

# Issues for stratospheric modelling and assimilation

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## 1 Dynamical balances

In the stratosphere, to a first approximation, waves propagate up and zonal-mean temperature anomalies propagate down; this is the basic physics behind the “downward control” of the wave-driven circulation (Haynes *et al.* 1991; see also Shepherd 2002). Temperature represents a balance between radiative relaxation and the wave-driven circulation, and the zonal wind is then determined from temperature by thermal wind balance. Thus, it is better to think of wave drag (or, more properly, angular momentum flux convergence) as driving radiative imbalance in the temperature which then shapes the zonal winds, rather than of wave drag as directly controlling the zonal winds (without thermodynamics): in the momentum equation wave drag is balanced by meridional flow, not by any particular value of the zonal wind.

In principle, the radiative component of the temperature should be modelled accurately in the stratosphere, where it involves clear-sky conditions. Rather surprisingly, stratospheric models show significant discrepancies of order 10 K in their global-mean temperatures throughout the stratosphere (Pawson *et al.* 2000), even though the global-mean temperature is essentially under radiative control. (Provided the static stability and radiative damping time scales are independent of latitude, then mass conservation implies that the meridional circulation can have no effect on global-mean temperature.)

Without wave driving from below, then, there would be essentially no radiative imbalance (apart from that associated with the seasonal cycle). The stratosphere, unlike the troposphere, is dynamically stable, and needs to be mechanically forced in order for a circulation to develop. An important exception is the stratospheric Hadley circulation in the tropics (Dunkerton 1989; Semeniuk and Shepherd 2001*a*), about which more will be said later.

A significant part of the wave drag comes from gravity waves, which are subgridscale and are not well constrained by observations. Since fractional errors in the TEM (residual) vertical velocity  $\overline{w}$  imply the same fractional errors in the radiative imbalance  $T - T_{\text{rad}}$ , the effect of gravity-wave drag can be significant where  $T - T_{\text{rad}}$  is large — notably in the polar night. Garcia and Boville (1994) showed that inclusion of gravity-wave drag in a zonally symmetric model increased wintertime Arctic stratospheric temperatures by over 5 K, and Antarctic temperatures by over 10 K. Beagley *et al.* (1997) showed that in the Canadian Middle Atmosphere Model (CMAM), a comprehensive GCM, nearly half the downwelling over the NH polar cap (60-90N) at 10 hPa arose from the parameterized orographic gravity-wave drag (in this case, there was no parameterization of non-orographic gravity-wave drag).

Because of the uncertainties in treating gravity-wave drag, most stratospheric models have serious polar temperature biases. An interesting diagnostic for investigating these biases is the relationship between wave forcing (e.g. vertical EP flux through 100 hPa) and polar temperature (e.g. at 50 hPa), with the temperature lagged by one month because of the finite radiative response time. Austin *et al.* (2003) compare these relationships in both hemispheres for various chemistry climate models. While some of the differences between the models may well be due to the different representation of resolved planetary-wave drag, it is likely that most of the differences are due to the models’ different representations of gravity-wave drag (including Rayleigh friction).

These temperature biases mean that the “perfect model” assumption generally used in data assimilation is problematical in the stratosphere. It would be very nice if the increments produced by data assimilation could be somehow used to infer the amount of gravity-wave drag in the real atmosphere, since direct measurements of gravity-wave drag are well beyond the reach of current instruments. However, most observations are of temperatures, so corrections are likely to occur in the temperature rather than in the momentum equation, even though the model errors are in the momentum equation. In this sense, measurements are likely to be fighting the natural direction of causality in the system, unless balanced wind increments are imposed at the same time.

Representation of drag processes should respect conservation of angular momentum; after all, Newton’s second law states that there are no external sources or sinks of angular momentum, and momentum transfers between different parts of the atmosphere are just that — transfers. In contrast, because of cooling to space the stratosphere is open from an energetic point of view, and energy provides little constraint on the system. For gravity waves, the angular momentum constraint is expressed in the steady-state balance

$$\bar{w}^* = \frac{-1}{a \cos \phi} \frac{\partial}{\partial \phi} \left\{ \frac{\overline{u'w'}}{2\Omega \sin \phi} \right\} \quad (1)$$

(Haynes *et al.* 1991). This relation states that the downwelling at any given level is determined by the net (mass weighted) momentum convergence above that level, *independent of where the waves actually break*. Thus, for example, changes in winds would change the location of gravity-wave breaking, but would lead to changes in  $\bar{w}^*$  only within the breaking region itself. In contrast, a non-conserving approximation to wave drag (e.g. Rayleigh drag) leads to spurious upward and downward influences which are associated with the addition of a “deus ex machina”. This problem is discussed in detail by Shepherd *et al.* (1996).

