Ozone climatological profiles for satellite retrieval algorithms

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[1] A new altitude-dependent ozone climatology has been produced for use with the version 8 Total Ozone Mapping Spectrometer (TOMS) and Solar Backscatter Ultraviolet retrieval algorithms. The climatology consists of monthly average ozone profiles for 10° latitude zones covering altitudes from 0 to 60 km (in Z^* pressure altitude coordinates). The climatology was formed by combining data from Stratospheric Aerosol and Gas Experiment II (SAGE II; 1988–2001) or Microwave Limb Sounder (MLS; 1991–1999) with data from balloon sondes (1988–2002). Ozone below 10 km is based on balloon sondes, whereas ozone at 19 km and above is based on SAGE II measurements. When SAGE data are not available (at high latitudes), MLS data are used. The ozone climatology in the southern hemisphere and tropics has been greatly improved in recent years by the addition of a large number of balloon sonde measurements made under the Southern Hemisphere Additional Ozonesondes program. The new climatology better represents the seasonal behavior of ozone in the troposphere, including the known hemispheric asymmetry, and in the upper stratosphere. A modification of this climatology was used for the TOMS version 8 retrieval that includes total ozone dependence, which is important in the lower stratosphere. Comparisons of TOMS ozone with ground stations show improved accuracy over previous TOMS retrievals due in part to the new climatology.

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1. Introduction

[2] Ozone climatologies are used for many purposes, and no single climatology will be optimum for all uses. A climatology developed by *Fortuin and Kelder* [1998] based on a combination of balloon and Solar Backscatter Ultraviolet (SBUV) data was, they note, intended mainly for climate simulations with general circulation models. *McPeters et al.* [1997] developed a climatology using SBUV data specifically for estimating the amount of ozone above balloon burst altitude so that total column ozone could be calculated from electrochemical concentration cell sonde measurements. Recently, *Lamsal et al.* [2004] developed a climatology to be used as an a priori for the Sciamachy optimal retrieval algorithm that has also been used in differential optical absorption spectroscopy retrievals. This climatology uses total column ozone to parameterize the profile shape.

[3] Satellite retrieval algorithms for backscattered ultraviolet (BUV) measurements have in the past used a relatively simple ozone climatology. The Total Ozone Mapping Spectrometer (TOMS) retrievals in version 7 used a total ozone-dependent climatology consisting of 26 profiles with ozone in Umkehr layers (~5 km) covering low-latitude, midlatitude, and high-latitude zones. That climatology and results of a study of the errors due to profile shape at high latitudes are discussed by *Wellemeyer et al.* [1997]. While such a climatology is adequate for accounting for stratospheric ozone profile shape changes, it has a relatively fixed tropospheric ozone climatology since tropospheric ozone does not correlate well with total column ozone. This has become a limitation on accuracy since tropospheric ozone variability has proven to be one of the largest sources of error in the current algorithms. These errors are discussed by *Bhartia* [2002] in the OMI Algorithm Theoretical Basis Document (ATBD).

[4] Ozone retrieval algorithms based on the optimal retrieval method [*Rodgers*, 2000] benefit from an accurate climatology in altitude regions where the measurement loses sensitivity, for example, in the lowest 10 km of the atmosphere for a TOMS total column ozone retrieval. The climatology also supplies information to such retrievals in the form of higher vertical resolution information than the retrieval itself can achieve. An SBUV retrieval derives a fairly accurate measure of the total amount of ozone between the ground and about 20 km, but has little information on how it is distributed. The climatology determines the distribution of ozone within this region in an SBUV retrieval.

[5] A good climatology can also be used when detailed day-to-day information is not necessary, such as in the

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calculation of average UV input to biological systems or calculations of average photolysis rates in atmospheric model calculations. The climatology described in this paper was originally developed to serve as a reference for comparison of stratospheric models used in environmental assessments of ozone response to chlorofluorocarbons, aircraft emissions, and other climate–chemistry interactions, a comparison referred to as Models and Measurements II [*Park et al.*, 1999]. The climatology was further developed to the form described in this paper for use in the version 8 TOMS and SBUV algorithms.

2. Data for the Climatology

[6] For the purposes of ozone retrieval using the BUV technique, a climatology is needed with four attributes: coverage from the surface to approximately 60 km, good vertical resolution, good latitudinal coverage, and seasonal time dependence.

[7] The BUV profile retrieval gives information on the ozone vertical distribution from approximately 30 to 1 hPa [*Bhartia et al.*, 1996], whereas the total column retrieval (using longer wavelengths) begins to lose sensitivity below about 10 km and has little sensitivity to ozone in the lowest 5 km of the atmosphere because of lack of penetration of backscattered sunlight in the ultraviolet. The difference between total column ozone and the integrated profile above the 30 hPa level is a fairly accurate estimate of ozone in the troposphere and lower stratosphere, but there is little information on how ozone is distributed in the troposphere. As *Bhartia* [2002] shows in the OMI ATBD, below the ozone maximum, "...the Rayleigh scattered radiation emanates... over a fairly broad region of the atmosphere (roughly 16 km wide at the half maximum point)." A climatology can be used as the a priori to supply a good guess as to the distribution. Vertical resolution in the range of 1–3 km is needed in the climatology to accurately represent the strong gradient in ozone in the upper troposphere–lower stratosphere region.

