Interpretation of Ozone Temperature Correlations

2. Analysis of SBUV Ozone Data

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In an effort to understand the behavior of ozone in the transition region, the terms in the perturbation continuity equation have been evaluated from solar backscattered ultraviolet ozone data, National Meteorological Center temperature data, and geostrophic winds derived from the temperature data at 2 mbar, winter 1978–1979. A linear parameterization is used to estimate the chemical source term. The perturbation ozone field calculated by integrating the net forcing evaluated from the data compares well with the measured perturbation ozone field. There are occasions during the winter when the sum of the dynamic terms is small due to cancellation, and the ozone and temperature perturbations are anticorrelated. The \(-1\) correlation between the ozone and temperature perturbations does not necessarily imply that chemical forcing is dominant.

1. INTRODUCTION

Remote sensing of the atmosphere has made it possible to examine the relationship between the stratospheric temperature, wind, and ozone fields in detail. Theoretical studies [Hartmann and Garcia, 1979; Garcia and Hartmann, 1980; Rood and Schoeberl, 1983a] indicate that ozone transport in the transition region, where both dynamical and photochemical forcing are important, is important to understanding observed features in the annual cycle of ozone. Previous observational studies have identified stratospheric transition regions, based on the observed change in the correlation of the deviations of ozone and temperature [Nagatani and Miller, 1984], or equivalently, on the change in the phase difference between ozone and temperature waves [Gille et al., 1980; Wang et al., 1983].

Recently, Rood and Douglass [1985] have shown that an anticorrelation between ozone and temperature deviations does not necessarily imply that the ozone deviation field is maintained by the rapid photochemical response of ozone to dynamically induced temperature perturbations. It was also shown that it is not possible to locate the transition region by considering only changes in the correlation of the deviations of ozone and temperature, because that correlation is the result of complex interactions between the wind field and the background gradients. Here, in order to understand the physical cause of the observed ozone temperature correlations, ozone and meteorological data are used to examine in detail the perturbation continuity equation

\[
\frac{\partial \gamma'}{\partial t} = -\left(\frac{u'}{u} + \frac{v'}{v} + \frac{w'}{w}\right) \frac{\partial \gamma'}{\partial x} - v \frac{\partial \gamma'}{\partial y} + \frac{\partial \gamma'}{\partial y} - w \frac{\partial \gamma'}{\partial z} + S'
\]  

The zonal, meridional, and vertical winds are given in \(u, v,\) and \(w,\) and the partial derivatives with respect to \(x, y,\) and \(z\) correspond to derivatives in the zonal, meridional, and vertical directions. The ozone volume mixing ratio is given by \(\gamma\) and \(t\) is time. An overbar indicates the zonal average, a prime the deviation from the zonal average. The rate at which the ozone perturbation is produced or destroyed by photochemical processes is given by \(S'.\)

It is common practice to assume that the nonlinear terms \(u' \frac{\partial \gamma'}{\partial x}\) and \(v' \frac{\partial \gamma'}{\partial y}\) are negligible compared with the linear terms \(\frac{\partial \gamma'}{\partial x}\) and \(\frac{\partial \gamma'}{\partial y}\) in (1). Here, the effects of these terms will be compared to determine if this assumption is valid. The vertical resolution of the ozone data is not sufficient to calculate \(\frac{\partial \gamma'}{\partial z}\), but the potential significance of the term \(w' \frac{\partial \gamma'}{\partial z}\) will be discussed. The terms \(u' \frac{\partial \gamma'}{\partial x}\) and \(w' \frac{\partial \gamma'}{\partial z}\) are presumed to be small compared with the other terms in (1) and are not considered.

The deviations of the measured ozone from the zonal mean value will be compared with the deviations calculated by integration of (1) for a 1-day time interval. The effects of errors in the terms on the calculated deviations will be determined. Comparison of the measured and calculated values of the perturbation field should reveal the existence of bias or systematic errors that have not been considered.

2. DATA SOURCES

Evaluating the terms in (1) requires synoptic measurements of ozone mixing ratio, temperature, and winds. The data sets used in this study are the same as used by Wu et al. [1985], where details about the data sources are given. In brief, the ozone data are derived from radiance measurements made by the solar backscattered ultraviolet (SBUV) instrument on the NIMBUS 7 satellite. Instrument and data processing information are given by Heath et al. [1973, 1975]. There are several days per month for which no ozone measurements are available, and for these days the missing data are linearly interpolated in time. The ozone data at 2 mbar, for the northern hemisphere winter December 1978 through February 1979, are used here because information is...
desired about the behavior of ozone in the transition region, and the ozone photochemical lifetime for middle latitudes winter at 2 mbar indicates that both dynamical and photochemical effects at this level are important.

The temperature data for the same period are provided at 18 standard pressure levels by NOAA/National Meteorological Center (NMC). The upper level temperatures (5, 2, 1, and 0.4 mbar) are derived from radiance measurements of the vertical temperature profiler radiometer (VTPR) on NOAA 5 and the stratospheric sounding unit (SSU) on Tiros-N. Below 10 mbar, conventional rawinsonde data are used. The temperatures derived from the satellite measurements are adjusted based on statistical comparison of derived temperatures with rocket measurements of temperature, following Gelman et al. [1983]. Details concerning this adjustment are given by Geller et al. [1984]. The zonal and meridional winds used in this work are computed geostrophically from height fields which are constructed from the temperature profiles.

