

Impact of Interannual Variability (1979–1986) of Transport and Temperature on Ozone as Computed Using a Two-Dimensional Photochemical Model

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Eight years of NMC (National Meteorological Center) temperature and SBUV (solar backscattered ultraviolet) ozone data were used to calculate the monthly mean heating rates and residual circulation for use in a two-dimensional photochemical model in order to examine the interannual variability of modeled ozone. Fairly good correlations were found in the interannual behavior of modeled and measured SBUV ozone in the upper stratosphere at middle to low latitudes, where temperature dependent photochemistry is thought to dominate ozone behavior. The calculated total ozone is found to be more sensitive to the interannual residual circulation changes than to the interannual temperature changes. The magnitude of the modeled ozone variability is similar to the observed variability, but the observed and modeled year to year deviations are mostly uncorrelated. The large component of the observed total ozone variability at low latitudes due to the quasi-biennial oscillation (QBO) is not seen in the modeled total ozone, as only a small QBO signal is present in the heating rates, temperatures, and monthly mean residual circulation. Large interannual changes in tropospheric dynamics are believed to influence the interannual variability in the total ozone, especially at middle and high latitudes. Since these tropospheric changes and most of the QBO forcing are not included in our model formulation, it is not surprising that the interannual variability in total ozone is not well represented in our model computations.

INTRODUCTION

A reasonably good qualitative representation of the total ozone seasonal behavior, when compared to total ozone measurements, has been achieved in several two-dimensional (2D) models in recent years, e.g., Pyle [1980], Garcia and Solomon [1983], Ko *et al.* [1984], Widhopf *et al.* [1984], Stordal *et al.* [1985], and Jackman *et al.* [1989a]; Jackman *et al.* [1989b], where the total ozone from several models are presented together; and Yang *et al.* [1991]. The transport-dominated features of measured total ozone such as the northern high-latitude late winter, early spring maximum, and the southern high-latitude off-the-pole maximum in early spring are represented qualitatively in model simulations. These models also simulate the low-latitude solar effects, with the minimum ozone in winter and maximum ozone in summer.

Model ozone profiles differ from measurements in several important respects. In the upper stratosphere, calculated ozone values are lower than measurements; equivalently, for models constrained by observations, calculated ozone loss exceeds production [e.g., Wofsy, 1978; Butler, 1978; Fredrick *et al.*, 1978; Johnston and Podolske, 1978; Jackman *et al.*, 1986; Natarajan and Callis, 1989; McElroy and Salawitch, 1989]. In the middle and lower stratosphere, calculated ozone values are generally greater than measured values. In spite of these model-observation ozone profile differences,

modeled total ozone has been compared carefully to measured total ozone because the measurements of total ozone comprise a long-term, reliable data set.

Two-dimensional residual circulation models (both with fixed circulation and coupled radiation, dynamics, and chemistry) are used to make predictions of future levels of ozone for many decades into the future [World Meteorological Organization (WMO), 1990], which are then used by policy makers in regulations of chlorine-containing source gases. Validation of these 2D models is important and is derived from many intercomparisons between model results and measurements. Another test of 2D models includes the ability of these models to predict past interannual changes in ozone over a several year time period.

We showed in a previous study [Jackman *et al.*, 1989a] that the total ozone calculated in a 2D model is sensitive to the vertical winds in the lower stratosphere. We compare in this study the 2D modeled ozone fields (calculated with interannual variability in input temperature and ozone fields) with measured ozone fields. We intend to determine if the use of a yearly changing residual circulation based on SBUV (solar backscatter ultraviolet) ozone and NMC (National Meteorological Center) temperature measurements results in an interannual behavior in ozone which is similar to the observed interannual behavior in ozone.