[8] In order to better account for tropospheric ozone variation, a latitudinal resolution of about 10° is desired. In the previous TOMS climatology, tropospheric ozone was identical in the two hemispheres, but ozone in the troposphere has been shown to be lower on average in the southern hemisphere than in the northern hemisphere [*Logan*, 1999]. This is included in the Labow, Logan, McPeters (LLM) climatology. A temporal resolution of about 1 month allows the a priori to track seasonal changes.

[9] It is also important for a climatology that will be used as an a priori to be representative of the period for which it will be applied. Global ozone decreased significantly during the 1980s [*WMO*, 1992, 1995]. While the decrease was not large other than in the region of the Antarctic ozone hole, only about 5% at midlatitudes and high latitudes, data for this climatology were averaged over the period 1988 through 2002 in order to better represent profile shapes in the current period. Since full recovery is predicted to take 50 years or more [*WMO*, 2003], this climatology should be appropriate for many years.

[10] No single instrument produces data that can meet all these criteria for creating a climatology. This climatology was created by combining sonde data for the troposphere and lower stratosphere with Stratospheric Aerosol and Gas Experiment (SAGE) and Microwave Limb Sounder (MLS) data for the stratosphere. Sondes are the only feasible source of ozone profile data for the lower troposphere since satellite instruments do not reliably measure ozone below 10 km. However, coverage is a serious problem with sonde data. In some 10° latitude zones, there is only a single sonde station to represent the entire zone. Fortunately in the tropics, where this could be a problem because of the well-known wave 1 structure in tropospheric ozone, coverage is much better because of the augmented sonde data from the Southern Hemisphere Additional Ozonesondes (SHADOZ) network.

[11] The SAGE II on the Earth Radiation Budget Satellite [*McCormick et al.*, 1989] is a good source for the stratospheric ozone climatology because of its 20-year record of observations, near global coverage (except in polar regions), and good vertical resolution (~1 km). Data from the MLS on the Upper Atmosphere Research Satellite do not have the vertical resolution of SAGE, but they have been used to fill in stratospheric ozone in the polar regions where SAGE has no coverage. While SBUV has excellent coverage, it has not been used because of its limited vertical resolution, no better than 6 km, decreasing to about 15-km resolution in the lower stratosphere and troposphere.

[12] A total of 23,400 ozone sonde profiles from 36 stations were averaged to create a climatology of the lower atmosphere—from the surface to 30-km altitude. Table 1 gives details on the stations that were used for each 10° latitude zone from 90°S to 90°N. Note that for the zone from 80°S to 90°S, there are no data for levels below 2 km because the South Pole station is located on the Polar Plateau, which is at more than 2-km elevation. Stations in each band are equally weighted to introduce as little longitudinal bias as possible. For example, Resolute and Ny Alesund in the 70°N to 80°N zone are given equal weight in the December zonal average even though Ny Alesund has three times as many sondes. There is an additional human factor problem in the Antarctic in the September–November time period in that balloons are more likely to be launched when things are "interesting," which can lead to ozone hole conditions being oversampled.

[13] Version 6.1 SAGE II data [*McCormick et al.*, 1989; *Cunnold et al.*, 2000] were used to create the monthly average stratospheric climatology from 20 to 60 km between 50°S and 50°N. Since SAGE measures ozone number density versus altitude, the conversion to a pressure scale introduces some uncertainty. A comparison of SAGE II with SBUV [*McPeters et al.*, 1994] documented this uncertainty but showed agreement generally within about 5%. Above 70° latitude, MLS version 5 data [*Waters et al.*, 1999] were used because of lack of coverage by SAGE. Between 50° and 70° latitudes, SAGE data are used for months when sampling was good—from March to September in the northern hemisphere and October to March in the southern hemisphere. Otherwise, MLS data are used. Since MLS measures only up to 83° maximum latitude, the 80–90° zones may be slightly biased.

Table 1. ECC Sonde Stations Used in Climatology Including Total Number of Sondes in Average