To avoid spurious vertical influence via the meridional circulation, a gravity-wave drag scheme must be momentum conserving. This means that any sponge layer which is implemented in the top few levels of a model in order to absorb upward propagating resolved waves, must act only on the waves and not on the zonal mean. It is, in fact, quite common for Rayleigh-drag sponge layers to act on the zonal mean as well, in order to control mean wind speeds (and thus act as a poor man’s gravity-wave drag), but this violates Newton’s second law and is therefore physically unjustifiable. Furthermore, any resolved or parameterized wave drag applied within a sponge layer which has a zonal-mean component to the sponge drag, will be almost completely absorbed by the sponge rather than inducing a meridional circulation — thus negating the real physical impact of the applied drag on temperatures below (Shepherd *et al.* 1996).

The stratospheric Hadley circulation was mentioned earlier as the one example of a thermally driven circulation in the middle atmosphere. In the tropics, inertial adjustment appears to be a real process. The distribution of ozone heating at solstice implies that  $T_{\text{rad}}$  has a non-zero meridional gradient at the equator, and thus cannot be realized because it cannot be in balance with any zonal flow. (Physically, the pressure gradient force then acts along the Earth’s axis of rotation, while the Coriolis and centrifugal forces act normal to the Earth’s axis of rotation.) This leads to a process of inertial adjustment, wherein a thermally direct circulation is set up which flattens the temperature gradient at the equator and causes heating on the winter side and cooling on the summer side of the equator (Dunkerton 1989). Unpublished work by Kirill Semeniuk (York University) shows that  $T - T_{\text{rad}}$  has a non-zero meridional gradient at the equator in the upper stratosphere, evidence of inertial adjustment since the wave-driven circulation cannot drive such a structure in the radiative imbalance (Semeniuk and Shepherd 2001a). The inertial adjustment is accomplished by stacked horizontal cells, which are analogous to inertial instability except that in this case, there is no steady state to go unstable to.

Inertial instability, like convection, has no natural scale selection apart from viscosity. Thus, in a model it tends to occur at the smallest vertical scale resolved by the model — yet it is a physical instability, not  $2\Delta z$  “noise”. An example is shown in Semeniuk and Shepherd (2001a), which persists even in the monthly mean. The Hadley circulation driven by this inertial adjustment is responsible for a significant fraction of the observed upwelling in the upper stratosphere (Semeniuk and Shepherd 2001b). In order to confirm the presence of inertial adjustment, one needs accurate estimates of the meridional gradient of the zonal mean zonal wind in the tropics. However, it seems that this quantity varies widely between different observational data sets (Randel *et al.* 2002).

In the lower stratosphere, in contrast, the upwelling appears to be driven mechanically rather than thermally (Plumb and Eluskiwicz 1999; Semeniuk and Shepherd 2001*b*), and is understood to be responsible for the annual cycle in tropical tropopause temperature — with upwelling being stronger in the NH winter than in the SH winter (Yulaeva *et al.* 1994). In fact, the annual cycle of 100 hPa temperature averaged over the tropics (30S-30N) and over the extratropics — which have equal mass — is almost exactly equal and opposite, indicating the role of the meridional circulation in driving this cycle. This then provides a key diagnostic for models. However, the tropical tropopause region has a very delicate radiative balance, with longwave warming rather than cooling, so the radiative timescales are very long and the balance can be difficult to get right. The Pawson *et al.* (2000) intercomparison of stratospheric climate models found an enormous range of behaviours in this respect.