TEMPERATURE AND OZONE DATA (1979–1986)

The ozone data used in this study consist of monthly values of ozone mixing ratio at a number of pressure levels from 100 mbar to 0.3 mbar measured from the SBUV

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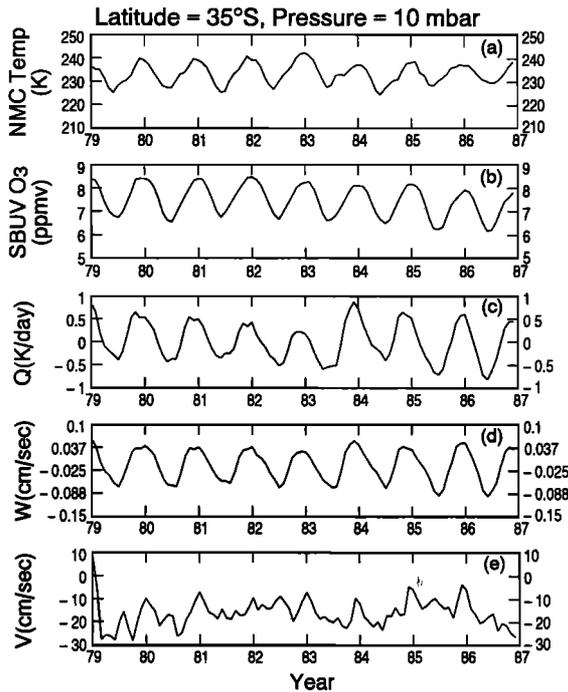


Fig. 1. Interannual changes at 10 mbar and 35°S for (a) NMC temperature in degrees Kelvin, (b) SBUV ozone in ppmv, (c) net heating rate Q in degrees Kelvin/d, (d) vertical velocity w in cm/s, and (e) meridional velocity v in cm/s.

spectrometer on the Nimbus 7 satellite and the total ozone measured from both the SBUV and total ozone mapping spectrometer (TOMS) instruments on the same satellite. They cover an 8-year time period from January 1979 to December 1986. These data are zonally averaged in 10° latitude bands and are the current version (version 5) of the processed data as described by Fleig *et al.* [1990]. The data below 30 mbar are based on climatology and constrained by simultaneous measurements of total ozone. The data above 0.3 mbar are based on climatology.

The NMC temperature covers the same time period and is given at 18 standard pressure levels from 1000 mbar to 0.4 mbar. The temperatures above 10 mbar are based on radiances measured from the vertical temperature profile radiometer (VTPR) on NOAA 5, and the stratospheric sounding unit (SSU) on Tiros N. The temperatures below 10 mbar are based on both the rawinsonde and satellite data.

The satellite-derived temperatures have been adjusted for possible instrument bias based on rocket-measured temperatures as described by Gelman *et al.* [1986]. This kind of correction is not possible for the SBUV instrument, which has degraded over this 8-year period due to the exposure of the diffuser plates to solar ultraviolet radiation [Watson *et al.*, 1988]. We have therefore carried out our study using both the original data (without removing the linear trends) and the detrended data. The linear trends were removed using a linear regression model at each pressure and latitude surface.

Although some of the ozone change in the upper stratosphere is instrumental, some of the ozone change is real, and total detrending overcompensates for the errors that are solely the result of the degrading instrument. The model studies in which the data with a trend were used were most appropriate when comparing to TOMS total ozone data.

Total ozone is mainly determined by the lower stratospheric part of the ozone profile and the heating rates in this part of the atmosphere are found to be most sensitive to temperature whose measured trend is not in question.

The radiative heating rates were calculated from the ozone and temperature data using a radiative transfer code described by Rosenfield *et al.* [1987], updated with a new parameterization for ozone infrared absorption [Rosenfield, 1991]. Seasonally averaged latent heating rates from Newell *et al.* [1974] were added to the radiative heating to derive net diabatic heating rates. Net heating rates and temperatures were then used to compute the monthly residual circulation following Dunkerton [1978].

The 8-year variation in the NMC temperature, SBUV ozone, net heating rate (Q), residual vertical velocity (w), and residual meridional velocity (v) are shown in Figures 1 and 2 at the two levels 10 and 3 mbar for latitude 35°S. This illustrates the typical interannual changes measured for NMC temperature and SBUV ozone and computed for heating rates, vertical velocities, and meridional velocities. A moderate degree of interannual change is observed in both the measured NMC temperature and SBUV ozone, but the yearly seasonal excursions are clearly larger than the interannual changes. Interannual changes input for the 2D model include the advection fields (w and v) computed with the use of the net heating rate (derived from the measured NMC temperature and SBUV ozone) and the NMC temperature.

