Climatology 2011: an MLS and sonde derived ozone climatology for satellite retrieval algorithms

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Abstract

The ozone climatology used as the a priori for the version 8 Solar Backscatter Ultraviolet (SBUV) retrieval algorithms has been updated. The Microwave Limb Sounder (MLS) instrument on Aura has excellent latitude coverage and measures ozone daily from the upper troposphere to the lower mesosphere. The new climatology consists of monthly average ozone profiles for ten degree latitude zones covering pressure altitudes from 0 to 65 km. The climatology was formed by combining data from Aura MLS (2004-2010) with data from balloon sondes (1988-2010). Ozone below 8 km (below 12 km at high latitudes) is based on balloons sondes, while ozone above 16 km (21 km at high latitudes) is based on MLS measurements. Sonde and MLS data are blended in the transition region. Ozone accuracy in the upper troposphere is greatly improved because of the near uniform coverage by Aura MLS, while the addition of a large number of balloon sonde measurements improves the accuracy in the lower troposphere, in the tropics and southern hemisphere in particular. The addition of MLS data also improves the accuracy of the climatology in the upper stratosphere and lower mesosphere. The revised climatology has been used for the latest reprocessing of SBUV and TOMS satellite ozone data.
1. Introduction

In 2007 McPeters et al. [2007] introduced an ozone climatology designed to be used in satellite retrieval algorithms for backscattered ultraviolet (buv) measurements. We use “buv” to designate the general technique, while a specific instrument such as SBUV is capitalized. This climatology, sometimes designated the LLM climatology, was used in the version 8.0 retrieval of ozone profiles from NASA SBUV and NOAA SBUV/2 instruments. The 2007 climatology was considerably more detailed than the simple climatology that had been used for previous versions of the SBUV and TOMS retrievals [McPeters et al., 1998], which consisted of only 26 profiles with ozone in Umkehr layers (~5 km) covering low, mid, and high latitude zones. While the 1998 climatology accounted quite well for changes in stratospheric ozone profiles, tropospheric ozone information was poor because tropospheric ozone does not correlate well with total column ozone. The 2007 climatology consisted of ozone profiles from the surface to 60 km pressure altitude (1 km steps) as a function of latitude (10° zones) and month. The climatology included an accurate tropospheric ozone variation derived from ozone sondes that was different in the southern hemisphere than in the northern hemisphere. A low vertical resolution version of this same climatology with total ozone dependence added was used for total column ozone retrievals from TOMS and OMI.

The revised climatology presented here was created in support of the upcoming version 8.6 reprocessing. The SBUV team is now engaged in reprocessing data from the entire series of SBUV instruments, from the original Nimbus 4 BUV instrument launched in 1970 through the SBUV/2 instruments on NOAA 16, 17, and 18 which are currently operating. For version 8.6 a consistent calibration has been applied so that a long term multi-instrument time series can be
created. New ozone cross sections, those of Brion et al. [1993] and Malicet et al. [1995] were used, and a new cloud height climatology [Vasilkov et al., 2008] based on OMI retrievals was used. To support this reprocessing the previous climatology needed to be updated.

We have updated the McPeters et al. [2007] climatology by using ozone profile data from the Aura MLS instrument, taking advantage of the excellent latitude coverage of MLS and its improved accuracy at low altitudes over the UARS MLS instrument. Also, nearly double the number of sonde profiles has been included in the new climatology, and several new stations have been added, greatly improving the accuracy of the tropospheric climatology. 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 ten kilometers of the atmosphere for a buv retrieval. The SBUV profile retrieval algorithm derives a very accurate measure of the total amount of ozone between the ground and about 25 km, but has little information on how it is distributed. Because the climatological a priori determines the distribution of the retrieved ozone within this region, improvements in the accuracy of tropospheric ozone in the revised climatology should improve the realism of the retrieved profiles.

