Final Report

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Research Activities

Our contributions to the SAGE II (and SAGE I) science team activities have focused on the validation of the ozone and NO_2 measurements. The objective has been to validate both the constituent concentrations and mixing ratios and the assigned error estimates. Here it should be noted that the sun-scanning capability, which is an integral part of the SAGE measurements, permits a profile by profile assessment of measurement precision. Our contributions to date have emphasized the comparison of ozone zonal mean and longitudinal variations between SAGE I and the Nimbus 7 SBUV (Cunnold, 1984; Cunnold et al, 1984), the comparison of SAGE I and ozone against umkehr ozone (Newchurch et al, 1986) and the study of preliminary SAGE II ozone and NO_2 data (Cunnold and Chu, 1986; copy attached).

During these validation activities some comparisons against three-dimensional numerical model results have also been made. Relationships between measured parameters, such as between ozone and temperature, have been studied. In these studies it is most important to separate variances having a natural origin from variances associated with measurement errors. In view of the roughly 10% precision of the SAGE measurements, the validation activities have taken precedence, and the scientific results regarding correlations between the measured parameters have so far been interpreted cautiously.

References

Cunnold, D., Comparison of ozone data derived from SBUV and SAGE wind emphasis on longitudinal variations, Adv. Spac Res., 4, 47-56, 1984.

Cunnold, D.M., M.C. Pitts, and C.R. Trepte, An intercomparison of SAGE and SBUV ozone observations for March and April 1979, J. of Geophysical Res., 89, 5249-5262, 1984.

Cunnold, D.M., and D.A. Chu, An analysis of preliminary SAGE II data on ozone and NO_2. Proceedings of COSPAR meeting, Toulouse, France, 1986. To appear in Adv. Space Research.

Newchurch, M.J., G. Grams, D.M. Cunnold, and J.J. DeLuisi, A comparison of SAGE I, SBUV, and Umkehr Ozone Profiles including a search for Umkehr aerosol effects. Submitted to J. of Geophysical Res., 1986.

AN ANALYSIS OF PRELIMINARY SAGE II DATA ON OZONE AND NO_2

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ABSTRACT

Zonal mean mixing ratios of ozone and NO_2 measured by SAGE II on several days in March and April, 1985 are compared against zonal means for this time of year previously measured by SAGE I, SBUV, and LIMS. After allowing for calculated diurnal variations of these gases, agreement within 15% is found for ozone and 20% for NO_2. It is noted that the profile error bars given on the SAGE II data tapes need to be carefully interpreted and that the measured tropical variances suggest that these error bars are being somewhat overestimated. Planetary waves in both ozone and NO_2 in the middle stratosphere should be derivable from the SAGE II measurements.

INTRODUCTION

SAGE II observations began in October 1984. A preliminary data set covering the period November 1984 to May 1985 has been distributed to the SAGE Science Team. From this data set the months of March and April 1985 have been selected because we previously analyzed SAGE I observations for March and April, 1979 /5/. Both the SAGE I and II ozone measurements are based on measurements of the earth's limb at 0.6 μm /6,2/. However, whereas the SAGE I NO_2 measurements were based on measurements at 0.45μm, the SAGE II NO_2 measurements are based on the differential absorption between two neighboring wavelengths close to 0.45 μm. This is expected to create a more accurate measurement of NO_2.

During the data retrieval vertical profiles have been smoothed over 5 km at heights where the extinction is less than 2×10^{-5}/km. This produces smoothing of all the NO_2 profiles and of ozone profiles above approximately 37 km altitude. In our analysis we have smoothed the ozone profiles below 37 km altitude in both SAGE I and SAGE II using

$$\bar{x}\,(Z_1) = \exp\left\{ \frac{1}{h} \int_{Z_1 - h/2}^{Z_1 + h/2} \ln x \, dZ \right\}$$

where x(Z) is the ozone mixing ratio at altitude Z and h = 5 km. The data has then been analyzed on the standard meteorological levels which are roughly 5 km apart.