Both of the data sets are interpolated from the standard NMC 65 x 65 rectangular hemispheric grid to a 2.5° latitude by 5° longitude grid. Because the two data sets are not obtained simultaneously, and because it is planned to integrate (1) for 24-hour time intervals, there is no possibility of comparing features that do not persist for at least 1 day. Therefore a 3-day running mean was calculated for both data sets, so that features of less than 1-day duration are suppressed in both the measured ozone distribution and the ozone distribution calculated by integration of (1).

3. EVALUATION OF DYNAMIC TERMS

Uncertainty in calculating the advective terms in (1) can come from both evaluation of the winds and evaluation of the gradients of the measured ozone. The gradients for the meridional advection, \( u'(\partial \gamma / \partial y + \partial \gamma / \partial y) \), are calculated with a fourth-order centered scheme:

\[
\frac{\partial \gamma}{\partial y} = \frac{2}{3} \left( \frac{\gamma (y + \Delta y) - \gamma (y - \Delta y)}{\Delta y} \right) - \frac{1}{12} \left( \frac{\gamma (y + 2\Delta y) - \gamma (y - 2\Delta y)}{\Delta y} \right)
\]

Because both gradients are multiplied by \( u' \), the separation of the meridional gradient into mean and perturbation components is necessary only to compare the effects of the two terms.

The zonal derivative of the perturbation field is required to calculate the zonal advection \( (u + u')\partial \gamma / \partial x \). Because the mean value is subject to smaller error than individual measurements, the derivative \( \partial \gamma / \partial x \) is less certain than the net meridional derivative. Moreover, because the zonal wind is frequently large, the effect of noise must be suppressed in calculating this derivative. The derivatives were calculated at each longitude using second-order accurate centered differences. These were then averaged with those at \( \pm 15^\circ \) longitude. This method was found to reduce the noise in the derivative without omitting or distorting any features expected in the derivative by examining the ozone field.

Because the gradients may be multiplied by large wind values, and because the terms in (1) are of varying sign, small random measurement errors may introduce large relative uncertainty in the net dynamical forcing, that is, the sum of the advective terms in (1). The random error \( \partial \gamma \) associated with an individual measurement \( \gamma \) is about 1%. Because the standard error of the mean value \( \gamma \) is smaller than the error associated with individual measurements, the mean value \( \gamma \) is taken to be precisely known, and all the uncertainty is assigned to the perturbation value. Because \( \gamma \) may be small, the error is approximated \( \delta \gamma = 0.01 \gamma = 0.01 \gamma \). The errors assigned to the derivatives \( \partial \gamma / \partial x \) and \( \partial \gamma / \partial y \) are thus taken to be \( 0.02 \gamma \Delta x \) and \( 0.02 \gamma \Delta y \), respectively. The errors associated with advection are significant whenever the winds \( u + u' \) or \( u' \) are large, particularly when there is partial balance among the dynamic terms.

Errors associated with the wind values are not included explicitly in this study; however, investigations by Quiroz [1981] and Elson [1985] indicate that the peak winds derived using the geostrophic approximation are larger than the ageostrophenically derived wind values, particularly at high latitudes during large planetary wave events. However, 60° is at the edge of the region of the greatest difference as calculated by Elson, and Elson’s results show both increases and decreases in the wind speed relative to the geostrophic wind speed at 60°, 2 mbar. Therefore it is not known whether the errors are random or systematic. Furthermore, the \( u' \) values may have a significant ageostrophic component equatorward of 60°. Because there is not a simple way to estimate the error associated with the geostrophic approximation, this error is not included in the error estimate for the zonal and meridional advection terms, but will be considered qualitatively.

The vertical transport term \( \partial \gamma \partial \partial \delta z \) is the least accurate of the dynamic terms due to uncertainties in both the vertical velocity and the vertical derivatives. Here \( w' \) is calculated from the thermodynamic equation

\[
\frac{\partial T}{\partial t} = - \frac{\partial T}{\partial x} - \frac{\partial T}{\partial y} - \frac{w' H N^2}{R} - a T'
\]

where the scale height \( H \) is 7 km, \( R \) is the gas constant for dry air, and \( N^2 \) is the buoyancy frequency squared, equal to \( 4 \times 10^{-4} \) s\(^{-2}\). For these calculations it is assumed that \( \partial T'/\partial t \) and the thermal relaxation \( a T' \) can be neglected.

Because of the poor vertical resolution of the data, \( \partial \gamma \partial \partial \delta z \) is highly uncertain. The standard mid-latitude ozone profile [Krueger and Minzner, 1976] indicates that the ozone gradient changes rapidly near the ozone mixing ratio peak, and is between \( -1.2 \times 10^{-4} \) and \( -3.6 \times 10^{-4} \) ppmv/m near 2.5 mbar. The data of McPeters et al. [1984] indicate that the ozone mixing ratio peak during winter is closer to the 2-mbar level than the peak of the standard profile, suggesting that the value of \( \partial \gamma \partial \delta z \) is at the smaller end of the range suggested by the Krueger-Minzner profile. Therefore for these calculations, \( \partial \gamma \partial \delta z \) is estimated to be \( -1.7 \times 10^{-4} \) ppmv/m; latitude dependence is neglected. Because of the strong altitude dependence it is possible that the error in \( \partial \gamma \partial \delta z \) may be as large as a factor of 2.