2. Data for the Climatology

Ozone retrievals using the backscattered ultraviolet (buv) technique benefit from an ozone climatology that has coverage from the surface to approximately 60 km, vertical resolution good enough to resolve the rapid ozone change in the upper troposphere/lower stratosphere, good latitudinal coverage, and seasonal time dependence. Data from the MLS instrument on the Aura
spacecraft come close to meeting all these criteria. Because the MLS retrieval loses accuracy
below the 215 hPa level [Froidevaux et al., 2008], sonde data are needed to produce the
climatology in the troposphere.

The revised climatology is very similar to the McPeters et al. [2007] climatology but uses
Aura MLS data rather than the SAGE II data used previously. SAGE had good accuracy and
very high vertical resolution, but its orbit produced limited sampling - monthly at most latitudes
and no sampling at all for some months at high latitudes. Moreover, since SAGE was a solar
occultation measurement, its sampling volume was always at sunrise or sunset. This can be a
problem in the upper stratosphere and mesosphere where diurnal variation is significant. Since
Aura is in a sun synchronous orbit with a 1:30 local equator crossing time, the Aura MLS has
nearly complete latitude coverage daily and its measurements are always near noon or near
midnight (except at high latitudes). We use daytime data only for the new climatology as most
appropriate for our solar backscatter ultraviolet retrievals.

The MLS instrument on Aura relies mostly on the 240 GHz band for its ozone retrievals.
This band gives much better accuracy in the troposphere than the UARS MLS instrument.
Comparisons with sondes [Jiang et al., 2007] show that MLS vsn. 2.2 has very good accuracy
down to at least the 215 hPa level. The vertical resolution of MLS is 2.7 to 3 km, from the upper
troposphere to the mid-mesosphere [Froidevaux, 2008]. Because of the good performance of
MLS in the lower mesosphere, we now extend the climatology up to 65 km. MLS version 3.3
data from late 2004 through 2010 were averaged to create the climatology. There is some
concern [Froidevaux, personal communication] that the version 3.3 ozone retrievals are
sometimes unstable in the tropical lower troposphere, but we use sonde data at the altitudes
where this appears to be a problem (see Figure 1, left panel).

A total of 54,782 ozone sonde profiles measured at 49 stations over the period 1988 - 2010
were averaged to create a sonde-based climatology of the lower atmosphere - from the surface to
approximately 30 km altitude. Table 1 gives details on the stations that were used for each ten
degree latitude zone from 90°S to 90°N. 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. Some records were combined. For example, sondes from three stations,
Yarmouth (43.9°N, 66°W), Kelowna (49.9°N, 119°W), and Egbert (44.2°N, 80°W), were
averaged and treated as though they came from one station (Canada) for the purpose of creating
the climatology. This was done in order to not overweight this longitude sector.

Coverage is a serious problem with sonde data. In some ten degree latitude zones, four in
the southern hemisphere and one in the northern hemisphere, there is only a single sonde station
to represent an entire latitude zone. Also notice that in some cases data from one station is used
in the averages of two latitude zones. Data from Hilo at 20°N latitude were used in both the 20°-30°N
zone and in the 10°-20°N zone, which has only one other sonde station. While the
tropospheric ozone distribution appears to be fairly uniform with longitude at mid and high
latitudes, this is not true of the tropics. Ziemke et al. [1996] have shown that there is an
asymmetry in the tropical southern hemisphere ozone distribution, with ozone higher by about 25
DU over the mid-Atlantic than over the mid-Pacific. Based on comparisons with MLS they argue
that this asymmetry is mostly in tropospheric ozone. In the tropics sonde station coverage is now
much better because of the augmented sonde data from the SHADOZ (Southern Hemisphere
Additional Ozone sondes) network [Thompson et al., 2003]. In the zone from the equator to 10°S
there are now 5 sonde sites that give fairly good sampling with longitude. Finally, notice that in
the zone from 80°S to 90°S there are no data for levels below 2 km. The Amundsen-Scott station
at the South Pole, the only station in this zone, is located on the Polar Plateau which is at more
than 2 km elevation.

The altitude variable used for the climatology is $Z^*$, a parameter frequently used in
comparisons of atmospheric chemistry models [Park et al., 1999]. $Z^*$, 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. The altitude spacing of the climatology is 1 km in $Z^*$ units.