The temperature data analyzed here is that accompanying each SAGE constituent profile. It is provided to the SAGE team by the Upper Air Branch of NOAA from the mapped data which is routinely derived from the TIROS satellites and radiosondes. These temperature profiles have generally been smoothed horizontally and vertically somewhat more than the SAGE constituent profiles. These profiles provide a reference height for each constituent profile and are used to relate geometric altitudes to pressure levels in the SAGE I data and in this version of the SAGE II data.

Horizontal variations in the SAGE data are analyzed as described in Cunnold /5/. Thus, each day of data (defined by Universal Time) is analyzed separately in terms of longitudinal Fourier components using generalized least squares estimation by which each measurement is inversely weighted according to the variance of the measurement. The components are assigned to the average latitude of the measurements on that day. Except at the extreme latitudes of the SAGE observations, a single day of observations typically traverses approximately 5° latitude. The observations are then grouped into 10° latitude bins. Because our interest is in longitudinal variations, we have selected only those days which contain no more than one orbit of missing data.

OZONE ZONAL MEANS

Figures 1 and 2 show a comparison of ozone zonal means for March and April at mid-latitudes and in the tropics. The preliminary SAGE II data for 1985 is being compared against two retrievals of SAGE I data for 1979 and SBUV data for 1979. Note that SAGE I version 1 is now officially non-existant and has been removed from the archives; the currently archived version (version 2), however, contains mixing ratio errors such that the correct ozone mixing ratios lie between those of versions 1 and 2 (but closer to 2). Note also that the SBUV data set is the original data which has not been adjusted for the Bass and Paur /1/ ozone cross section measurements. Although there are several versions of each satellite data set (including a new version of SAGE II now being produced) these adjustments typically change the concentrations by a factor of less than 10% in a way which is only weakly dependent on latitude and height. Thus, in particular, longitudinal variances normalized by the zonal mean concentrations do not differ significantly from one version to another.

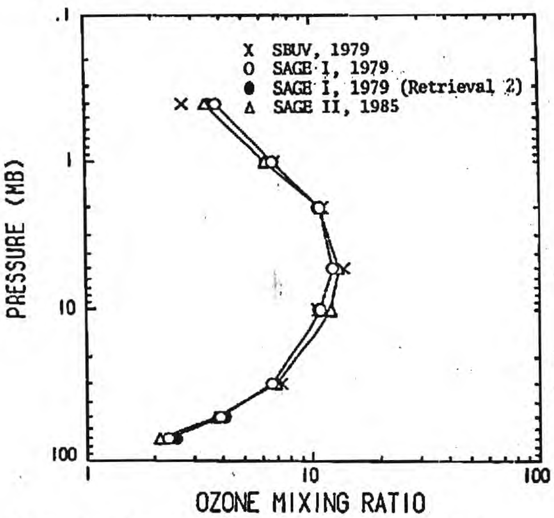

Fig. 1. Zonally-averaged ozone mixing ratios (μg/g) at 40–50°S for several days in March and April.

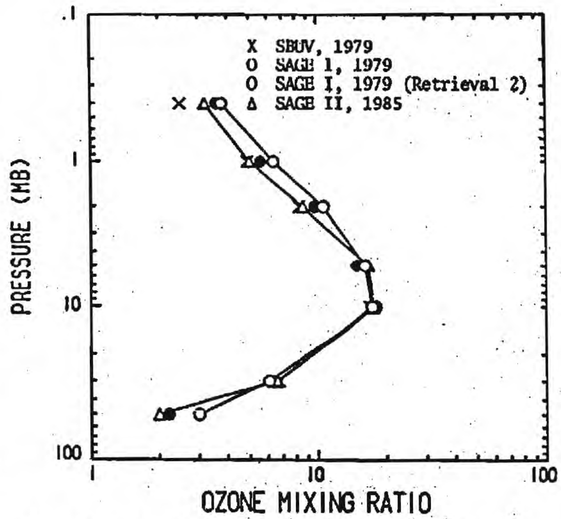

Fig. 2. Zonally-averaged ozone mixing ratios (μg/g) for 20°N–20°S for several days in March and April.