TWO-DIMENSIONAL MODEL DESCRIPTION

The residual circulation computed from the 96 months (8 years) of ozone and temperature data, as described above, is used in a 2D model [Douglass *et al.*, 1989] for several experiments. The vertical extent of the model is between the

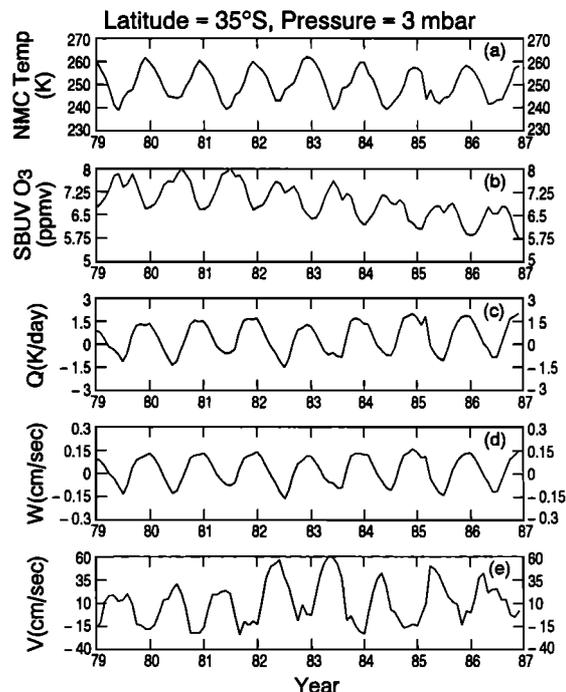


Fig. 2. Interannual changes at 3 mbar and 35°S for (a) NMC temperature in degrees Kelvin, (b) SBUV ozone in ppmv, (c) net heating rate Q in degrees Kelvin/d, (d) vertical velocity w in cm/s, and (e) meridional velocity v in cm/s.

ground and 0.23 mbar (approximately 60 km), equally spaced in log pressure, with about a 2-km grid spacing and from 85°S and 85°N with a 10° grid spacing.

The lower boundary conditions are given in Table 1 for the model background cases used: a simulation of year 1980 with ~ 2.5 ppbv Cl_x input at the ground. The upper boundary conditions were assumed to be zero flux for all species. Most reaction rates and photodissociation cross sections are taken from *DeMore et al.* [1987] and presented by *Dougllass et al.* [1989]. Another reaction which was included, but inadvertently left out of Table 2 in *Dougllass et al.* [1989], was $\text{OH} + \text{CH}_3\text{CCl}_3 \rightarrow 3(\text{Cl}) + \text{Fragments}$ with $k = 5.0 \times 10^{-12} \exp(-1800/T) \text{ cm}^3 \text{ s}^{-1}$ from *DeMore et al.* [1987].

Eddy diffusion was also specified in the 2D model. The K_{yy} values were taken from *Newman et al.* [1988] and *Jackman et al.* [1988] and were determined from a computation of the potential vorticity using seasonally averaged NMC temperature data over the 4-year period from December 1, 1978, to November 30, 1982. The K_{yz} distribution simply relates the mixing on isentropic surfaces to the mixing on pressure surfaces [*Jackman et al.*, 1988]. Both K_{yy} and K_{yz} are seasonally varying but have no interannual change. We fix K_{zz} to $2 \times 10^3 \text{ cm}^2 \text{ s}^{-1}$ in the stratosphere with K_{zz} increasing with decreasing altitude in the troposphere to $1 \times 10^5 \text{ cm}^2 \text{ s}^{-1}$ at the ground.

The 2D model was run for 20 years to a seasonally repeating steady state for the model background cases. We ran 5 years of 1979 dynamics to a seasonally repeating steady state before starting with 1980, 1981, etc. because the model results for a particular year were somewhat sensitive to the previous years' dynamics (also noted by *Schneider et al.* [1991]). We likewise focused on the results of the later years (1982–1986) rather than the early years (1979–1981) when comparing our model results to the interannual behavior of ozone. Thirty-three other minor species besides ozone were computed in our model [*Dougllass et al.*, 1989], however, ozone is the only species for which global data are available for all 8 years of the model study. Therefore ozone is the only species for which we compare model results with measurements.