	Station	Latitude	Longitude	Number	Time Period
80–90°N	Alert	82.5	−6	787	1988–2002
70–80°N	Ny Alesund	78.9	12	1190	1990–2002
	Resolute	74.7	−10	566	1988–2002
60–70°N	Sodankyla	67.4	27	894	1988–2001
	Churchill	58.7	−94	659	1988–2002
50–60°N	Edmonton	53.5	−114	664	1988–2002
	Goose Bay	53.3	−60	708	1988–2002
	Lindenberg	52.2	14	908	1988–2002
	Uccle	50.8	4	1736	1988–2001
40–50°N	Hohenpeissenberg	47.8	11	1818	1988–2002
	Payerne	46.8	7	2023	1988–2002
	Sapporo	43.0	141	518	1988–2001
30–40°N	Boulder	40.0	−105	571	1988–2002
	Wallops	37.9	−75	577	1988–2002
	Tateno	36.0	140	755	1988–2002
20–30°N	Kagoshima	31.6	131	501	1988–2002
	Naha	26.2	128	471	1989–2002
	Hilo	19.7	−155	629	1988–2002
10–20°N	Hilo	19.7	−155	629	1988–2002
0–10°N	Paramaribo	5.8	−55	175	1999–2002
0–10°S	Nairobi	−1.3	37	290	1996–2002
	Braz/Ascen	−4.3	15	416	1990–1992, 1997–2002
	Natal	−5.8	−35	498	1978–1992, 1996–2002
	Galapagos	−0.9	−91	237	1998–2002
	Java	−7.5	112	138	1998–2002
10–20°S	Samoa	−14.2	−171	415	1986–1990, 1996–2002
	Tahiti/Fiji	−17.5	−149	363	1995–2002
	Reunion	−20.0	55	223	1992–2002
20–30°S	Irene	−25.2	28	276	1990–1993, 1998–2002
30–40°S	Laverton	−37.9	145	524	1988–2002
40–50°S	Lauder	−45.0	170	979	1988–2002
50–60°S	Macquarie	−54.5	159	300	1994–2002
60–70°S	Marambio	−64.2	−57	345	1988–1998
	Syowa	−69.4	40	752	1988–2002
70–80°S	For/Neumayer	−70.8	−8	990	1988–2002
	McMurdo	−77.9	167	420	1988–1998
80–90°S	S. Pole	−89.9	−25	922	1988–2002

[14] The altitude variable used here is Z^*, a parameter frequently used in comparisons of atmospheric chemistry models. Z^*, sometimes called pressure altitude, is in units of kilometers but really should be considered a pressure variable. It is defined as:

$$Z^* = 16 \times \log\left(\frac{1013}{P}\right)$$

where P is pressure in units of hPa. In an isothermal atmosphere, Z^* would correspond closely to altitude.

[15] The monthly average data from SAGE or MLS were merged with data from sondes to create the climatological profiles. As shown in Figure 1 (left panel), SAGE and sonde data were merged over the Z^* layers 10–18 km (240–76 hPa). It is important to use the satellite data to as low an altitude as possible because of their more uniform longitudinal sampling. In a few zones, near 55°N in March or near 65°S in October, for example, the sonde data available were unrepresentative of the zone and produced erroneous total column ozone when used for the lower stratosphere. The MLS data can be considered very reliable down to the 20-hPa level, but lose accuracy by the 100-hPa level [*Waters et al.*, 1999]. Consequently, for MLS, the merge is done between Z^* layers 20 and 28 km (50–20 hPa) as shown in Figure 1 (right panel).

3. Ozone Morphology

[16] The new climatology, hereafter referred to as the LLM climatology, captures the average behavior of ozone as a function of altitude, latitude, and season. Figure 2 shows the annual average ozone in partial pressure for each 10° zone for the southern (left) and northern (right) hemispheres. The variation with latitude is, as expected, very systematic, with the strongest, highest altitude peak being in the tropics, whereas the high-latitude profiles have more ozone at lower altitudes. The striking north–south asymmetry seen at high latitudes is likely due in part to the greater stability of the polar vortex in the southern hemisphere.

[17] Figure 3 shows ozone variation with month for two zones—40–50°N and 70–80°S. Note the systematic change in profile shape in the 40–50°N zone from late winter to late summer as total ozone decreases, and the factor-of-3 change in ozone near 12 km. The curve for October at 75°S shows the results of ozone destruction in the Antarctic ozone hole. This climatology is based on averaging data for years 1988–2002, a period during which the ozone hole was large most years. This represents an