Figure 1 exhibits excellent agreement between the four data sets with 15% being the range of the zonal means except at 0.4 mb. At this level the smaller SBUV values almost certainly reflect the diurnal variation of ozone which should be neglible at altitudes below 1 mb but which should have a magnitude of roughly 25% at 0.4 mb (e.g., /7/). In the tropics there exists a wider spread in the measurements at 2, 1 and 0.4 mb. This difference between the SBUV and SAGE I measurements was previously noted by Cunnold /5/. Note, however, the excellent agreement between SAGE II and SBUV and the closer agreement with SAGE I version 2 than with version 1. Assuming that version 2 is more correct than version 1, the spread between the data sets in both tropics and mid-latitudes (excluding SBUV measurements at 0.4 mb) is 15%.

We thus consider the SAGE II ozone data for this time period to have been validated to 15%. Using simultaneous SBUV II measurements and improved SAGE II retrievals, we hope to be able to validate the SAGE II data at all heights and latitudes to better than 10%. The projected accuracy of the SAGE II measurements is similar to that of the SAGE I measurements and is approximately 5%. If percentage differences at 1, 2, 5, 10 and 30 mb are averaged for both the tropics and mid-latitudes (including 50°N, not shown), there is less than 1% difference between the SAGE II and the SBUV ozone measurements on average and the SAGE II measurements are approximately 2% smaller than those for SAGE I version 2.

TROPICAL VARIANCES OF OZONE

An estimate of the precision of the SAGE measurements is obtained by examining the longitudinal variances of ozone in waves 1 through 4 in the tropics where we should expect that physically-generated variations are small. Figure 3 shows these values for both SAGE I and SAGE II. The noise in SAGE ozone measurements consists of an uncertainty of approximately 0.25 km in the reference height for the profile and measurement noise which dominates the uncertainties above 2 mb (there are about equal contributions at 2 mb; see /5/). SAGE II evidently contains a slightly smaller (10-20%) uncertainty in the reference height than SAGE I, and at altitudes above 2 mb, measurement noise is less for SAGE II (by roughly a factor of 5 in variance at 0.4 mb).

These uncertainties may be compared against the profile error bars supplied on the data tapes. Those error bars, however, refer to 1 km vertical resolution. In comparing the results in Figure 3, the "theoretical" profile error variances need to be reduced by a factor of 2 because we are retaining only 4 waves (8 out of 15 degrees of freedom) and, at heights above 2 mb, they should also be reduced by a factor of 5 to reflect the vertical averaging over 5 km. Note that at lower altitudes, where the reference height uncertainty dominates, vertical averaging should not affect the error bars. The smaller measurement noise for SAGE II is reflected in the error variances at 0.4 mb and after a reduction by a factor of ten these error variances are slightly larger than the measured tropical variances. Since the error bars are derived assuming a vertical correlation between measurements of 1 km, this suggests that this correlation distance is being over-estimated. At lower altitudes, the reference height uncertainty in the tropics is evidently less than 0.25 km (perhaps only 0.15 km). It is not obvious how to extrapolate this uncertainty to middle latitudes because of the more intense large scale wave activity at mid-latitudes which might increase the reference height uncertainty there. Overall, the error variances provide a conservative estimate of the observed ozone uncertainties. Note that at 50 and 70 mb the reference height uncertainty results in large variances because of the large vertical ozone gradient in the tropics.

Between 0.4 and 30 mb, the combined variability in the 4 waves is 20×10^{-4}. A wavenumber breakdown, given in Table 1, shows that, where the reference height uncertainty dominates, much of this variability is in wave 1 and in the zonal mean. This is probably associated with the dominance of wave 1 variations in temperature and geopotential height which are mapped into reference height uncertainties also in wave 1. In contrast, at 0.4 mb, where measurement errors dominate, the spectrum is fairly white but the substantial variance in the zonal mean may be noted, which suggests that there may be longer term (> 1 day) variations in noise level. Table 1 suggests that ozone wave amplitudes need to exceed 3% in wave 1 and 2% in wave 1-4 to be observable (i.e., the longitudinal variance must exceed approximately 20×10^{-4}).

