q). \qquad (5.3)$$

This is an immediate consequence of the well-known kinematical relations between Q, $\mathbf{q}_a$ and circulation. An alternative, slightly different and self-contained route to the same result is as follows. Let I_1 and I_2 be the upper and lower isentropic surfaces bounding L, $\mathbf{n}_1$ and $\mathbf{n}_2$ the upward normals, and θ_1, θ_2 the corresponding constant potential temperatures. From (3.6),

$$A_{L_N}(Q) + A_{L_S}(Q)$$
$$= A_L(Q) = \iiint_L \mathbf{q}_a \cdot \nabla\theta dV$$
$$= \iiint_L \nabla\cdot(\mathbf{q}_a\theta)dV = \theta_1 \iint_{I_1} \mathbf{n}_1 \cdot \mathbf{q}_a dA$$
$$- \theta_2 \iint_{I_2} \mathbf{n}_2 \cdot \mathbf{q}_a dA = 0. \qquad (5.4)$$

The third last step uses the fact that $\nabla\cdot\mathbf{q}_a = 0$, as noted below (3.7). The second last step uses the divergence theorem and the fact that θ_1 and θ_2 are constants. The last step uses Stokes' theorem to show that each of the surface integrals vanishes, because of the fact that the isentropic surfaces I_1 and I_2 do not intersect the ground and therefore have no boundary.

It is easy to devise thought experiments in which diabatic processes localized in northern high latitudes change the radioactive tracer amount $A_{L_N}(\chi)$ contained in the northern part of L where Q is positive, while conditions elsewhere are imagined to remain adiabatic. Such processes clearly cannot change $A_{L_S}(Q)$; and it follows from (5.3) that they cannot change $A_{L_N}(Q)$ either.

Both this last fact, and the immutability of $A_L(Q)$ itself, are of course fully in accord both with the impermeability theorem and with the relationship be-

tween PV and Kelvin–Bjerknes circulation [e.g., Hoskins et al. 1985, Eq. (4.4)]. By contrast, these same facts would seem mysterious from any perspective in which the right-hand side of (3.2) was assumed independent of the left-hand side. Such an assumption would ignore the fact that the same heating field $H(\mathbf{x}, t)$ shapes the diabatic contributions to both sides of (3.2) simultaneously, namely the contribution from advection by the diabatic velocity field $\mathbf{u}_{\text{diab}}(\mathbf{x}, t) = \mathbf{u} - \mathbf{u}_{\theta\perp} - \mathbf{u}_{\parallel}$ on the left, representing motion relative to isentropic surfaces, and the contribution from the $\rho^{-1}\mathbf{q}_a \cdot \nabla H$ field on the right. This is one of the ways in which (3.2) and its equivalent form (3.3) differ profoundly from (3.8).

Note also that the vanishing of integrals like that on the last line of (5.4) implies that any material volume, large or small, that is surrounded by a closed isentropic surface, contains a net amount of PVS that is precisely zero. This again is profoundly different from chemical behavior, and bears on the question of small-scale turbulent transport to be considered next. It suggests at once that conventional scaling and mixing-length arguments, which envisage, explicitly or implicitly, the bodily advection of tracer-bearing blobs of fluid on the large-eddy scale, will give wrong answers if used to estimate turbulent eddy fluxes of PV in cross-isentropic turbulent mixing.

6. Small-scale turbulence: Does the notion of "adiabatic mixing" make sense?

Suppose that, as seen from a coarse-grain perspective, mass is being entrained across an isentropic surface by small-scale turbulent mixing, for example at some location near the lower edge of a tropopause fold that is not touching the earth's surface. It is assumed in D and its predecessors that PVS would then be turbulently transported across the isentropic surface by what is referred to as "adiabatic mixing" [e.g., D (4.8–12)] and, presumably, that this would result in changes in the total amounts of PVS above and below that surface, in much the same way as would tend to occur with any chemical substances that may be present. The mathematical facts set out in HM87 and in the foregoing imply, however, that no such change in the total amounts of PVS can take place.[1] How is the disagreement to be resolved?

Part of the answer is that, in physical reality, the notion of "adiabatic mixing" used in D and its predecessors is self-contradictory, if the term "mixing" is to be understood in its usual sense as a process leading to thermal and chemical contact between previously

separate constituents. In reality, there is a diabatic heating field, dominated at the turbulent microscales by heat conduction.