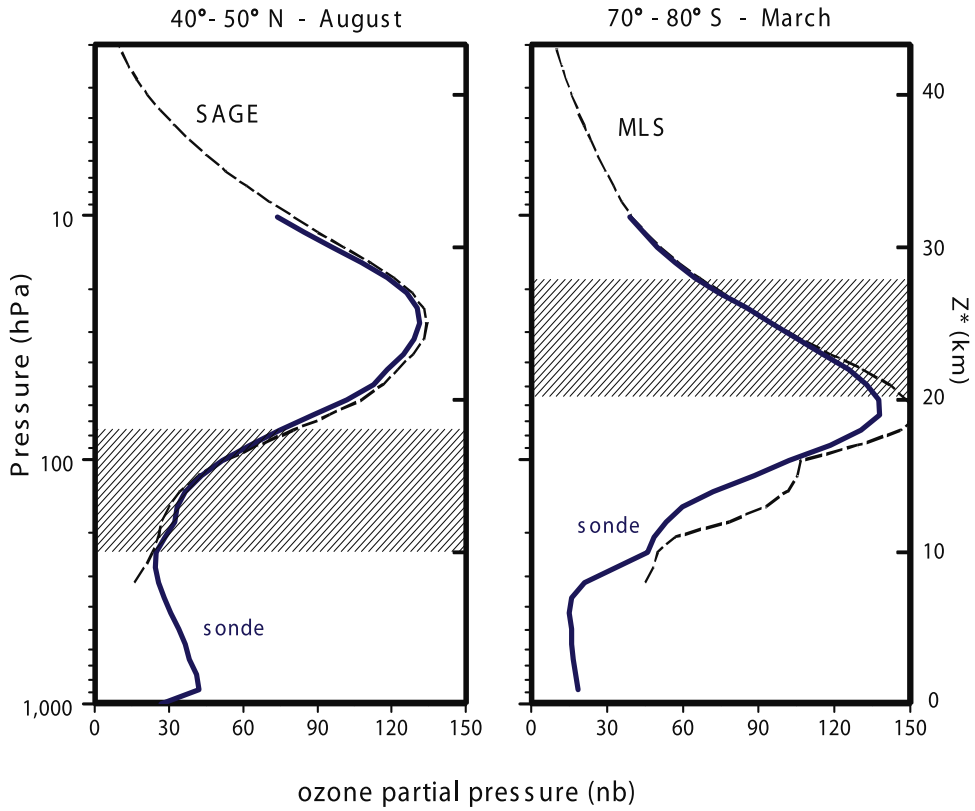

Figure 1. Zonal average sonde data are merged into the zonal average SAGE data between 10- and 18-km altitude region (example on left). At high latitudes, where MLS data must be used, the merge is done in the 20- to 28-km region (right example).

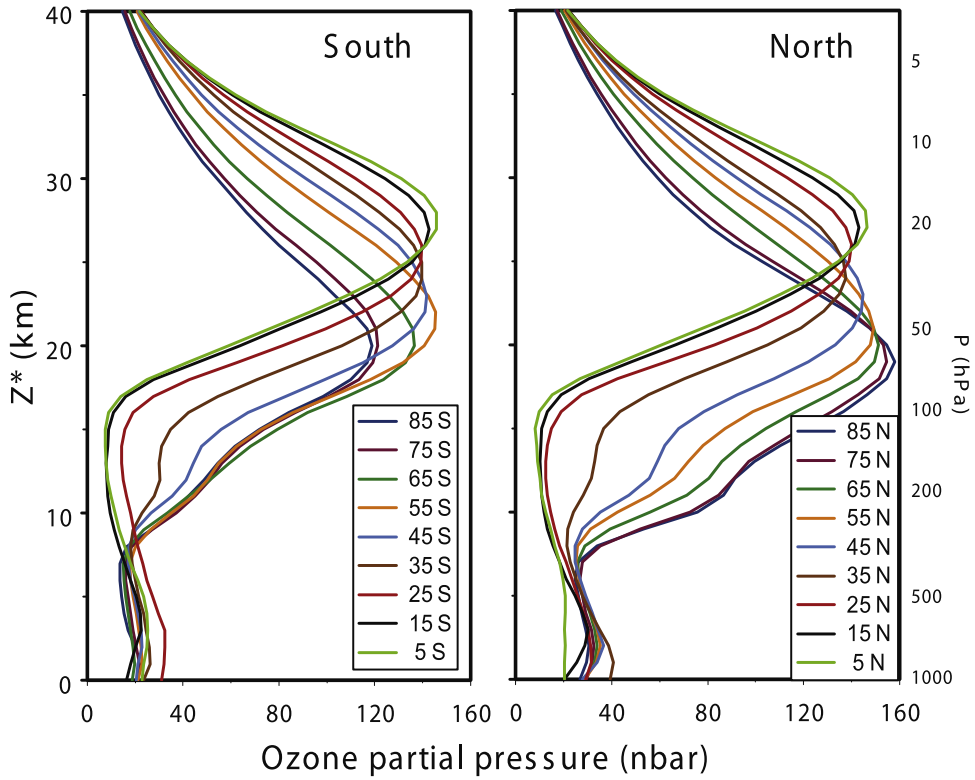

Figure 2. A comparison of the annual average ozone climatological profiles for 10° zones for the southern and northern hemispheres.