TABLE 1 Wavenumber breakdown of tropical variances (20°N-20°S)

(a) Ozone ($\overline{\text{ratio to zonal mean}^2}$) (SAGE II March/April 1985)

mb	Wave 1	Wave 2	Wave 3	Wave 4	Variance of zonal mean
30.0	11.0	2.0	1.0	1.0	13.0
5.0	6.0	4.0	2.0	1.0	3.0
0.4	8.0	5.0	3.0	4.0	37.0

(b) Temperature ($\overline{°K^2}$) (Coincident with SAGE II, April 1985)

mb	Wave 1	Wave 2	Wave 3	Wave 4	Variance of zonal mean
30.0	0.14	0.14	0.09	0.09	0.18
5.0	0.61	0.24	0.08	0.17	0.01
0.4	0.90	0.41	0.13	0.29	0.71

MID-LATITUDE OZONE VARIATIONS

Table 2 shows considerable ozone activity in excess of the measurement noise levels at mid-latitudes in March and April. A significant minimum in ozone activity is found at 30 mb, a tendency which is also found in our 6 wave numerical model of the atmosphere /4/. Similar levels of activity are found in the 2 SAGE observations and in the model. Note, however, that the model exhibits a minimum of activity at 5 mb but is absent in the observations. In the model this is associated with different irregularity production mechanisms operating at 2 and 10 mb and is related to a correlation between ozone and temperature of approximately zero at 5 mb. If this correlation is examined in the SAGE observations (see Table 3), the transition between heights at which ozone variations are in phase with temperature variations and heights where the variations are out of phase seems to vary in the atmosphere. Note that if variations between latitude bins are included (see Table 3), the SAGE I and SAGE II results are not significantly different at most levels. The brackets at 0.4 mb for SAGE II (in Table 3) reflect the lack of activity there in April 1985 and thus the probable dominance of measurement noise at that time.

Apart from the variability from day to day in the real atmosphere which could be smoothing out the ozone variance minimum at approximately 5 mb, the correspondence between observed and modeled ozone-temperature covariances is acceptable. Additional studies should indicate whether it is possible to use measured factors similar to those given in Table 3 to derive conclusions about atmospheric chemistry and transport.

TABLE 2 Variances of ozone at mid-latitudes (40-70°N) expressed as a ratio to the zonal mean squared x 10^4.

Pressure level (mb)	SAGE II March/April 1985	SAGE I March/April 1979	6 wave model
50	227	126	1000
30	34	31	120
10	66	44	155
5	115	58	55
2	190	79	170
1	70	166	190

TABLE 3 Ratio of amplitudes of longitudinal ozone variations to the amplitudes of correlated temperature variations (= $r\sigma_{O3}/\sigma_T$) at mid-latitudes of the Northern Hemisphere.

Pressure level (mb)	SAGE II (April, 1985)	SAGE I (March/April, 1979)	3D (6 wave) model (April)
50.0	6.8 ± 4.4	3.6 ± 0.5	4.2
30.0	4.0 ± 0.5	2.5 ± 0.2	2.6
10.0	0.5 ± 1.7	2.8 ± 0.4	2.1
5.0	-2.0 ± 1.6	2.6 ± 1.3	-0.3
2.0	-3.8 ± 0.9	-1.8 ± 2.5	-3.7
1.0	-2.4 ± 0.3	-4.3 ± 1.5	-5.6
0.4	(-0.3 ± 1.1)	-4.5 ± 0.2	-3.6