The term \( \partial \gamma \partial \delta z \) is omitted from (1) because poor vertical resolution precludes accurate evaluation of \( \partial \gamma \partial \delta z \) from the data. However, it is possible to estimate \( \partial \gamma \partial \delta z \) from the 2- and 1-mbar perturbation fields, and by comparison with \( \partial \gamma \partial \delta z \), determine the potential significance of the omission. Results are given in Table 1. The value of \( \partial \gamma \partial \delta z \) is only 2-6 times larger than these estimates. Thus the nonlinear term, \( \partial \gamma \partial \delta z \), is potentially significant, especially when contribution to the net forcing due to vertical advection is
significant. Because only the term \( w' \phi_0 \) is considered, the error assigned to this term is taken to be the same size as the term itself. This may be an underestimate of the error, however, for most of the winter, the term \( w' \phi_0 \) is small, and the inaccuracy of this term does not have a large effect on the prediction calculation.

4. Evaluation of Chemical Forcing

Because simultaneous measurements of all relevant species are not available, and because computing resources are limited, it is not possible to consider exact expressions for the photochemical forcing \( S' \) in (1). Instead, \( S' \) is parameterized in terms of the perturbation temperature \( T' \) and the ozone volume mixing ratio \( \gamma \) according to

\[
S' = -\Gamma \gamma - \theta T'
\]

A parameterization of this type was used by Hartmann and Garcia [1979]; their values of \( \Gamma \) and \( \theta \) were derived from a simple Chapman chemistry scheme, with reaction rate coefficients modified to account for catalytic loss cycles affecting ozone. Here, the parameters \( \Gamma \) and \( \theta \) are calculated by the method of Stolarski and Douglass [this issue] using a scheme that explicitly accounts for the temperature and odd oxygen dependencies of the catalytic loss processes involving chlorine, odd nitrogen, and odd hydrogen. The parameters \( \Gamma \) and \( \theta \) indicate the response, in a 24-hour averaged sense, of an ozone perturbation to perturbations in the ozone mixing ratio and temperature. Although the photochemical model used in determining these parameters does not reproduce the observed mean ozone at 2 mbar, the parameters were used successfully by Stolarski and Douglass to predict \( (\gamma_M - \gamma_d) \) from \( (T_M - T_d) \), where the subscripts \( M \) and \( d \) denote the monthly mean and daily values, respectively. This suggests that the dependence of the odd oxygen loss processes on temperature and odd oxygen mixing ratio is correctly represented. These parameters, evaluated monthly at latitudes of 40\(^\circ\), 50\(^\circ\), and 60\(^\circ\), using appropriate temperature profiles, solar zenith angles, and concentrations of water, odd nitrogen species, and chlorine species, are given in Table 2. Except at 60\(^\circ\), the monthly changes in \( \Gamma \) and \( \theta \) are not extreme. It will be shown in a subsequent section that the photochemical terms at 60\(^\circ\) are small compared with the dynamic terms in winter, and large errors in \( \Gamma \) and \( \theta \) at 60\(^\circ\) have small consequences for the whole system. Therefore for this study, more frequent evaluation of the parameters is unnecessary.

This estimate of the chemical forcing considers only local deviations in ozone and temperature and neglects changes in the local response that are due to ozone changes above, i.e., opacity effects. Simple tests, using a one-dimensional steady state model, indicate that errors in the parameters due to opacity effects are not large. For 2 mbar during winter at 40\(^\circ\)-60\(^\circ\) latitude, the parameter \( \theta \), which indicates the response of \( \gamma \) to temperature perturbations, was found to be nearly independent of the vertical scale of the odd oxygen perturbation. The parameter \( \Gamma \), which indicates the response of \( \gamma \) to odd oxygen perturbations, is dependent on this vertical scale. For an odd oxygen perturbation of 10\%, the value of \( \Gamma \) calculated for a local change in odd oxygen differs from the value calculated for a perturbation applied to all levels by less than 15\%.

Other factors that affect the accuracy of this estimate of the chemical source term, discussed more fully by Stolarski and Douglass [this issue], include the nonlinearity of the ozone response to temperature perturbations, and the sensitivity of \( \Gamma \) and \( \theta \) to the conditions of ozone, temperature, and trace species concentration for which they are derived. The parameters respond in the same way to changes in these conditions, indicating that errors in \( \Gamma \) and \( \theta \) are highly correlated.

Because random measurement errors affecting \( \gamma \) and \( T' \) are small compared with the possible errors \( \Gamma \) and \( \theta \), the errors associated with the parameterization are considered the total error in the photochemical forcing. Considering the factors affecting the parameters detailed above, as well as the good agreement between the predicted and measured deviations of the daily zonal mean ozone from the monthly mean ozone, a maximum error of 25\% is assigned to \( \Gamma \) and \( \theta \). This error estimate reflects all of the difference in the estimated response from the (unknown) true response. The ability of this analysis to predict the next day’s perturbation field therefore is a test of the parameterization as well as a test of the ability to calculate ozone transports from satellite-derived ozone, temperature, and wind fields.