The corresponding diabatic contribution $\mathbf{u}_{\text{diab}}(\mathbf{x}, t)$ $= \mathbf{u} - \mathbf{u}_{\theta\perp} - \mathbf{u}_{\parallel}$ to the velocity field is the means whereby mass is carried across isentropic surfaces during turbulent mixing. It would also carry PVS across isentropic surfaces, were it not for the compensating effects of the nonadvective diabatic terms in (3.2), (3.3) and (3.9) implied by the results of section 4. To revert temporarily to the language used in D, the heat conduction gives rise to a strong microscale "self-cancelling source and sink" that conspires to oppose the effects of the advective contribution to the transport of PVS across isentropic surfaces.[2]

In a coarse-grain description, the cancelling effects of the advective and nonadvective diabatic terms on the turbulent microscales will manifest themselves indirectly, in terms of cancelling eddy correlations on the scales of larger eddies. The analysis already given is sufficient to show this—for instance, one can apply the impermeability theorem of section 4 directly to any coarse-grain description in which the turbulent $\mathbf{u}$, ρ and θ fields are averaged sufficiently to leave a coarse-grain θ field that is stably stratified. Then all the analysis of HM87, and the analysis presented above, applies rigorously, and without modification, to the coarse-grain $\mathbf{u}$, ρ and θ fields, and to the PV and PVS defined by substituting those fields into (3.6), provided only that the eddy flux convergences arising from finer scales are included in the diabatic heating field H and the nonconservative force field $\mathbf{F}$.

Note especially that the impermeability theorem, in the form derived in section 4, applies rigorously since we are dealing with a stably stratified coarse-grain θ field, so that isentropes always move with finite velocities $\mathbf{u}_{\theta\perp}$ and (4.1) is mathematically well-behaved everywhere. This holds independently of any assumptions about the detailed nature of the fine-scale motion. It would hold, indeed, even if such a thing as "adiabatic mixing" were to occur, although in that (very hypothetical) event the relationship between the coarse-grain and fine-grain θ and Q fields would be even more complicated than in real mixing, and not, for instance, statistically stationary.

The following example shows in another way that these points are not merely academic.

7. Small-scale turbulence due to breaking gravity waves

One of the acknowledged causes of small scale, three-dimensional turbulence in the real atmosphere is the breaking of internal gravity waves. The convergence of the radiation stress or effective wave-induced mean

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[1] We reiterate that, as will be discussed in section 8 (item 6), there is no conflict with the observed facts described in the available literature, which we do not question. For instance, strong *mixing-ratio* correlations within tropopause folds can be expected to result from dilution.

[2] This means for instance that one cannot ignore turbulent eddy correlations in the first terms on the right of D(4.10) and D(4.12).

momentum flux, generally associated with breaking waves, gives rise to a net wave drag in accordance with well-established theoretical principles. Such drag may be significant for example in the stratosphere over mountainous regions. A particularly clear laboratory demonstration of the physical reality and robustness of the wave drag due to breaking internal gravity waves is that reported in Delisi and Dunkerton (1989). The field-observational evidence for the atmosphere is also very strong, and includes results from the classic airborne studies of mountain waves by Lilly and others. A convenient review is given in section 4 of Palmer et al. (1986).

When gravity wave drag is significant in some region of the atmosphere, it must, in turn, cause significant modifications to coarse-grain isentropic distributions of PV on the same regional scale. The general nature of these modifications was discussed for instance in HM87 (p. 831, item 6; see also Zhu and Holton 1987). The fact that the effects in question must come about through a complicated interplay of wavelike and turbulent dynamics, which must ultimately involve the turbulent microscales on both the right-hand and left-hand sides of Eq. (3.2), does not make them any the less real, as the experiments and observations clearly show. It is clear moreover that the effect of breaking gravity waves on the Q field is generally quite different from the accompanying effect on the X field representing the distribution of a chemical tracer substance, contrary to what is implied by the arguments in D.