ZONAL MEANS OF NO_2

Figures 4 and 5 show the zonal means for SAGE II NO_2 versus those for SAGE I (version 2). One way to discuss the differing sunrise and sunset comparisons is to consider the mean of sunrise and sunset values together with the sunset/sunrise ratio. Figure 4 shows that at mid-latitudes at 5 and 10 mb (the mixing ratio peak where NO_2 concentrations are measured most precisely), SAGE II measurements are 40% larger than those for SAGE I; however, in the tropics there is excellent agreement between the SAGE I and SAGE II measurements (Figure 5). Furthermore, at mid-latitudes the SAGE II measurements lie within the range of balloon measurements and, more particularly, are in excellent agreement with the LIMS measurements at 32°N at 1:30 pm for May 1979. Based on Chu and McCormick /3/, NO_2 mixing ratios in May should be similar to those in March and April except at 5 mb where they are expected to be approximately 10% larger. The discussion of the diurnal variation of NO_2 by Roscoe /8/ indicates that mixing ratios at 1:30 pm should be approximately a factor of 2 smaller than this average at 2 mb but equal to the average at 5, 10 and 30 mb. Given that all these measurement techniques have an accuracy of approximately 20%, we consider that Figures 4 and 5 constitute validation of the SAGE II NO_2 measurements to this accuracy.

The sunset/sunrise ratios shown in Table 4, on the other hand, are not in such good agreement. The SAGE I ratios have been found to be in good agreement with theory /3/ but the SAGE II ratios are considerably smaller. Part of this problem in the SAGE II measurements has already been identified as an error in the reference altitudes for sunrise measurements (sunrise ozone measurements, for example, are 4-7% larger than sunset measurements at all levels). Correction of this problem may produce agreement with Sage I values at 30, 10 and 5 mb leaving a problem at 2 mb only.

TABLE 4 NO_2 Sunset to Sunrise Ratios

Pressure level mb	SAGE II 30-40°N Mar/Apr 1985	SAGE II 50°N Mar 31, 1985	SAGE I 30-40°N Mar/Apr 1979	SAGE I 35°N Mar 12, 1979
30	1.00	1.04	1.19	1.03
10	1.24	1.31	1.62	1.66
5	1.33	1.28	1.67	1.80
2	0.44	0.54	0.91	1.25

TROPICAL VARIANCES OF NO_2

SAGE measurements of NO_2 are expected to be both less accurate and less Precise than SAGE O_3 measurements. Figure 6 contains a comparison of the tropical NO_2 variances with the profile error variances given on the data tapes. The tropical variances indicate that the SAGE II measurements of NO_2 are 3 or 4 times more precise than those of SAGE I. The error variances suggest that they are just twice as precise at 5 and 10 mb but we are currently unsure how to relate these error variances to the measured variances. Figure 6 suggests that it is unlikely that longitudinal variations in NO_2 could have been observed by SAGE I but that such variations should be observable between 1 and 10 mb in the SAGE II measurements. In contrast to the ozone measurements, the tropical variance appears to be roughly independent of wavenumber. We conclude that 0.3 ppbv variations (3% of the zonal mean) should be observable at 5 mb (and 10 mb) and 2 ppbv fluctuations (4% of the zonal mean) should be observable at 2 mb. This suggests that the precision of the SAGE II NO_2 measurements is excellent.

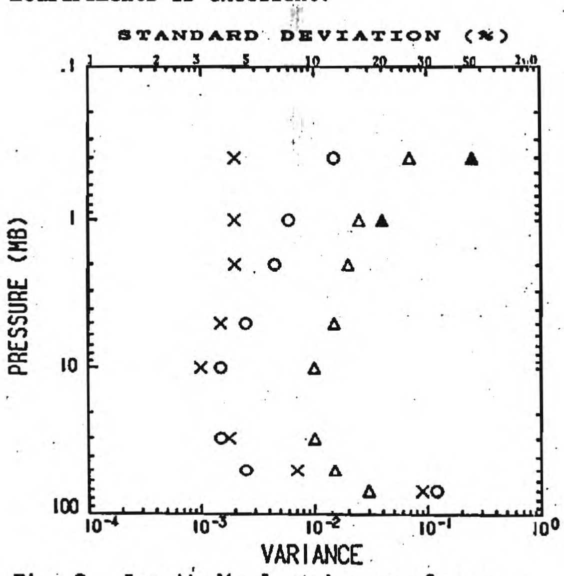

Fig. 3. Longitudinal variances of ozone (normalized by the zonal-mean squared) and standard deviations (as % of the zonal mean) in the tropics for several days in March and April. SAGE I values are denoted by O's, SAGE II values by X's. Also shown are the measurement error bars given on the data tapes for SAGE II (Δ) and, where different, for SAGE I (▲).