We completed a number of model runs, both for the data with a trend and the detrended data. All the model experiments were run for 12 years of model time. In the troposphere, only the temperatures and radiative heating rates

TABLE 1. Lower Boundary Conditions for All Transported Species

Species	Type of Boundary Condition	Unit	1980 Value
N_2O	mixing ratio	ppbv	300
CH_4	mixing ratio	ppmv	1.6
CO	mixing ratio	ppbv	100
H_2	mixing ratio	ppbv	500
CH_3OOH	flux	$\text{cm}^{-2} \text{ s}^{-1}$	0.0
CH_3Cl	mixing ratio	pptv	700
CH_3CCl_3	mixing ratio	pptv	100
CCl_4	mixing ratio	pptv	100
CFCl_3	mixing ratio	pptv	170
CF_2Cl_2	mixing ratio	pptv	285
O_x	deposition velocity	cm s^{-1}	0.1
HNO_3	mixing ratio	pptv	90
NO_y	mixing ratio	pptv	100
Cl_x	flux	$\text{cm}^{-2} \text{ s}^{-1}$	0.0

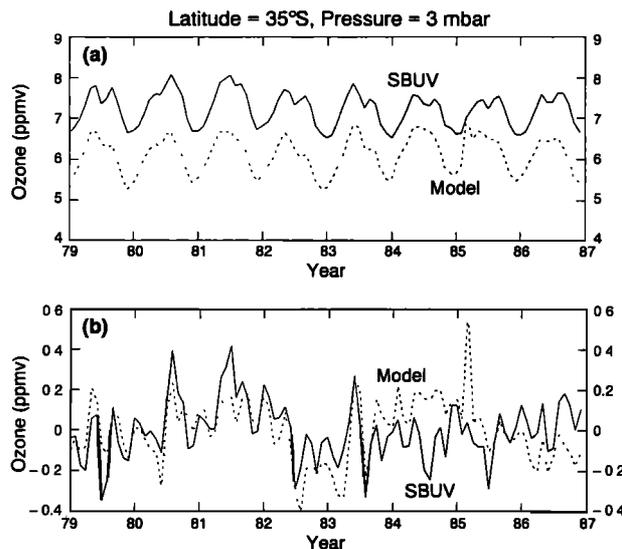


Fig. 3. (a) Ozone (ppmv) at 3 mbar and 35°S from detrended SBUV data (solid line) and model experiment using detrended SBUV ozone and NMC temperature data (dashed line). (b) Ozone (ppmv) residual deviations in the model and data after annual and semiannual components are removed.

had interannual variation; the diffusion coefficients, the latent heat, and the tropopause height were all fixed.

Solar cycle ultraviolet (UV) flux variation was not accounted for in any of our computer simulations. Some variation is expected in the background species' abundance because of the solar cycle UV flux variation. We do not include this UV change, so that it is possible to analyze more easily the straightforward influence of interannual dynamics behavior.

MODEL SIMULATION USING DETRENDED OZONE AND TEMPERATURE DATA

The model results using the detrended data provide the best comparison between model profile ozone and SBUV data, since there is such a large trend in the SBUV data over the 8-year time period. The largest calculated changes in ozone are found in the lower stratosphere/upper troposphere.

In the upper stratosphere, where photochemistry is more important than transport, the model O_3 is 15–20% lower than the SBUV data at 3 mbar, but the behaviors are in qualitative agreement. The detrended SBUV data (solid line) and model ozone (dashed line) given in Figure 3a at 3 mbar and 35°S exhibit annual and semiannual changes caused by the annual and semiannual temperature swings. The correlation coefficient between model and data in Figure 3a is at a very high value of 0.87 (significant to the 99% confidence level). We have removed the annual and semiannual components of both model and SBUV ozone and present the residual changes in Figure 3b. These smaller residual ozone changes are similar in both the model and SBUV data and are primarily caused by inverse temperature variations associated with the temperature dependence of reactions which destroy odd oxygen. The correlation coefficient for the model and data compared in Figure 3b is at a moderate value of 0.48 (significant to the 99% confidence level).