Consider for instance a thought experiment in which the initial Q and X distributions are both spatially uniform, in some statically stable region within which gravity waves are about to break. Suppose also that radiative heat transfer is negligible and that the nonadvective tracer flux N_x in Eq. (3.8) is wholly diffusive. If the wave-breaking event results in net drag being exerted in, say, a westward direction, then a dipole pattern must appear in the regional-scale distribution of PV on each isentropic surface that intersects the wave-breaking region, with a cyclonic PV anomaly in the southern half and an anticyclonic PV anomaly of compensating strength in the northern half of the region, the associated transport of PVS along isentropes being upgradient. Similar dipole patterns have been seen in isentropic distributions of PV from numerical weather prediction experiments incorporating parameterizations of gravity-wave drag (A. J. Simmons, personal communication). No such pattern, on the other hand, can possibly form in the tracer mixing ratio distribution if N_x is wholly diffusive. Being spatially uniform, the X distribution cannot then be changed at all by the turbulent mixing. The contrasting behavior of the Q and X fields is, and can only be, a consequence of the different ways in which molecular effects enter into the right-hand sides of Eqs. (3.2) and (3.8).

It should be noticed incidentally that both terms on the right of (3.2) are likely to be involved in the creation of the PV dipole pattern. Because the kinematic mo-

lecular viscosity and heat diffusivity coefficients of air have comparable orders of magnitude, scaling considerations strongly suggest that the viscous and diabatic terms on the right of (3.2) will both tend to become important simultaneously as length scales diminish toward the Kolmogorov turbulent microscale. In particular, it would be a formally inconsistent "approximation" to neglect the viscous term $\rho^{-1}(\nabla \times \mathbf{F}) \cdot \nabla \theta$ in examples like that just described, while retaining the contribution from heat conduction to the diabatic term $\rho^{-1} \mathbf{q}_a \cdot \nabla H$.

There exist unequivocal demonstrations, both from laboratory experiments (Plumb and McEwan 1978) and from theoretical calculations (McIntyre and Norton 1990), showing that the viscous term $\rho^{-1}(\nabla \times \mathbf{F}) \cdot \nabla \theta$ on the right of (3.2) is, in fact, capable by itself of producing upgradient (in fact, gradient-independent) PV transport along isentropes. The theoretical calculations show in detail how this transport arises, as an eddy correlation effect, in the case of laminar, predominantly viscous dissipation of internal gravity waves under laboratory conditions in a stratified salt solution. The laboratory experiments verify the physical reality of the effect. There also exist detailed theoretical calculations showing similarly that wave dissipation by heat conduction alone can cause upgradient PV transport, and how this comes about (McIntyre and Norton 1990). These calculations show clearly that the diabatic term $\rho^{-1} \mathbf{q}_a \cdot \nabla H$ on the right of (3.2) is likewise, by itself, capable of producing upgradient or gradient-independent PV transport along isentropes.

None of the foregoing could occur if the suppositions in D about PV behavior in general, and about the effects of molecular diffusion in particular, were correct. Indeed, if those suppositions were shown to be true, then the entire edifice of observational, laboratory, and theoretical work on wave-mean interaction would be overthrown, including the classic work of Lord Rayleigh and others on acoustic streaming. The latter phenomenon, it should be noted, can involve upgradient *vorticity* transport by molecular diffusion; for the detailed evidence, and an extensive bibliography, the reader is referred to the paper by McIntyre and Norton cited above. The examples given in that paper illustrate, for instance, the distinction noted earlier between body torque (stress-tensor asymmetry) and force-curl $\nabla \times \mathbf{F}$, in terms of easily observable phenomena.

8. Some specific points raised in D

A few further comments are called for regarding some of the points raised in D.

1) It is not strictly speaking correct to say that the definition (3.6) of PV is "unique" (D, near end of section 2). As Ertel himself pointed out, and as dynamical theories confirm, the PV concept refers to the entire class of quantities

$$Q_{f(\theta)} = \rho^{-1}\mathbf{q}_a \cdot \nabla\{f(\theta)\}. \qquad (8.1)$$

The use of (3.6), the case $f(\theta) = \theta$, as a representative of that class, is only a convention. It is a convenient and useful convention when applying the PV concept to the earth's atmosphere, but that is for purely practical reasons, not for reasons of general principle. It happens that, when $f(\theta) = \theta$, a constant value of Q marks the position of the extratropical tropopause to fair approximation (Reed and Danielsen 1959, Danielsen 1968; WMO 1985, Chapter 5; Hoskins et al. 1985) the value being in the region of one or two "PV units" of 10^{-6} m^2 s^{-1} kg^{-1} K. As Danielsen has rightly pointed out in earlier publications, this makes better sense than defining the extratropical tropopause from vertical θ gradients alone. It is likely, in fact, that a different choice for the function $f(\theta)$ in (8.1) would be still better, on average, for tropopause-marking purposes; but we shall not pursue that question here.