## 2 Tropical winds

In the tropics, geostrophic balance becomes problematical because of the vanishing Coriolis parameter, and assimilation schemes that use geostrophic balance to couple the wind and mass fields generally decouple the fields in the tropics. This, together with the paucity of direct wind measurements, may explain why tropical winds are so poorly represented in analyses (Randel *et al.* 2002). Unpublished comparisons between NCEP/NCAR analysed wind speeds and direct ER-2 measurements between 70 and 45 hPa in 2000 by Paul Newman (NASA GSFC) show that in the tropics there is enormous scatter, with a standard deviation to the difference of over 5 m/s. Unpublished comparisons between ECMWF analysed tropical wind speeds and direct winds measured from a high-altitude balloon at 60 hPa in 1998 by Albert Hertzog (LMD) show a similar discrepancy. In contrast, the same comparisons in the extratropics show much better agreement.

However, one expects an anisotropy in the tropics, with the zonal length scales being much longer than the meridional length scales. In this case, a *semi-geostrophic* balance results, with the zonal flow being in geostrophic (or, more accurately, gradient wind) balance, and the meridional flow being ageostrophic. This is the same kind of anisotropic balance as results in fronts or for coastal flows, and holds even for order unity Rossby number so long as the aspect ratio of length scales is small. It is thus not the case that geostrophic balance necessarily fails in the tropics; it just fails for the meridional velocity. True, geostrophic balance itself just gives zero equals zero at the equator ( $fu = -\Phi_\phi/a$ ), but if one takes the meridional derivative of the meridional momentum equation then geostrophic balance takes the form  $\beta u = -\Phi_{\phi\phi}/a^2$ , which is perfectly well-defined. Including all terms, gradient wind balance of the zonal flow takes the form

$$2\frac{uu_\phi}{a}\tan\phi + \frac{u^2}{a}\sec 2\phi + 2\Omega\cos\phi u + 2\Omega\sin\phi u_\phi + \frac{1}{a}\Phi_{\phi\phi} = 0. \quad (2)$$

In this anisotropic limit, the vorticity is dominated by the meridional derivative of the zonal velocity, and an appropriate measure of Rossby number at the equator is  $U/\beta L^2$ , where  $L$  is the meridional length scale. Then if this Rossby number is order unity, the anisotropic scaling should have errors of order  $\delta^2$  where  $\delta$  is the ratio of meridional to zonal length scale.

Unpublished analyses by Matt Reszka (University of Toronto) show that in the CMAM, the meridional and zonal autocorrelation lengths of the zonal wind in the tropical stratosphere are about 1600 km and 3900 km respectively, for which  $\delta = 0.4$ . In fact, normalized rms gradient-wind imbalance of the zonal wind in the tropics in CMAM appears to also be about 0.4, and a similar result is found for UKMO analyses (Matt Reszka, personal communication). While these numbers are less than unity, they are not particularly small. Thus, while semi-geostrophic balance may provide some constraint on the tropical winds, it may not be a very strong one. However, the constraint is more accurate for the longest zonal waves, and of course for the zonal mean. On the other hand, it only applies to the zonal velocity.

### 3 Transport of trace species

As well as being responsible for departures from radiative equilibrium, the diabatic circulation is responsible for tracer transport. For about 25 years it has been known that the TEM velocity provides some sort of approximation to Lagrangian motion, at least for small-amplitude waves, based on the mixing-length approximation (Dunkerton 1978). However there has been some doubt about the quantitative accuracy of this relationship given the violation of the separation in scale needed for the mixing-length approximation. (Mixing in the stratospheric surf zone occurs over length scales much larger than, rather than much smaller than, the tracer gradient length scales.) In a recent study of planetary-wave-induced transport in a mechanistic 3-D model, Pendlebury and Shepherd (2003) found  $\overline{w}^*$  to be quantitatively extremely close to the mean Lagrangian vertical motion, even in the surf zone. The Lagrangian meridional motion, in contrast, is much more complex, and in the surf zone is dominated by mixing rather than by bulk transport.