5. Calculation of Ozone Perturbation Field and Error Analysis

To test the overall accuracy of this approach, the day to day changes in the ozone perturbation are calculated from (1) and compared with measured values. The net forcing \( A \) for each day is evaluated at each grid point according to

\[
A(t_i) = -(\bar{u} + u') + v' + (\frac{\partial \gamma}{\partial x} + \frac{\partial \gamma}{\partial y}) \frac{\partial T'}{\partial x} + \frac{\partial \gamma}{\partial z} - \theta T'
\]

using the \( i \)th day values for all time dependent quantities. The time dependent forcing is replaced in (1) by the 24-hour
average value \([A]\) of the forcing \(A(t)\) given in (4). The continuity equation (1) may now be written
\[
\frac{\partial y'}{\partial t} = [A] - \Gamma y' \tag{5}
\]
which has the solution
\[
y'_c = \frac{[A]}{\Gamma} (1 - e^{-\Gamma t}) + y'(0) e^{-\Gamma t} \tag{6}
\]
where \(y'(0)\) is the initial value of the ozone perturbation. The approach outlined in (4)–(6) was tested against a variety of other methods for predicting day to day ozone changes using the model results of Rood and Schoeberl [1983b]. It was found that whenever the day to day changes in the forcing were not large, the ozone perturbation evaluated in this way agreed well with the exact model calculation, even though the exact model transport calculation uses 15-min time steps compared with the 24 hour time steps used here.

It is important to consider the effects of the errors in individual terms on the result. The general method for combining the different errors that all contribute to the uncertainty in the final result is outlined by Clifford [1973]. Each error \(\sigma\) is subscripted to indicate the source of the error. The errors in the dynamic terms are assumed to be uncorrelated. The errors \(\sigma_1\) and \(\sigma_2\) in the chemical forcing are correlated; the net error due to uncertainty in the chemical forcing \(\sigma_c\) is calculated according to
\[
\sigma_c = \left( \sigma_1 \frac{\partial y'}{\partial \Gamma} \right)^2 + \left( \sigma_2 \frac{\partial y'}{\partial \theta} \right)^2 + 2 \sigma_1 \sigma_2 \frac{\partial y'}{\partial \Gamma} \frac{\partial y'}{\partial \theta} \right)^{1/2}
\]
The total error \(\sigma\) in the system is estimated by determining the sensitivity of the result to each source of error \(\epsilon_i\); for example, the error associated with the zonal gradient of the perturbation field \(\partial y'/\partial x\) is the sensitivity of \(\gamma'_c\), given by (6), to \(\sigma_{zax}\), that is, \(\partial y'/\partial x(\partial y'/\partial x)\), multiplied by the estimated error in the zonal gradient \(\sigma_{zax}\). The errors are combined according to
\[
\sigma = \left( \sum \left( \frac{\partial y'}{\partial \epsilon_i} \sigma_i \right)^2 \right)^{1/2}
\]
Sources of error not considered in evaluating \(\sigma\) include the uncertainty in the meridional and zonal advection terms because of the use of geostrophic winds instead of the actual winds.

A typical comparison of the measured values of the ozone perturbation field with the predicted values, calculated using (6), is given in Figure 1a. The estimated errors in the calculation are also given. The calculated ozone contains more structure than the measured ozone because no effort was made to suppress high-frequency components in the forcing due to inclusion of nonlinear terms. The measured ozone is within the estimated errors of the calculated ozone at most longitudes. Where this is not true, the measured deviation is generally smaller than the predicted deviation, but in the same direction. The ozone perturbation calculated from the temperature field without dynamics, the photochemical equilibrium estimate
\[
\gamma_{pe'} = -\frac{\theta}{\Gamma} T \tag{7}
\]
is compared with the predicted ozone distribution and the measured ozone in Figure 1b. A comparison of the prediction \(\gamma'_c\) to the photochemical equilibrium estimate \(\gamma_{pe'}\) shows that the changes introduced by including the dynamic terms are all in the correct sense. Because the prediction calculated according to (6) produces an ozone distribution that reflects the features of the measured distribution, Figure 1a is considered a case of good agreement of measurement and theory. Not all predictions are so successful. Figure 1c is an example of poor agreement between measurement and prediction. The estimated errors are large because the small uncertainty in the zonal derivative is multiplied by a large zonal wind, but the measured ozone is not within the estimated errors for 140°–220° longitude. The magnitude of the calculated deviation far exceeds the measured deviation; however, even in this case, the actual deviations are in the same sense as the predicted deviations, and except for 140°–220°, \(\gamma'_c\) is a better reflection of the true ozone than \(\gamma_{pe'}\). The individual terms of (1) are given in Figure 1d for the case of Figure 1c; the magnitude of the meridional advection is very large; acting alone, it would produce a maximum ozone change of 3 ppmv/d. Meridional advection is responsible for the predicted large value of \(\gamma'\) at about 175° longitude in Figure 1c. In general, cases of poor agreement occur when the forcing due to one dynamic term, most commonly the meridional advection \(\nu' \partial y'/\partial y\) but occasionally the zonal advection \((\bar{u} + u') \partial y'/\partial x\), is large; this is seen most often at 60° latitude. It is possible that the forcing has been overestimated by using geostrophic winds to calculate the advection terms.