What is fundamental, dynamically speaking, is the sharp isentropic gradient of PV that often marks the extratropical tropopause. This morphological feature exists independently of the choice of $f(\theta)$.

2) HM87 did not recommend changing the definition of PV by omitting the factor ρ^{-1} from (3.6) or (8.1), nor deny the usefulness of either quantity as an approximate air-mass marker. What HM87 did recommend (p. 830-1, item 4) was the use of the flux form of the PV equation, e.g. (3.9) above, for the purpose of discussing the budget of PV as a conserved quantity, that is to say for keeping track of total amounts and locations of the generalized tracer substance here referred to as PVS. The same item 4 recognized and discussed the connection with Rossby's isentropic "vorticity."

3) We agree of course that PV values can change, as D (4.19) illustrates, and that PV isopleths can move relative to the air. Both things are true also of the mixing ratio χ of an exactly conserved tracer substance, as was illustrated below Eq. (3.8).

4) We entirely agree that there are circumstances in which the material tendency DQ/Dt is locally small despite nonzero H, and that this can be useful in particular case studies. For instance, turbulent mixing might be absent, and radiative diabatic temperature tendency approximately proportional to $p^{0.286}$, so that $H \approx$ constant and the field $\rho^{-1}\mathbf{q}_a \cdot \nabla H$ on the right-hand side of (3.2) takes small values in some location. A case in point would be stratospheric air parcels that have neither encountered turbulent mixing, nor been closer than a kilometer or so to underlying cirrus clouds. [Closer than that, the high opacity of CO$_2$ in the 15 μm band can give rise to significant vertical gradients in H; e.g., Liou (1986), W. E. Ward (personal communication).] We agree that persistently small stratospheric DQ/Dt and $D\chi/Dt$ values might help explain the correlations between Q and chemical tracer mixing ratios χ often seen in aircraft data for the lower stratosphere.

5) Such correlations might be made even stronger, in particular cases, by redefining the PV. One could exploit the arbitrariness in (8.1) and tailor the function $f\theta)$ to reduce the magnitude of the field $\rho^{-1}\mathbf{q}_a \cdot \nabla\{Hf'(\theta)\}$ that then replaces $\rho^{-1}\mathbf{q}_a \cdot \nabla H$ on the right of (3.2). But such procedures have a certain ad hoc flavor, as against the general principles discussed in sections 3 and 4, which apply for instance to (8.1) as well as to (3.6), for any $f(\theta)$, and apply also in the presence of small-scale turbulence. The correlations just mentioned, and those within tropopause folds, can of course be understood in terms of the same general principles, as can cases where the correlations are not maintained (e.g., Keyser and Shapiro 1986; WMO 1985, section 5.2.4).

6) In particular, if tropospheric air is mixed across an isentropic surface into a tropopause fold, as must happen for instance when the fold is penetrated by cumulonimbus clouds (e.g., Danielsen 1968, pp. 508–512), then stratospheric tracers like ozone in the fold will be diluted by ozone-poor tropospheric air. But the circulation theorem, and the impermeability theorem, both tell us that tropospheric air entering the fold across isentropes will have the same dilution effect as if it carried zero PV with it. This was shown in various ways in sections 4–6. For PV in a tropopause fold, therefore, the dilution effect will be slightly enhanced over that expected from admixture of tropospheric air that is merely "PVS-poor." Even with the best available quantitative information it would be difficult to distinguish observationally between these two slightly different degrees of dilution, for instance in the fold situation discussed in Danielsen et al. (1987).

7) We agree entirely that a coarse-grain description, allowing for eddy correlations arising from finer scales, is needed for use with observational data. That is why HM87 pointed out the direct applicability of the conservation and impermeability theorems to the coarse-grain PV field, Q_c say, constructed by substitution of coarse-grain $\mathbf{u}$, ρ and θ fields into (3.6) or (8.1). Related points are made in a forthcoming paper by Keyser and Rotunno (1990). As Keyser and Rotunno point out, in the presence of three-dimensional turbulence it could be very important to distinguish Q_c from the $\bar{Q}$ of D (4.10) and D (4.12).