Stratospheric chemical transport models (CTMs) tend to have serious problems with their diabatic circulation when driven by analyzed winds. Part of this is that the vertical motion represents a small difference of large terms, and is not well represented in analyses. Computing the vertical motion in isentropic coordinates using an independent radiation code improves matters, but still can lead to problems. For example, a systematic radiative error would generate systematic vertical motion, if observed temperatures were continuously imposed. In contrast, a systematic radiative error in a GCM equilibrates locally and would just lead to an error in  $T_{\text{rad}}$  and hence in  $T$  itself, rather than generating a persistent circulation (e.g. Shepherd *et al.* 1996). It seems likely that an assimilating model is more like a CTM than a GCM in this respect.

A key test of transport is the “tropical tape recorder” (Mote *et al.* 1996). Model tape recorders tend to ascend too rapidly. Part of the problem may be the overly coarse representation of inertial adjustment, and part may be vertical diffusion from inaccurate transport. For example, the tape recorder in the CMAM ascends from the tropopause to the stratopause in about 12 months (Shepherd 2002), which is characteristic of free-running models, while in the observations it is closer to 24 months. In contrast, the tape recorder in the ECMWF model run in assimilation mode appears to be even faster — more like 6 months.

Another key test involves “mixing barriers” as are observed to occur at the edge of the tropical pipe, at the extratropical tropopause, and at the edge of the wintertime polar vortex. A striking example is provided by the isolation of aerosol within the tropical pipe following the Mt. Pinatubo eruption, observed by Ed Browell’s airborne lidar (Grant *et al.* 1994). Such structures are characterized by strong horizontal gradients (Sparling 2000). The latter do not necessarily imply transport barriers, but represent strongly inhomogeneous meridional structure in mixing; there is nothing to prevent a constant mass flux right through a “mixing barrier” (Shepherd 2002). A striking example is provided by the mechanistic study of Pendlebury and Shepherd (2003). Mixing barriers are reflected in distinct regions in chemical correlation diagrams (Sankey and Shepherd 2003). It seems that high horizontal resolution is not necessarily required to obtain this kind of structure. Even at T32 resolution, the CMAM has a well isolated tropical tape recorder (Shepherd 2002) — in fact, more isolated than the real tape recorder! — and distinct tropical  $\text{N}_2\text{O}:\text{CH}_4$  correlations which agree well with those observed from space by ATMOS (Sankey and Shepherd 2003).

It is notable that CMAM, which is a spectral model, uses spectral transport, driven by the desire to have a consistent treatment of advection of both mass and tracers. Unpublished work by Jean de Grandpré (McGill University) found that implementing a semi-Lagrangian scheme in CMAM led to excessive horizontal diffusion, with too much transport across the edge of the Antarctic polar vortex. Of course, the CMAM with its Eulerian dynamics and rather short time step (10 minutes) is probably an unsuitable model in which to implement semi-Lagrangian transport, which is known to be highly diffusive because of interpolation when used with short time steps.

The seasonality of the diabatic circulation in the stratosphere is very strong, because of the seasonality of planetary-wave drag. Within each hemisphere, ozone builds up in winter from transport, and decays photochemically through summer. This photochemical decay can be quantified in regression coefficients between

ozone anomalies at different times of the year (Fioletov and Shepherd 2003). It turns out that late-spring total ozone anomalies in midlatitudes are remarkably persistent, with significant correlations lasting through summer and early fall, until the next winter’s buildup begins. This would seem to be a robust diagnostic which models ought to be able to replicate. In fact, this seasonal persistence of ozone anomalies appears to account for the seasonality of the long-term ozone trends observed in the NH midlatitudes (Fioletov and Shepherd 2003).

A great hope of four-dimensional data assimilation is to be able to obtain wind information from the evolution of trace species. Whether this can really be done is, however, not so obvious. First, from such an analysis it is only possible to obtain one component of the wind — that which is parallel to the tracer gradient. Unfortunately, tracer gradients tend to align normal to the wind. Thus, the amount of wind information that can be obtained will depend on the autocorrelation time of the winds not being too long. On the other hand, if it is too short then one is in a diffusive limit and it is hard to invert tracer evolution to get the winds. So, the nature of the velocity field is an important constraint. Finally, to obtain wind information it is necessary to have a non-zero tracer gradient. It is unfortunate that while wind information is most desperately needed in the tropics, most tracers tend to have very flat spatial distributions in the tropics. Thus, there are likely to be considerable challenges in this endeavour.