In an isothermal atmosphere $Z^*$ would correspond closely to altitude.

The monthly average data from MLS were merged with monthly average data from sondes
to create the final climatological profiles. For low and mid latitudes, between 40°N and 40°S, the
sonde and MLS profiles are merged for $Z^*$ levels between 8 km and 16 km (320 hPa to 101 hPa).
Between 40° latitude and the pole in each hemisphere, the profiles are merged somewhat higher
in the atmosphere, for $Z^*$ levels between 13 km and 21 km (156 hPa to 49 hPa). It is useful to
use MLS data to as low an altitude as possible because of its complete longitudinal coverage, but
at higher latitudes we frequently see discrepancies between sonde and MLS below approximately
133 100 hPa. The high variability of tropospheric ozone at these latitudes as sampled by a small
134 number of sonde stations is the likely cause of the discrepancies, but the merge process needs to
135 be done at an altitude where the profiles are a bit more consistent. Figure 1 shows examples of
136 the merging process, near the equator in June and at high southern latitudes in October. In the
137 70°- 80°S zone for example (Figure 1, right panel) the profile between the ground and Z*=13 km
138 (pressure level 156 hPa) is an average of balloon sonde profiles from 2 stations, at Neumayer and
139 at McMurdo. From Z*=21 km to 65 km (pressure level 49 hPa to 0.09 hPa) the profile is a zonal
140 average of MLS profiles. In the merge zone between 13 km and 21 km the climatology is
141 weighted linearly, from 100% sonde at 13 km to 100% MLS at 21 km.
142
143 3. Ozone Morphology
144 The new climatology, which we will henceforth designate the ML climatology, captures
145 the average behavior of ozone as a function of altitude, latitude and season. Figure 2 shows the
146 annual average ozone in partial pressure for each ten degree zone for the southern (left panel)
147 and northern (right panel) hemispheres. The variation with latitude is, as expected, very
148 systematic, with tropical ozone peaking near 27 km while high latitude ozone peaks down near
149 20 km. There is also a clear north-south asymmetry seen at high latitudes which is likely due in
150 part to the greater stability of the polar vortex in the southern hemisphere.
151 Examples of the seasonal behavior of the climatology are given in Figure 3, which shows
152 the monthly variation in the 70° to 80°S zone (on left) and the 40° to 50°N zone (on right). The
153 change at high latitudes in the south is the most extreme because of the development of the
154 ozone hole each October. The extremely low ozone between 12 km and 25 km is a result of the
well known ozone destruction within the polar vortex each spring [WMO, 2003]. Neumayer
station (71°S, 8°W) tends to be outside the vortex in October while McMurdo station (78°S,
167°E) is more likely to be inside the vortex. This sonde sampling problem is somewhat
alleviated by the influence of the well-sampled MLS contribution down to about 15 km. At mid-
lattitudes in the north ozone above the ozone maximum shows only a small variation, while ozone
at lower altitudes follows the seasonal variation from high ozone in the spring to low ozone in
the fall.

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 to mid latitudes, increasing to as much as 25% at
high latitudes. In the troposphere the standard deviations can range from 25% to 50% at mid and
high latitudes. Figure 4 shows the variance of ozone in the 30° to 40°N zone for March when
variance is high, and in August when variance is low. Notice that near 10 km in March the
variance is high and ozone is very low, leading to a standard deviation that can approach 100%.

4. Comparisons

The revised climatology should be more accurate than the previous climatology because of
the use of Aura MLS data which have nearly full global coverage on a daily basis, and because
of the addition of more sonde data. Data from the Aura MLS instrument can reliably be used
down to the 215 hPa level, leading to much better coverage in the upper troposphere / lower
stratosphere region. The climatology of tropospheric ozone benefits from the inclusion of new
stations, especially in the tropics, and nearly double the number of sonde profiles as before. The
ozone above the stratopause should also be more accurate, allowing us to extend the new
climatology up to 65 km.