8) It follows that there are two serious inconsistencies in D. The first is that already discussed in section 6, namely the use of the self-contradictory idea of "adiabatic mixing." The second amounts to using $\bar{Q}$ when deriving the theory, as in D (4.10) and D (4.12), but replacing $\bar{Q}$ by Q_c when considering the application of that theory to observational data. It is only Q_c, of course, that can be determined observationally.

9) There is a further inconsistency in D related to coarse-graining. A formulation presented in D section 4 relies on choosing a volume of integration containing an exactly constant mass of air. The mathematical notation used in D does not show clearly what functional dependencies and mathematical operations are in-

tended. But it seems likely from the discussion that the motion of each boundary point of the volume of integration is taken to be the center-of-mass velocity of a similar (albeit not precisely defined) volume centered on the boundary point [see line below D (4.3)]. That is, the boundary velocity is taken to be the local value ·of the mass-weighted mean velocity field, itself defined as some kind of running mean over finite volumes. There is then no way to justify all the steps in D(4.5): and counterexamples can easily be constructed showing that it cannot be true in general. In order to overcome this difficulty an additional assumption, such as that of scale separation, would have to be introduced.

10) Further to point 3 above, note again that movement of Q or X isopleths need not be simply related to transport, by any definition. A sufficient example would be that described below Eq. (3.8). Another example, in a laboratory context, would be the motion of solute mixing-ratio isopleths during osmosis of a solvent across a stack of semi-permeable membranes. The isopleths generally move because of dilution or concentration of the solute by the solvent, even though the cross-membrane transport of solute is zero at all times.

9. Concluding remarks

The viewpoint we have advocated, based on Eqs. (3.9) and (4.1) and related discussion, is arguably the simplest correct statement of the analogy between PV and chemicals that has universal validity, is numerically well conditioned, and permits PV behavior to be discussed in the same language as chemical tracer behavior.

In chemical language, the evolution of isentropic distributions of PV can be described exactly, and completely, in terms of PVS being advected or otherwise transported along a layer between two isentropic surfaces, and being diluted or concentrated (in the chemist's sense) when mass leaks diabatically into or out of that layer. Instead of being located everywhere, the sources and sinks of PVS are located only where isentropic surfaces intersect boundaries. This simplification follows logically when the words "source" and "sink" are used in the chemist's sense, which is also the physicist's sense used when speaking of the budgets of other conservable quantities like energy. Some of the implications may seem strange at first sight, but in reality are no stranger than the facts about PV seen from any other viewpoint, as the basic examples of section 5–7 well illustrate.

"Otherwise transported" may include nonadvective ·upgradient transport, as was clearly illustrated by the wave-breaking example of section 7 and supported by the laboratory and other evidence cited there.

. The complementary viewpoint in terms of material tendencies or air-mass transformation rates, based on equations of the form

$$DX/Dt = \text{right-hand side}, \quad (3.1), (9.1)$$

is also useful. However, for the reasons explained in section 3, and illustrated in sections 6 and 7, it tends to conceal some fundamental differences between PV behavior and chemical behavior. When speaking of PV and chemical mixing ratios together, it would clearly be useful if the right-hand sides of equations like the above were referred to not as sources but as, say, material tendencies, or air-mass transformation rates.

One can point to phenomena in the real atmosphere in which—again in chemical language—the PVS dilution and concentration effects are remarkably strong. An extreme example of PVS dilution is seen in the pools of zero-PV air that continually spread out in the stably stratified tropical upper troposphere from major cumulonimbus convection sites. An extreme example of PVS concentration is seen in the midlatitude "explosive cyclogenesis" that is commonplace in the maritime lower troposphere in winter. In explosive cyclogenesis, latent heat release allows mass to be drawn upwards across isentropic surfaces, leaving cyclonic PVS behind to be concentrated rapidly into a small central region, together with additional PVS being advected in from the surrounding reservoir of cyclonic PVS.

It is perhaps lucky that no chemical pollutant can be concentrated in this way.

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