## 4 Structure of dynamical fields

In the stratosphere, the flow is dominated (in the extratropics) by large-scale, low-frequency motion, a result of Charney-Drazin filtering. A consequence is that autocorrelation times of velocity derivatives are much shorter following Lagrangian motion than they are for the flow itself in the Eulerian frame (Ngan and Shepherd 1999). This is the hallmark of what is often called “chaotic advection” (strictly, chaotic particle paths generated by a time-periodic velocity field). It is a special case of spectrally non-local dynamics, wherein the tracer evolution at small scales is driven by the velocity field at large scales, and there is a single time scale (Shepherd *et al.* 2000). This aspect of tracer evolution in the stratosphere is well known, and is the basis for the successful Match technique for identifying chemical ozone loss (Rex *et al.* 1998). It is also the ideal context within which to apply semi-Lagrangian dynamics.

In the upper stratosphere and mesosphere, however, we expect the flow to become increasingly unbalanced as upward propagating gravity waves reach large amplitude. Direct global observations of this phenomenon do not exist, and analyses tend to filter gravity waves, but a comparison of free-running middle atmosphere GCMs found that all models exhibited a shallow spectrum of kinetic energy at sufficiently high altitude (Koshyk *et al.* 1999), associated with unbalanced motion (i.e. divergence comparable to vorticity). Even a model with T32 horizontal resolution will exhibit a shallow spectrum in the mesosphere. This shallow spectrum means that the tracer problem becomes spectrally local: the tracer evolution at a given scale is determined by the structure in the velocity field at that same scale, and the time scale gets shorter for smaller length scales.

In this regime, the Eulerian autocorrelation time becomes comparable to the Lagrangian autocorrelation time, and both become very short (Shepherd *et al.* 2000). In this case, it would seem impossible to get winds out of tracers, for example. The increasing dominance of gravity waves with altitude will pose a serious challenge for mesospheric data assimilation. In principle, it also calls into question the validity of semi-Lagrangian dynamics. However, unpublished work by John Koshyk (formerly of University of Toronto) showed that when the semi-Lagrangian dynamical core was used in place of the spectral core in the NCAR MACCM, the shallow kinetic energy spectrum disappeared and the spectrum dropped sharply with wavenumber! So, semi-Lagrangian dynamics appears to be highly dissipative of high-frequency motion.

The stratosphere itself is somewhat special in being controlled by the large scales. Near the tropopause, the kinetic energy spectrum exhibits a power law scaling close to  $k^{-3}$ , and this is marginal for spectrally non-local dynamics: the rms strain rate diverges logarithmically as  $k \rightarrow \infty$ . Here, small-scale tracer evolution is significantly affected by small-scale structure in the velocity field (Shepherd *et al.* 2000). At sufficiently small horizontal scales, the kinetic energy spectrum at the tropopause also shallows, and this mesoscale regime is

then analogous to the mesospheric regime — albeit without the very short time scales.

## 5 Interactive ozone

In the upper stratosphere, ozone is highly interactive with the temperature field, with a negative correlation. A positive temperature anomaly increases ozone loss rates and thus induces a negative ozone anomaly. The radiative feedback acts in the opposite sense and is thus stabilizing. Since both the radiative and photochemical time scales are very short in the upper stratosphere (days or less), the feedback is strong. It is in striking contrast to the *positive* ozone-temperature relationship observed in the lower stratosphere, which to a first approximation is purely coincidental — downward motion increases ozone through transport while also increasing temperature through adiabatic warming — although there are positive feedbacks on longer time scales. The different nature of the correlation at different altitudes is beautifully illustrated in analyses of planetary-wave structures from the CRISTA instrument (Ward et al. 2000).

The strong coupling between ozone and temperature in the upper stratosphere suggests that models of this region really ought to have fully interactive ozone. It is interesting to note that by making the ozone in the CMAM fully interactive with radiation, a persistent warm bias at the summer stratopause was nearly eliminated (de Grandpré *et al.* 2000). Since the summer stratopause is essentially under radiative and photochemical control, the interpretation of this result was that the ozone climatology being used by the model in non-interactive mode was not sufficiently accurate in the upper stratosphere, and that in this region it may be easier to model ozone (so long as it is interactive) than to observe it!

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