The SBUV ozone is best between 30 and 1 mbar; thus we

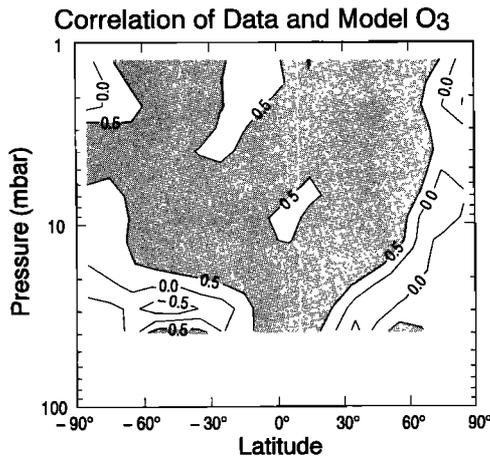


Fig. 4. Correlation coefficient of SBUV ozone data with modeled ozone simulation using detrended SBUV ozone and NMC temperature data for all months together in years 1982–1986. Cross-hatched areas indicate values where correlation coefficient is larger than 0.5. The value for the 95% confidence levels for the 60 months that are included in this calculation is 0.21.

only show model-measurement comparisons in that region. We computed the correlation coefficient between the data (detrended) and detrended model run for the last 5 years of the run (1982–1986), which is shown in Figure 4. The 95% confidence level is 0.21 for Figure 4 (which includes 60 months of data). In Figure 4 the seasonal behavior of ozone drives the correlation and a very high level of correlation (0.5–0.9) is achieved in the middle to upper stratosphere and in the middle to low latitudes. The modeled and measured ozone values in the middle to lower parts of the stratosphere are largely uncorrelated. The correlation is reduced when the annual and semiannual cycles are filtered out from both the model and measured ozone values, as illustrated in Figure 3b. The correlation in the upper stratosphere which results after filtering out the annual and semiannual cycles is in the range of 0.3–0.6 compared to values of 0.5–0.9 shown in Figure 4.

MODEL SIMULATION USING OZONE AND TEMPERATURE DATA WITH THE TREND

We used ozone and temperature with the trend in a model simulation to compare modeled total ozone with data (TOMS). We found that the temperature differences from year to year are the major contributors to the calculated differences in the lower stratospheric heating rates and circulation, in agreement with *Schneider et al.* [1991]. Before discussing the results of the interannual comparisons in total ozone for the model experiments, we first show a comparison of modeled total ozone with TOMS data. This is illustrated in Figure 5, where both the TOMS data and the modeled total ozone are presented for 1986.

There is qualitative similarity between the model and measurements, but significant difference in detail. The model represents the northern hemisphere high-latitude late winter peak qualitatively, although the model's higher values extend to lower latitudes than indicated in the TOMS data. The low-latitude solar zenith angle effect is observed in both model and data, with higher ozone values observed in both hemispheres during summer and lower ozone values during