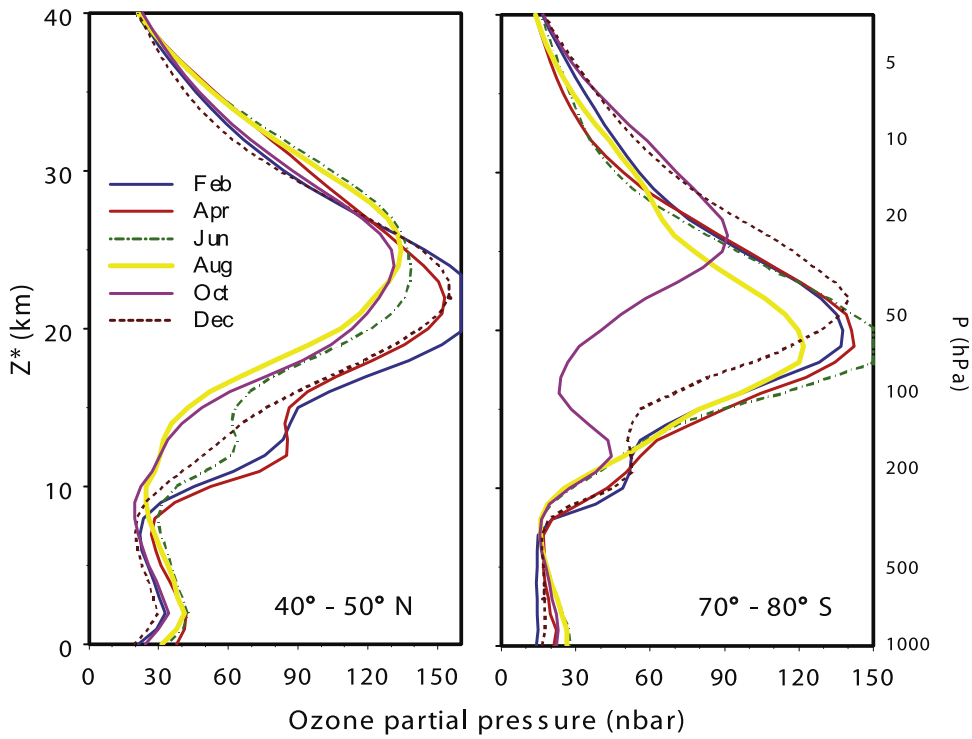

Figure 3. Sample profiles of ozone partial pressure plotted for different months for the 40–50°N zone (left) and for the 70–80°S zone (right).

extreme case where poor sampling by the sonde stations is a problem. Neumayer station (71°S, 8°W) tends to be outside the vortex in October, whereas McMurdo station (78°S, 167°E) is more likely to be inside the vortex. The average of the two to describe zonal ozone below 20 km is likely to be somewhat in error, as will be seen later in the total ozone comparison.

[18] The climatological standard deviations are much as expected, showing low variance in the stratosphere and high variance in the troposphere. At altitudes above 20 km, the standard deviations are generally less than 10% at low latitudes to midlatitudes, increasing to almost 15% at high latitudes. In the troposphere, the standard deviations increase to 20% to as much as 50% at midlatitudes and high latitudes, with the highest variance being seen in the 200- to 400-hPa region.

[19] Perhaps the most significant improvement for the TOMS and SBUV ozone retrievals is the inclusion of more realistic tropospheric ozone. Because the BUV ozone retrieval loses sensitivity in the lowest 10 km of the troposphere, an accurate climatology is particularly important in this region [*Bhartia*, 2002]. Figure 4 shows that annual average ozone in the lower troposphere is lower in the southern hemisphere than in the northern hemisphere. Near 75° latitude, ozone below 15 km is almost 75% higher in the northern hemisphere than in the south. However, this is seasonally dependent, varying from 30% larger in the fall to as much as three times larger in late spring when the Antarctic ozone hole is present. Near 45° latitude, ozone below 15 km is 36% larger in the north than in the south, varying from 15% larger in the winter to 70% larger in the summer. The blue squares indicate the ozone in the troposphere and lower stratosphere used in the previous V7 TOMS algorithm.

[20] Below 30° latitude, there is little difference in tropospheric ozone between north and south. However, *Ziemke et al.* [1996] showed that, while there is little variation of stratospheric ozone with longitude in the tropics, there is a strong variation of tropospheric ozone with longitude, the well-known wave 1 variation of tropical ozone. The variation is about 25 DU amplitude with maximum tropospheric ozone near 0° longitude and minimum near 180°. In the interest of simplicity, we have chosen not to include this longitude variation in the climatology, but the user could account for this variation to first order by applying a simple harmonic function to tropospheric ozone in the tropics.

4. Comparisons

[21] To show that the new climatology accurately represents the atmosphere, integrated total column ozone from the climatology each month is compared with zonal average ozone (version 8) measured by TOMS instruments for the period 1988–2002. As shown in Figure 5, the difference exceeds 4% in only a few areas. Differences greater than 4% are seen mostly at high latitudes and are likely due to the sonde sampling problem noted earlier. MLS measurements, which must be used at high latitudes where there are no SAGE measurements, do not retrieve ozone below 20 km, whereas the sonde data used at low altitudes are derived from only one or two stations and cannot accurately represent the ozone variation within these zones. The largest differences are seen in the southern hemisphere above 70° latitude in October and November, where spatial variability is large because of the presence of the ozone hole.