Because the agreement between prediction and measurement is usually good in the sense that the predicted ozone distribution reflects the features of the measured distribution as detailed above for Figure 1a, it is concluded that the method of calculating the dynamic terms and estimating the photochemical forcing is good and that assuming that the net forcing is nearly constant, to allow integration of (5), is acceptable. The agreement between prediction and measurement suggests that the effects of the terms that have been neglected are usually small.

6. COMPARISON OF TERMS

In order to show that the 2-mbar level is appropriately designated part of the transition region, it is necessary to devise a method to compare the terms in (1). Calculation of the root-mean-square (rms) value facilitates comparison because the squares of the terms are always positive and have nonzero zonal averages. The rms value, defined here to be the strength, was evaluated on a daily basis for each of the five terms according to
\[
R_j = \left( \frac{\sum_{i=1}^{N} \text{(term)}_i^2}{N} \right)^{1/2} \tag{8}
\]
where \(i\) is the longitude index. The strength may be interpreted as an indication, in a zonally averaged sense, of the relative ability of each term to affect the perturbation ozone mixing ratio. Results of the calculation are given in Figures 2a and 2b for 40° and 60° latitude for December–February. At 40°, the strengths of all five terms are the same order of magnitude; the strength of the vertical advection is generally 2–5 times smaller than that of the largest term. At 60°, strengths of the photochemical terms are generally smaller than the strengths of the zonal and meridional advection.
1. **Measured ozone distribution** $\gamma'$, ozone distribution calculated from (6) $\gamma_c'$, and the error limits of the calculated distribution $\gamma_c \pm \sigma$ for January 24, 1979, at 2 mbar, 50° latitude. (b) Measured ozone distribution $\gamma'$, the photochemical estimate $\gamma_{pe}'$ calculated from (7) and the ozone $\gamma_c'$ calculated from (6) for the time and location of Figure 1a; $\gamma_c'$ is much closer to $\gamma'$ than $\gamma_{pe}'$. (c) Same as Figure 1a for February 4, 1979, 2 mbar at 60° latitude. The calculated ozone perturbation is much larger than the observed deviation at about 180°. (d) The terms in the perturbation continuity equation (1) for the time and location of Figure 1c. The large value of the meridional advection produces the large ozone perturbation at 180° in Figure 1c.

7. **Importance of the Nonlinear Terms**

It is common practice to neglect terms such as $u'\partial y'/\partial y$ and $u'\partial y'/\partial x$ in model calculations which trace the time evolution of constituents, under the assumption that these terms are small compared with terms that are linear in the perturbation quantities. To test this assumption, the rms terms. This supports the statement that the possible large errors in the chemical response parameters at 60° latitude are not highly significant to the end result. Even so, adopting the criterion that the strength of a term must be an order of magnitude smaller than the strength of the largest term to be negligible, neither the chemical terms nor the vertical advection is negligible for the entire winter. Thus the 2-mbar level during winter 1978–1979 is appropriately considered part of the transition region for the latitudes 40°–60°. The dynamic terms do not become small compared with the photochemical terms at any time from the beginning of December to the end of February.
RMS VALUES (2mb; 40°N)

![Graph showing RMS values for 40°N]

RMS VALUES (2mb; 60°N)

![Graph showing RMS values for 60°N]

Fig. 2. (a) The strength $\Gamma$ given by (8) at 2 mbar, 40° latitude, December 1, 1978 to February 26, 1979, for each of the terms in the perturbation continuity equation (1). The photochemical and dynamic terms are all about the same order of magnitude; the vertical advection is 3–5 times smaller than the rest of the terms. (b) Same as Figure 2a but for 60° latitude. Here the zonal and meridional advecti aren dominate for much of the winter.

value, given by (8), is calculated for the linear and nonlinear terms each day for the month of January and given in Figure 3. These quantities are compared rather than calculating ratios of the nonlinear terms to the linear terms because ratios may be of either sign and also because ratios become large when the linear terms become small, giving a false sense of the importance of the nonlinear term. The zonal transport terms are compared in Figure 3a and 3c, and meridional terms in Figures 3b and 3d. At 40°, the nonlinear terms may be larger than the linear terms. In Figure 3b the nonlinear component $v'\partial\gamma'/\partial y$ dominates the linear component $v'\partial^2\gamma/\partial y^2$ at the end of January because the mean ozone gradient is very small. At 60°, where the dynamic terms are larger, neglect of the nonlinear terms compared with the linear terms is sometimes justified. However, even at 60°, the strength of the nonlinear terms if often comparable to the strength of the linear terms, indicating that the nonlinear terms should be retained. The comparisons between $\gamma'$ and $\gamma''$ are improved when the nonlinear contribution to the dynamical forcing is included.