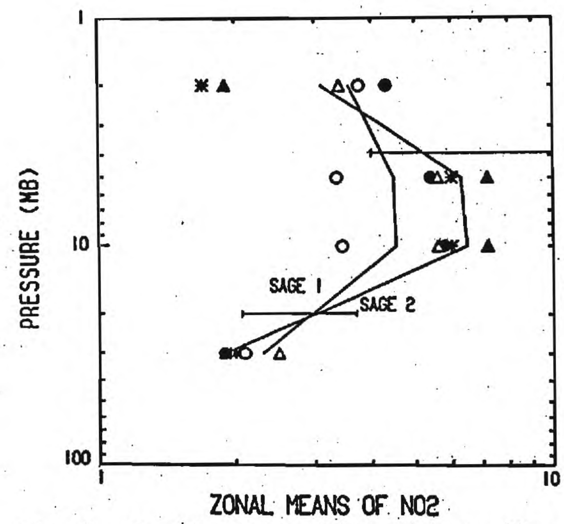

Fig. 4. Zonally-averaged NO_2 mixing ratios (ppbv) at 30-40°N for several days in March and April. The horizontal lines indicate the range of climatological measurements by balloons in this latitude range. LIMS measurements in May 1979 at 32°N at 1:30 pm (local time) are denoted by an "*" (from /9/).

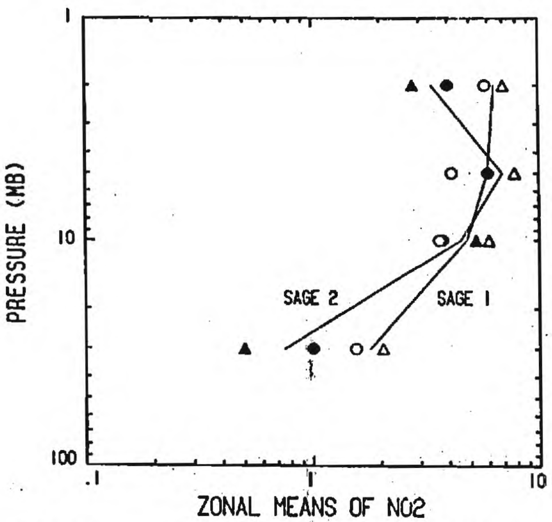

Fig. 5. Zonally-averaged NO_2 mixing ratios (ppbv) in the tropics for several days in March and April. The continuous profiles join the averages of the sunset and sunrise values.

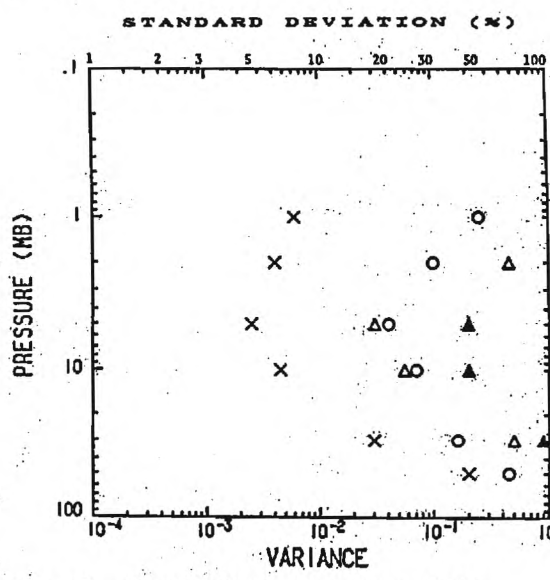

Fig. 6. Longitudinal variances of NO_2 (normalized by the zonal-mean squared) and standard deviations (as % of the zonal mean) in the tropics for several days in March and April. SAGE I values are denoted by O's, SAGE II values by X's. Also shown are the measurement error bars given on the data tapes for SAGE II (Δ) and, where different, for SAGE I (▲).