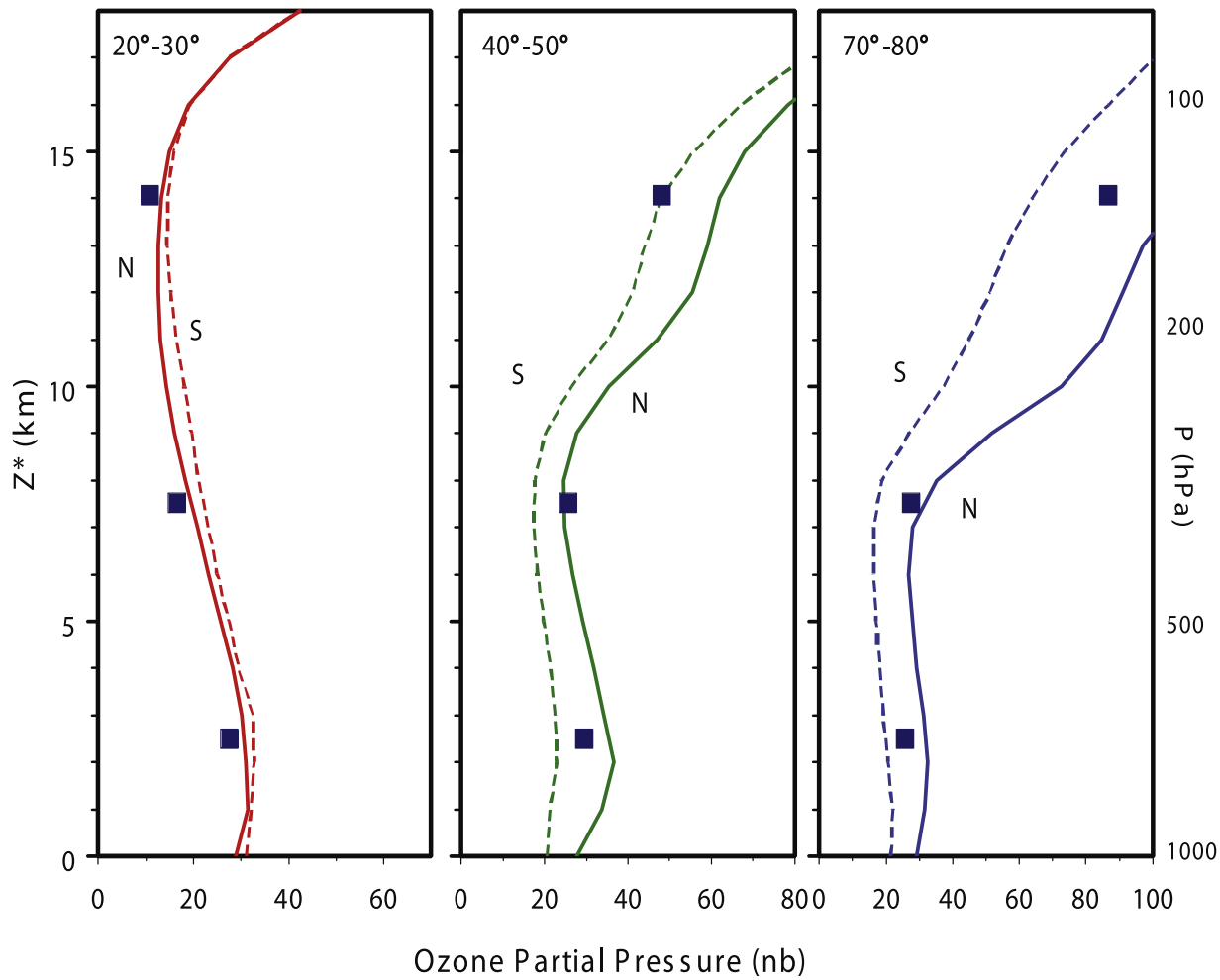

Figure 4. Average tropospheric/lower stratospheric ozone for the northern hemisphere (N) and southern hemisphere (S) compared in three latitude zones. Squares indicate the old climatology used for TOMS V7 processing.

[22] Next, the climatological ozone profiles are compared with profiles from SBUV/2 to assess the consistency of the vertical distribution. NOAA 11 SBUV/2 version 6 (NOAA, National Oceanic and Atmospheric Administration) data from 1989 through 2000 were averaged for comparison. The version 8 SBUV algorithm used this climatology for its a priori, so the comparison was done with version 6 data in order to avoid the appearance of circular reasoning, though the a priori only drives the final profile retrieval in regions where there is no information content in the measurements. Figure 6 shows a height–latitude cross section of ozone mixing ratio from the LLM climatology (upper panel) and the percent difference from NOAA 11 SBUV/2 (bottom panel). Mixing ratio is a useful variable to plot in order to better show ozone variation in the middle and upper stratospheres. The comparison is shown only down to 20 km because the SBUV retrieval is determined mostly by the a priori at lower altitudes. Agreement is mostly within 10% except near 50 km and southward of 70°S latitudes. When Nimbus 7 SBUV profiles were compared with SAGE II profiles [*McPeters et al.*, 1994], agreement was mostly within 10%, so these results might have been expected. The differences at high southern latitudes may result from a difference between SBUV/2 and MLS, which is used at high latitudes, but a similar difference is not seen at high northern latitudes. It is also possible that there is a subtle instrument artifact in SBUV/2 data in the southern hemisphere.