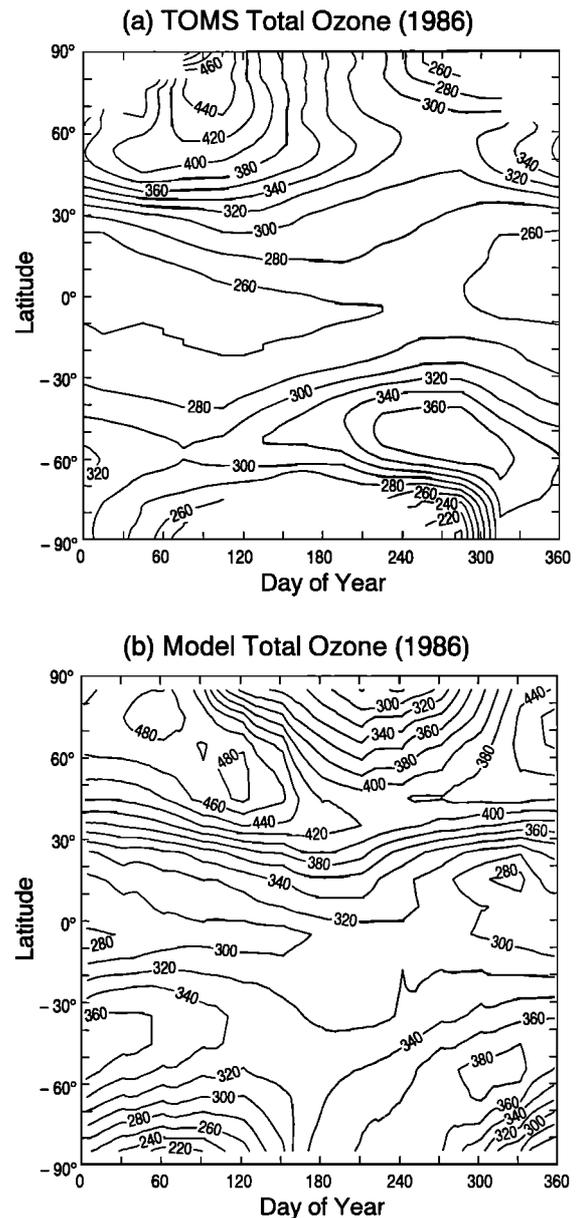


Fig. 5. Total ozone for 1986 in Dobson units from (a) TOMS (total ozone mapping spectrometer) and (b) from model results using SBUV ozone and NMC temperature data including the trend.

winter. A quantitative difference is apparent in the lower latitudes with the model predicting up to 40 Dobson units more ozone than indicated in the data. An off-the-pole southern hemisphere winter maximum occurs in both model and TOMS data; however, the model ozone differs significantly from TOMS at southern high latitudes. Among the factors that probably contribute to this disagreement are the omission of polar heterogeneous chemistry and the errors in the SBUV ozone profiles in the Antarctic region [*McPeters et al.*, 1986]. *Rosenfield et al.* [1988] show that lower stratospheric heating rates and vertical advection in the Antarctic springtime are very sensitive to ozone amounts and the vertical gradient of the ozone mixing ratio profile.

The ratios of the seasonally averaged total ozone from the TOMS data to the model values are given in Figure 6 as a function of latitude for 1982–1986. There are some absolute

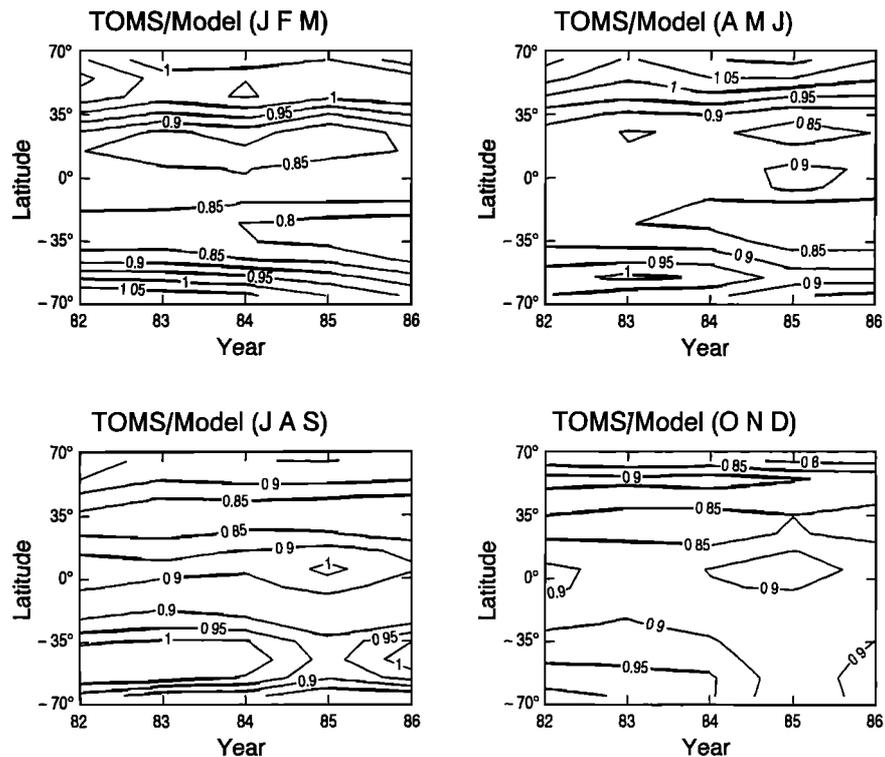


Fig. 6. Total ozone from TOMS divided by the model computed total ozone for January-February-March (J F M), April-May-June (A M J), July-August-September (J A S), and October-November-December (O N D).

differences between the data and model values, indicated by the range of contours from 0.8 to 1.1. The interannual variations are much different in the model and data, as the contours are much different from the straight lines that would indicate agreement between modeled and observed variability. Although some latitudes and seasons (e.g., OND (October-November-December) northern latitudes) compare more favorably than others (JAS (July-August-September) southern latitudes 1984–1986), the overall comparison is poor and suggests that physical processes important to the observed interannual variability of total ozone are not included in this model.