8. INTERPRETATION OF TEMPERATURE CORRELATIONS

In Rood and Douglass [1985], it was shown that the correlation between the ozone and temperature perturbations in the transition region is the result of complex interactions between the wind field, the ozone background mixing ratio gradients, and the chemical forcing. To illustrate this conclusion, the linear correlation coefficients for the temperature and ozone perturbations for the three latitudes and 3 months under consideration were calculated, and are given in Table 3. These values are generally consistent with those reported by Nagatani and Miller [1984], although in that work the correlations were for standing wave components only. The daily linear correlation coefficients for the months of December 1978 and February 1979 are given in Figure 4. A linear correlation coefficient of approximately $-1$ has been interpreted to imply photochemical equilibrium between the ozone and temperature perturbations. The correlations given in Figure 4 are often found to be close to $-1$, even though the comparison of the strengths of the terms (Figure 2) clearly indicates that the dynamic terms are not negligible compared with photochemical terms. The photochemical terms do not dominate the perturbation continuity equation at any time between the beginning of December and the end of February; furthermore, there is no obvious relationship between the relative sizes of the terms and the observation of a strong anticorrelation.

Rood and Douglass [1985] concluded that dynamic forcing can produce a wide range of correlations between ozone and temperature perturbations. This conclusion is supported by comparison of the strengths (Figures 2a and 2b), the monthly correlation coefficients (Table 3), and the daily correlation coefficients (Figure 4). For example, at 2 mbar, 40°, the photochemical and dynamic terms are the same size (Figure 2a), suggesting that this is approximately the center of the transition region, yet the monthly correlation coefficients are strongly negative, ranging from $-0.80$ to $-0.93$. This is contrary to the assumption of Nagatani and Miller [1984] that a zero correlation is the center of the transition region. Furthermore, the transition region located by comparison of strengths is at a higher altitude than the region identified by considering the change in the phase difference between ozone and temperature waves [Gille et al., 1980; Wang et al., 1983].

To understand the possible range of interactions between the terms in (1) which produce the anticorrelations, three situations will be addressed in detail. In the first situation, the correlation between the ozone and temperature perturbations is not close to $-1$. This situation is found for much of the winter at 50° and 60° latitude, but infrequently at 40° latitude. An example is given for each latitude.

The first example is 40° latitude on December 4, 1978, one of only 17 occasions out of the 90 days when the correlation
between ozone and temperature deviations is not -0.75 or less. In Figure 5a, which gives the terms of (1), the zonal and meridional advections are dominant. Both the ozone and temperature deviations are small in this example, which explains the dominance of the dynamic terms. At 40°, whenever the correlation coefficient is not close to -1, the maximum ozone deviations are small, usually around 0.5 ppmv. The correlation between the ozone and temperature perturbations in this case is moderate, -0.69, and there is no obvious out-of-phase relationship between the dynamic terms, although there is some cancellation. Neither the photochemical estimate \( \gamma_{pe} \) (Figure 5b) nor the ozone \( \gamma \) calculated according to (6) (Figure 5c) compares particularly well with the measured ozone \( \gamma \). The measured ozone lies within the bounds \( \gamma \pm \sigma \), but the estimated errors here are large compared with the maximum ozone deviation.
Although the comparisons between the predicted and measured ozone perturbation fields are given here for only a few cases, these comparisons are good throughout most of the winter. It is correct to conclude that the moderate correlation between ozone and temperature perturbations implies at least partial dynamic control of the ozone perturbation.

In the second situation, the anticorrelation is strong, and the photochemical estimate of the ozone perturbation field is good, but the dynamic terms are not small compared with the photochemical terms. This is observed when balance exists between some combination of the dynamic terms, and is found under a variety of circumstances. Two typical examples of balance are given here.

In the first example, the net dynamic forcing is small compared with the photochemical forcing. The dynamic and photochemical terms for 40°, February 19, 1979, are given in Figure 8a. There is an out-of-phase relationship between meridional and vertical advection, which provides a maximum of about 20% cancellation because the meridional advection is much larger than the vertical advection. There is also partial cancellation between the meridional and zonal advection. The correlation coefficient between the ozone and temperature deviations is −0.96, and the photochemical estimate \( \gamma_{pe}' \) (Figure 8b) reflects the features of the measured ozone distribution \( \gamma \). The ozone calculated according to (6) also reflects the features of the measured ozone, largely because the sum of the dynamic terms is small compared with the photochemical terms.

In the second example, which is observed at 50°, there is a nearly in-phase relationship between vertical and meridional advection. These combine to partially cancel the zonal advection. Again, the chemical forcing terms are not large compared with the dynamic terms (Figure 9a), the anticorrelation is strong (−0.92), and the photochemical estimate compares well with the measured ozone field (Figure 9b). As in the above example, the prediction calculation also reproduces most features of the ozone field. In some sense, for both examples, the photochemical estimate could be considered superior to the result of the prediction calculation (Figure 9c); however, it should be noted that the relative errors in this sort of calculation are largest when the net forcing is smaller than the individual terms due to cancellation. These two examples are given to show that, through the dependence on the background gradients, different terms may combine to produce dynamic balance and large anticorrelations. This clearly demonstrates that the existence of a large negative correlation is not sufficient proof that ozone and temperature are in photochemical equilibrium, with photochemical forcing dominating the perturbation continuity equation.