5. Climatology Modification for TOMS

[23] While the LLM climatology was used directly in the SBUV V8 algorithm, a modified climatology was used in the TOMS V8 algorithm. For the TOMS retrievals, it was important to include a total ozone dependence, making this in effect a four-dimensional climatology (latitude–month–altitude–ozone). In this climatology, the altitude variation reverts from Z^* (1-km resolution) to Umkehr layers (5-km resolution) since better vertical resolution is not necessary for the total ozone retrieval. Variation with total ozone is included: 225–325 DU in the tropics, 225–575 DU at midlatitudes, and 125–575 DU at high latitudes, with 50-DU steps in each case. Ozone between 30 and 300 hPa is well correlated with total ozone. By contrast, the mean ozone density above and below these altitudes varies primarily with season and latitude, with no discernable

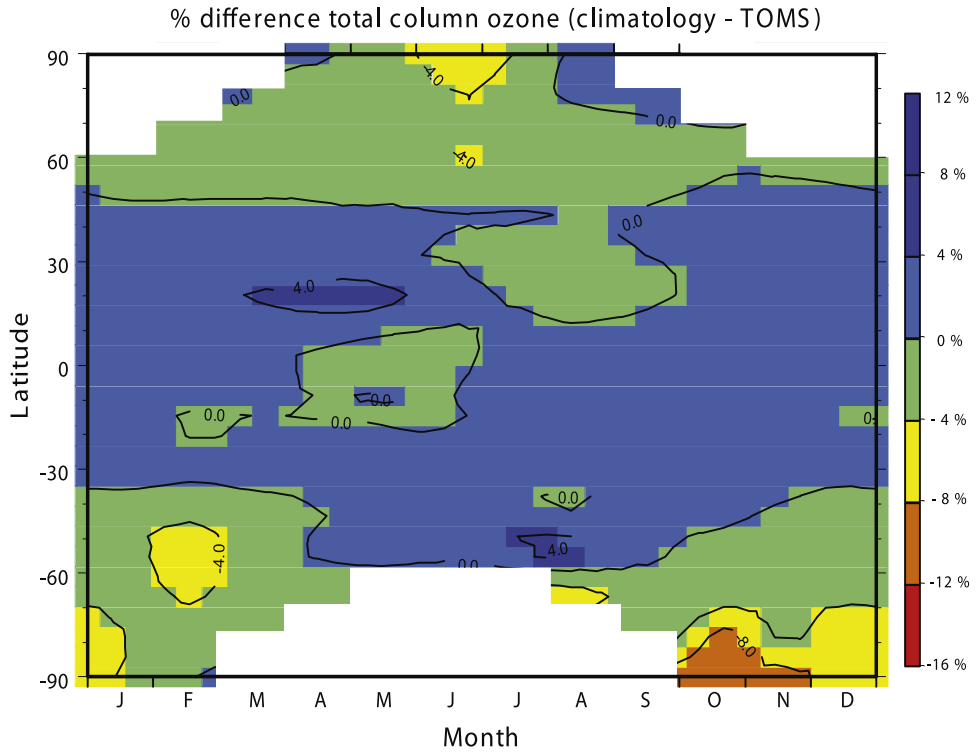

Figure 5. Percent difference between integrated total column ozone from climatology and TOMS total ozone.

correlation with total ozone. In those altitude regions, the TOMS climatology is identical to the LLM climatology. The modified climatology combines the benefit of the old climatology by including total ozone-dependent profile shape changes in the lower stratosphere with the benefits of the LLM climatology in following seasonal ozone changes in the troposphere and upper stratosphere. The SBUV retrieval derives profile shape changes in the lower stratosphere directly, so the total ozone dependence is not needed. A three-dimensional temperature climatology (latitude–month–altitude) was used for the TOMS retrievals.

6. Data Availability

[24] Both the LLM climatology and the TOMS modified climatology are available online. The data can be accessed via anonymous ftp from toms.gsfc.nasa.gov. The data are in the directory pub/LLM_climatology. A copy of the OMI ATBD [*Bhartia*, 2002] is included in the directory for the convenience of the user.

[25] The LLM climatology is available in three forms: an ASCII table of ozone mixing ratios (ppmv), a table of ozone layer amounts (Dobson units), and both variables in an Excel spreadsheet. An ancillary table of mixing ratio standard deviations (ppmv) is also included. The TOMS modified ozone climatology is an ASCII table of ozone layer amounts (Dobson Units) with an accompanying table giving the temperature climatology used.

[26] We have also updated our climatology [*McPeters et al.*, 1997] for estimating the amount of ozone above balloon burst altitude so that total column ozone can be calculated from balloon sonde measurements. The new balloon sonde climatology is the file "new sonde add-on table.txt."

7. Conclusions

[27] The LLM climatology is useful because it captures the significant variations in both stratospheric and tropospheric ozone as a function of latitude and season. This climatology was used to produce the version 8 TOMS and SBUV data sets. Because the new climatology is dependent on latitude (10° zones) and month, it better represents the average state of the atmosphere than the previous climatology that was an annual average for only three zones—low latitude, midlatitude, and high latitude. Better a priori information is particularly important for the lower troposphere because poor penetration of UV leads to lack of sensitivity in the total column ozone retrieval. Also, at high solar zenith angles (greater than 80°), the TOMS total column ozone retrieval becomes profile-shape-dependent. The new climatology comes closer to representing the average state of the atmosphere and should produce more accurate ozone retrievals.