There are a number of possibilities which could explain the poor comparisons between the interannual behavior in model predictions and measurements. These are (1) the input ozone values are not true measurements below 30 mbar, but rather rely on climatology and the measurement of total ozone, (2) the horizontal eddy diffusion rates vary monthly, but they have no interannual behavior, (3) the QBO is not represented with only the input temperature changes [Gray and Pyle, 1989; Gray and Chipperfield, 1990], and (4) tropospheric interannual changes are not well represented (e.g., the latent heat changes monthly but with no interannual behavior).

Use of climatological ozone rather than measured ozone below 30 mbar is not believed to be very important in the interannual changes under investigation here; below 30 mbar the heating rate changes are influenced mainly by temperature changes [Schneider et al., 1991]. We did complete two other sets of model experiments in order to investigate the sensitivity of our results to interannual heating rate changes, interannual temperature changes, and interannual horizontal eddy diffusion changes.

In the first set of model experiments, we compared three model transport and temperature formulations: (1) the interannual heating rate and temperature changes together were both included (the model base simulation), (2) only the interannual heating rate changes were included, together with a fixed annual cycle of temperature, and (3) only the interannual temperature changes were included, together with a fixed annual cycle of heating rates. We found from these model simulations that the total ozone is more dependent on the heating rate changes than on the temperature changes.

In the second set of model experiments we compared two model calculations: (1) the model base simulation with K_{yy} values from Newman et al. [1988] and Jackman et al. [1988] along with the interannual heating rate and temperature changes; and (2) a model simulation including self-consistent K_{yy} computed from the residual meridional velocity (see section 5 of Jackman et al. [1988]) along with the interannual heating rate and temperature changes. We found that our model results were relatively insensitive to these horizontal eddy diffusion changes. Yang et al. [1990, 1991] indicate that the interannual K_{yy} changes corresponding to interannual transport changes can be computed more exactly than undertaken here. An indication of these interannual K_{yy} changes can be found in Figure 15 of Yang et al. [1990]. These large interannual changes in K_{yy} computed by Yang and coauthors suggest that corresponding large interannual changes in total ozone might be possible from only the interannual K_{yy} variations. The sensitivity of 2D model results to interannual K_{yy} changes requires further study before a final judgment can be made on the K_{yy} and their significance in determining total ozone amounts.

The QBO forcing and the tropospheric interannual

changes are two of the largest interannual atmospheric changes which are not well represented in our model computation. There is a clear signal of the quasi-biennial oscillation in the tropical total O₃ and zonal wind [see Lait *et al.*, 1989]; no such signal is present in the heating rates and derived vertical winds in that region. Although the tropospheric interannual changes in temperature are included through the NMC data set, the more important interannual variations in the tropopause height, weather systems, and wave actions are not represented in these model computations.

SUMMARY AND CONCLUSIONS

The seasonally averaged climatological behavior of total ozone is fairly well represented with a 2D model residual circulation formulation. Such formulations have been previously shown to have a large sensitivity of total ozone to the circulation. We have used 8 years of SBUV ozone data and NMC temperature data to examine the sensitivity of modeled ozone interannual variability to interannual changes in ozone and temperature. The magnitude of the modeled ozone variability is similar to the observed variability, but the observed and modeled year-to-year variations are mostly uncorrelated. Two major problems are apparent: (1) the quasi-biennial oscillation in low-latitude total ozone is not present in the model calculations, and (2) the interannual variability in tropospheric forcing of the stratospheric circulation is not represented and is important in determining the year-to-year variations.

Future work in this type of detailed model-measurement comparison should use a more complete data set for the interannual ozone and temperature behavior, a better representation of the QBO signal, and a better representation of the interannual behavior of the troposphere. Detailed studies of this nature, however, can be of use for certain well-posed problems concentrating on specific areas of the atmosphere.

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