CONCLUSIONS

The preliminary version of the SAGE II ozone data has been compared against SAGE I data and SBUV data for the same months in 1979. The comparison shows agreement within 15% for all three data sets except at two locations. At 0.4 mb the SBUV measurements are approximately 25% smaller corresponding presumably to the diurnal variation of ozone there. In the tropics above 5 mb, the SAGE I (version 2) results which have been corrected for temperature biases in the NOAA data are in significantly better agreement with the SBUV and SAGE II data than was true for the SAGE I (version 1) results.

The longitudinal variations in the SAGE II measurements in the tropics indicate that the SAGE II ozone measurements are more precise than the SAGE 1 ozone measurements. This feature is reflected in the profile error bars provided with the data. These error bars are nominally for 1 km resolution and need to be adjusted above 2 mb by $\sqrt{n}$ for a resolution of n km. The tropical variances indicate that the precision of the measurements is being somewhat underestimated and is dependent on the planetary wavenumber. Between 0.4 and 30 mb, variations having a magnitude of 3% of the zonal mean in wave 1 and 2% in waves 2-4 should be observable in the SAGE II ozone data. Mid-latitude variations exceeding these magnitudes roughly exhibit the expected (i.e., modeled) variation with altitude and covariances with temperature.

The preliminary SAGE II NO_2 sunset-sunrise average measurements exhibit agreement with SAGE I NO_2 measurements at tropical and mid-latitudes for the same months in 1979 to better than 20%. Even better agreement is found with the May, 1979 mid-latitude LIMS measurements for 1:30 pm local time at 30, 10, and 5 mb. SAGE II NO_2 sunset-sunrise ratios are found to be too small but these may be corrected when the sunrise retrievals are adjusted for reference altitude errors. The tropical variances of NO_2 indicate that the SAGE II NO_2 measurements are substantially more precise than those of SAGE I and that planetary wave activity exceeding 3% of the zonal mean may be observable at the NO_2 mixing ratio peak (5-10 mb).

ACKNOWLEDGEMENT

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REFERENCES

1. Bass, A.M. and R.J. Paur, UV absorption cross sections for ozone: The temperature dependence, EOS Trans. AGU, 63, 331, 1982.

2. Chu, W.P. and M.P. McCormick, Inversion of stratospheric aerosol and gaseous constituents from spacecraft, solar extinction data in the 0.38-1.0 μm wavelength region, Appl. Opt., 18, 1404-1413, 1979.

3. Chu, W.P., and M.P. McCormick, SAGE observations of stratospheric nitrogen dioxide, J. Geophys. Res., 91, 5465-5476, 1986.

4. Cunnold, D.M., F.N. Alyea, and R.G. Prinn, Preliminary calculations concerning the maintenance of the zonal mean ozone distribution in the Northern Hemisphere, Pageoph, 118, 329-354, 1980.

5. Cunnold, D.M., M.C. Pitts and C.R. Trepte, An intercomparison of SAGE and SBUV ozone observations for March and April 1979, J. Geophys. Res., 89, 5249-5262, 1984.

6. McCormick, M.P., T.J. Swisler, E. Hilsenrath, A.J. Krueger, and M.T. Osborn, Satellite and correlative measurements of stratospheric ozone: Comparison of measurements made by SAGE, ECC balloons, chemiluminescent and optical rocketsondes, J. Geophys. Res., 89, 5315-5320, 1984.

7. Prather, M.J., Ozone in the upper stratosphere and mesosphere, J. Geophys. Res., 86, 5325-5338, 1981.

8. Roscoe, H.K., B.K. Kerridge, L.J. Gray, R.J. Wells, and J.A. Pyle, Simultaneous measurements of stratospheric NO and NO_2 and their comparison with model predictions, J. Geophys. Res., 91, 5405-5420, 1986.

9. Russell, J.M., III, J.C. Gille, E.E. Remsberg, L.L. Gordley, P.L. Bailey, S.R. Drayson, H. Fischer, A. Girard, J.E. Harries, and W.F.J. Evans, Validation of nitrogen dioxide results measured by the Limb Infrared Monitor of the Stratosphere (LIMS) experiment on Nimbus 7, J. Geophys. Res., 89, 5099-5108, 1984.