[28] The new climatology agrees with the TOMS total column ozone to within 4% except in the area near the Antarctic ozone hole. The profiles agree with NOAA 11 SBUV/2 profiles in the 20- to 50-km region to within about 10% except near 50 km and at high southern latitudes. In the northern hemisphere, the average difference between TOMS V7 and a network of Dobson and Brewer stations was 1.55%. In version 8, this offset dropped to −0.03% [*Labow et al.*, 2004]. For the southern hemisphere, the improvement was from 2.14% to 0.05%.

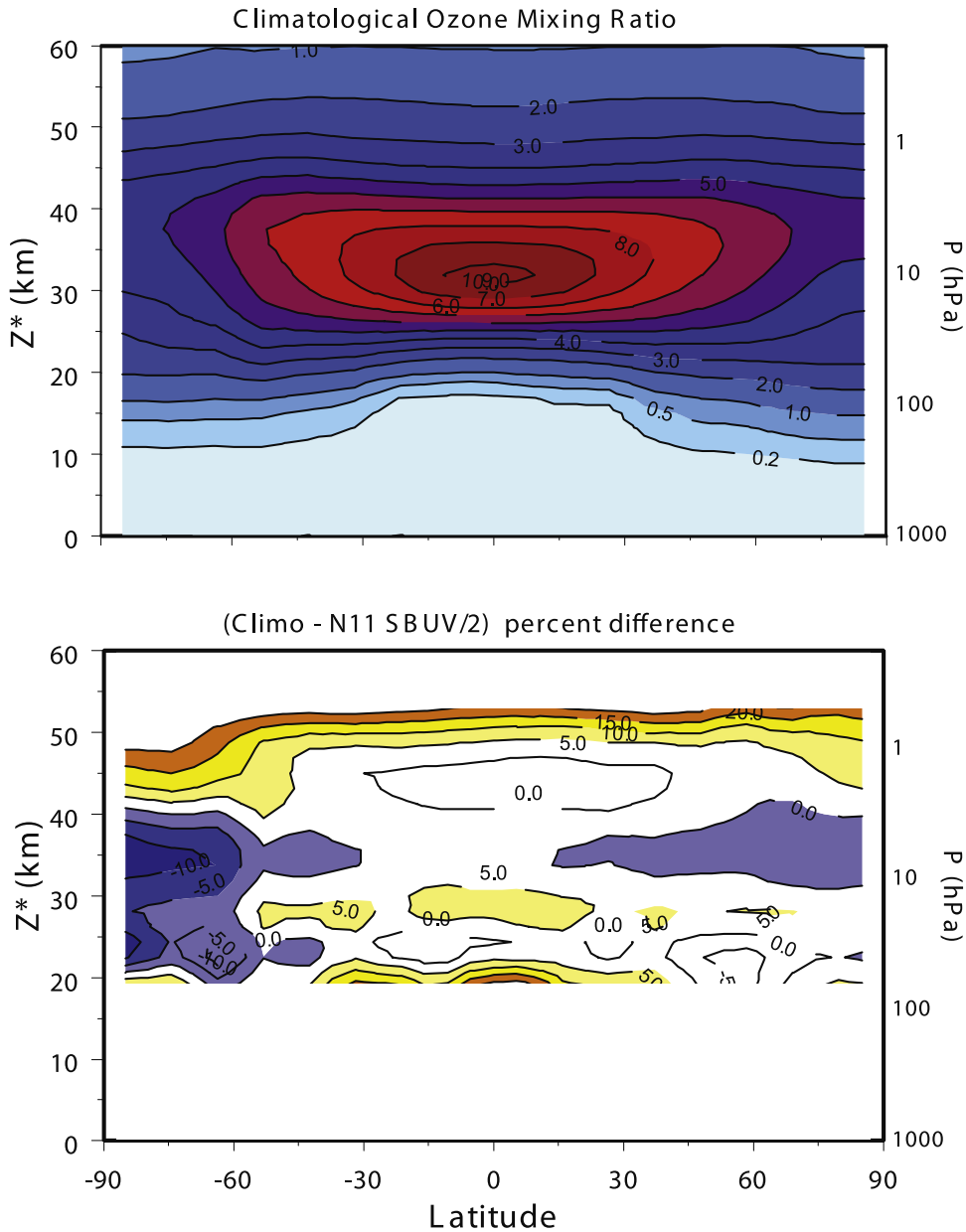

Figure 6. A height–latitude cross section of annual average ozone mixing ratio from the climatology (top) and the percent difference from NOAA 11 SBUV/2 ozone.

Much of this better agreement came from calibration improvements, but the extra half percent improvement in the southern hemisphere might be attributed to the improved climatology. While this is not a large improvement, it is significant if our goal is to achieve 1% accuracy in the ozone retrievals.

[29] **Acknowledgments.** The latest SAGE II data were obtained from the SAGE team at NASA, whereas balloon sonde data were obtained from the WOUDC in Canada and from the SHADOZ team at GSFC. Langley. J. A. Logan was supported by the NASA/ACMAP program.

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