The third situation is illustrated by the snapshot of the forcing terms (Figure 10a), the photochemical equilibrium estimate (Figure 10b), and the predicted ozone distribution (Figure 10c) calculated from (6). The anticorrelation between the ozone and temperature deviations is pronounced (−0.95), but the photochemical estimate of the ozone perturbation field derived from the temperature field deviates from the measured ozone by as much as 1 ppm. The ozone calculated from the net dynamic forcing compares somewhat more favorably with the measured ozone distribution. In this case, the advection by the mean zonal wind and the advection by the perturbation meridional wind are in approximate

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<tr>
<th>Latitude</th>
<th>December</th>
<th>January</th>
<th>February</th>
</tr>
</thead>
<tbody>
<tr>
<td>40°N</td>
<td>−0.88</td>
<td>−0.80</td>
<td>−0.93</td>
</tr>
<tr>
<td>50°N</td>
<td>−0.46</td>
<td>−0.67</td>
<td>−0.77</td>
</tr>
<tr>
<td>60°N</td>
<td>+0.24</td>
<td>+0.04</td>
<td>−0.55</td>
</tr>
</tbody>
</table>

TABLE 3. Monthly Correlation Coefficients

Fig. 4. The daily linear correlation coefficients between ozone and temperature at 40° latitude and 60° latitude for December 1978 and February 1979. The correlation coefficient at 40° is commonly close to −1, and also becomes large and negative at 60° during February.
balance, but the net dynamic forcing is important in calculating the next day’s ozone according to (6). The success of this calculation supports the premise that the difference between the photochemical estimate and the observed ozone is not necessarily the result of an error in the calculation of the chemical response parameters. Not only does this situation indicate that a large negative correlation does not imply photochemical equilibrium (as did the previous situation), but also that, if photochemical equilibrium were assumed and these data used to estimate the chemical response parameters, the temperature dependence of the ozone chemistry could be incorrectly assigned. This possibility was discussed by Rood and Douglass [1985].

9. DISCUSSION AND CONCLUSIONS

Rood and Douglass [1985] show that the correlation between ozone and temperature deviations could take on a
wide variety of values depending on dynamic and photochemical parameters and the characteristics of the constituent field. They also suggest that under particular conditions, a -1 correlation could be observed as a result of dynamic forcing alone. Though supporting the first result, the current analysis indicates that the atmosphere responds in a more limited fashion than was suggested by Rood and Douglass. The -1 correlation is found when there is balance between the dynamic terms. Thus while the anticorrelation is not a result of dominance of the dynamic terms by photochemical forcing (a traditional interpretation), neither does it result because a particular dynamic term forces a correlation that mimics photochemistry.

Examination of the data show that the correlations have a tendency to be closer to -1 at 40° than at 60° and that the correlations become more negative as time progresses from winter to spring. Both of these results would be expected from photochemical theory. At 40°, where the correlation between ozone and temperature deviations is close to -1 for most of this winter, and there is good agreement between...
Fig. 7. (a) The terms in the perturbation continuity equation (1) for December 14, 1978, 60° latitude. The correlation coefficient between $\gamma'$ and $T'$ is +0.22. (b) The measured ozone $\gamma'$ for the time and location of Figure 7a does not compare well with the photochemical estimate $\gamma_{pc}'$. (c) The measured ozone distribution $\gamma'$ for the time and location of Figure 7a lies within the error limits of the ozone distribution calculated from (6) $\gamma_{pc}' = \sigma$. 

Both $\gamma_{pc}'$ and $\gamma'$ with the measured ozone, close examination indicates that the net dynamic forcing is small compared with the photochemical forcing. The individual dynamic terms are not dominated by the photochemical forcing, and the appearance of the photochemical signature arises because of compensating dynamic terms.

At 50° and 60°, while there are times that the dynamic terms do balance, the dynamic contribution to the correlation between the ozone and temperature deviations is usually large. This is manifested in the data by positive and moderate negative correlations during much of the winter. Since much of the dynamic activity is associated with transient planetary waves, the effects of time averaging the data were considered by Rood and Douglass [1985]. In the model it was seen that over the course of a 10-week time average, the dynamic contribution to the ozone temperature correlation was significant well above 40 km. The presence of correlations that are persistently removed from −1 (Figure 4) suggests that time averaging the data does not eliminate the dynamic effects.
Perhaps the most important result is that the correlation of the ozone and temperature deviations is a rapidly varying function of time, depending often upon balances between large dynamic terms. A small change in this balance therefore can create large changes in the measured correlation. There is no time during the winter between 40° and 60°N when the photochemical forcing dominates the dynamic forcing. The role of the balances is particularly well illustrated by two cases at 60° (Figures 7a–7c and 10a–10c). In the first case, the balance between zonal and meridional advection is dramatic, except at about 120°–210° longitude. The ozone and temperature deviations, both maintained by dynamic effects, are weakly correlated, and the value of $\partial \gamma'/\partial t$ is significant. In the second case, the balance between zonal and meridional advection is more complete, the correlation between ozone and temperature deviations is close to -1, and the value of $\partial \gamma'/\partial t$ is close to zero.

The role of the balances is further illustrated by substituting for $w'$, as calculated from (2), in the perturbation continuity equation (1):
During those times when the anticorrelation is strong and the photochemical estimate is good, the last two terms on the right cancel, and the time derivative $\frac{\partial \gamma'}{\partial t} = 0$. By substitution of $\frac{\partial T'}{\partial x} = -(\Gamma' \partial \theta' / \partial x)$, $\frac{\partial \gamma'}{\partial y} = -(\Gamma' \partial \gamma' / \partial y)$, (9) becomes

$$0 = -\left\{ \tilde{\alpha} \left( 1 + \frac{R}{HN^2} \frac{\partial \gamma' \Gamma}{\partial \theta} \right) + u' \right\} \frac{\partial \gamma'}{\partial x} - u'$$

The term $(\tilde{R}/HN^2)(\Gamma' \partial \gamma' / \partial \varepsilon)$ is generally on the order of $-0.2$. The balance required to produce the appearance of
Fig. 10. (a) The terms in the perturbation continuity equation (1) for February 24, 1979, 60° latitude. The correlation coefficient between $\gamma'$ and $T'$ is $-0.95$. (b) There are significant differences (>1 ppmv) between the measured ozone $\gamma'$ and the photochemical estimate $\gamma'_{PE}$ for the time and location of Figure 10a, but the positions of the peaks are in good agreement. (c) The measured ozone distribution $\gamma'$ for the time and location of Figure 10b lies within the error limits of the ozone distribution calculated from (6) $\gamma' = \sigma$.

Photochemical equilibrium is therefore between the net zonal advection and the net meridional advection. There is no a priori reason for expecting this balance; therefore the observed correlation between ozone and temperature is expected to change rapidly as this balance changes.

The data analysis indicated two regimes in which balance between zonal and meridional advection, modified by vertical advection, yielded a result that simulated photochemical equilibrium. In an attempt to produce a generalized statement on when such balances might be expected to occur, the transport model of Rood and Schoeberl [1983b] was analyzed in the same manner as the data.

The model results are in qualitative agreement with the data in that the dynamic terms are larger than the chemical terms at 60° and are the same size at 40°. Further, the correlation between ozone and temperature perturbations produced by the model is a strongly fluctuating function of time, and the greatest contribution to the forcing is consistently meridional advection. In the model at 60°, it is possible to define three distinct regimes, a wave growth period during
which the meridional eddy advection and the zonal mean advection oppose each other, the onset of the warming when the zonal mean advection is small but the meridional advection is large, and the postwarming stage when the zonal mean advection is large and the meridional advection is small. It was attempted to find similar regimes in the atmospheric data, in particular periods of wave growth associated with the balance of the advection by the mean zonal wind with that by the meridional eddy wind. No unique correspondence was found between the observed balances in the dynamic terms and wave growth or any other parameter. While part of the failure to identify the conditions under which a particular balance may be expected to occur may be related to the inability of the model to simulate the winter stratosphere properly and the omission of nonlinear terms from the model, it is felt that no general rule can be derived from the data as to when to expect certain balances among the dynamical terms.

The results presented here also indicate that the transition region is not identified by some particular correlation value that lies between +1 and -1. For example, the strengths given in Figure 2b suggest that at 60°, 2 mbar is the bottom of the transition region during December and January, yet the corresponding monthly correlation coefficients are +0.24 and =0. For all 3 months, the strengths of Figure 2a indicate that 2 mbar is about the center of the transition region at 40°, yet the monthly correlation coefficients are all -0.8 or less. The transition region, located by comparison of the strength of the dynamic terms to the photochemical terms, is consistently at a higher altitude than the transition region identified by other authors.

In evaluation of the dynamic terms it was found that inclusion of the nonlinear terms in the calculation improved the comparison of the ozone, \( \gamma' \), to the measured ozone, \( \gamma \). When the nonlinear terms were calculated, no effort was made to suppress high wave number components that are not present in the measured ozone field; therefore \( \gamma' \) appears noisy compared with \( \gamma \). Comparison of the strengths of the linear to the nonlinear terms shows that the nonlinear terms are significant elements of the net dynamic forcing throughout the winter.

There may be significant errors in the calculation due to the neglect of terms in both the chemical and dynamic formulation of the above analysis. In particular, as discussed previously, the use of geostrophic winds may misrepresent the actual winds [Elson, 1985]. This may explain the fact that, for cases of poor agreement between the calculated and measured ozone deviations (e.g., Figure 1c), the dynamic/photochemical estimate generally overestimates the amplitude of the ozone perturbation. If ageostrophic effects are found to systematically reduce the wind speed, the comparison of the predicted ozone with the measured ozone should improve. The fact that good agreement is generally observed suggests that errors associated with ageostrophy are not consistently large at these latitudes; day to day ozone variations can usually be predicted from satellite data within calculated error limits. When the net dynamical forcing is small, then the photochemical estimate is often quite good, indicating the accuracy and the value of the Stoelarski and Douglass [1985] parameterization in studying ozone data. When the photochemical estimate is poor, the inclusion of the dynamic forcing consistently improves the estimate, producing an ozone deviation field that reflects the important features of the measured distribution even when the magnitudes of the deviations do not agree. The results indicate that dynamic/photochemical interaction is strong throughout all of the winter and that the dynamic terms must be evaluated in the study of the correlations of ozone and temperature perturbations.

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