4.1 Total Column Ozone

To show that the new climatology accurately represents the atmosphere, integrated total
column ozone from the climatology is compared with zonal average ozone measured by the
OMI instrument on Aura for the period 2005 through 2008. OMI has proven to be a stable, well
calibrated instrument as shown by validation against the ground networks [McPeters et al.,
2008]. In 2009 partial blockage of the field of view became a problem, the so called row
anomaly problem, so the initial four year period was used. A four year period also minimizes any
possible effect of QBO variation. Data from a special processing using the Brion, Daumont, and
Malicet ozone cross sections [Malicet et al., 1995] were used in order to eliminate the small bias
(1.3%) resulting from ozone cross section differences.

As shown in Figure 5, the difference between the climatology and OMI total column ozone
exceeds 3% in only a few areas. Differences of 3% to 6% are seen in the northern tropics,
possibly due to the sonde sampling issues noted earlier. 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. In an area weighted average, the ML
climatological ozone is 1.2% higher than OMI total column ozone.

4.2. Tropospheric Ozone
The addition of new sonde stations and the near doubling of the number of sondes used have significantly improved the tropospheric ozone in the new climatology. For example, there are now five sonde stations in the SHADOZ program [Thompson et al., 2003] in the 0° to 10°S latitude zone. In Figure 6 we compare the climatological average to profiles from the individual stations in this zone for the month of September 2001. This is a zone in which we expect longitudinal asymmetry in the tropospheric ozone distribution such that ozone in the mid-Atlantic is higher than that over the mid-Pacific [Ziemke et al. 1996]. This is seen in Figure 6 where ozone from the Atlantic stations, Ascension Island and Natal, is higher than the climatology in the lower troposphere, while ozone from Pacific stations, Java and San Christobal, is lower in the lower troposphere than the climatology. The climatology represents a good average of the longitudinal distribution from the sonde stations. The sonde data in Figure 6 also show that the asymmetry is much smaller in the upper troposphere. This was part of the reason for our choice to use MLS data in the climatology down to 16 km (100 hPa) and blend MLS and sonde data between 16 km and 8 km. The difference between climatology and the sondes chosen for this comparison in the 16 - 18 km region may be due to the ~3 km vertical resolution of MLS, but it could also be due to differences in this one month at these discrete locations.

4.3 Mesospheric Ozone

The SBUV instruments infer an ozone profile by measuring backscattered sunlight in the ultraviolet. Consequently in the mesosphere, where there is a significant diurnal variation of ozone, the MLS daytime ozone is more appropriate for forming the climatology for use in buv
retrievals than the night observations or an average of the two. An accuracy assessment in this altitude region is difficult because of limited data and disagreement among the data sets that do exist. In Figure 7 we compare the climatology with observations by SAGE II, SABER, and Nimbus 7 SBUV. SAGE II [Chu et al., 1989, McCormick et al., 1989] observations made in March in the 40° to 50°N latitude zone between 1985 and 2005 show good agreement near 45 km but are 25% higher than the MLS climatology at 60 km. The SABER (Sounding of the Atmosphere using Broadband Emission Radiometry) instrument on TIMED in the 2004-2007 period derives ozone in the mesosphere to as high as 80 km altitude. The average of March observations between 9:00 and 15:00 local time also shows agreement with climatology near 45 km but is 30% higher than the ML climatology at 60 km. The Nimbus 7 SBUV profiles from March 1983 agree well with the climatology between 48 km and 55 km. While there might be concern that the 55 km point (0.5 hPa) is influenced by the a priori climatology, the ozone between 0.7 and 2 hPa is determined almost totally by the SBUV measurement itself.

The difference between SAGE II and the MLS-based climatology might be expected because of the diurnal variation of ozone, since a sunrise/sunset SAGE II occultation measurement is being compared with a near-noon MLS observation, and ozone in the mesosphere is higher at night than in the day [Ricaud et al., 1996]. In contrast, the SBUV observations are usually near-noon and agree well with MLS at all altitudes. When orbit drift leads to late afternoon or early morning observation times, we see significant differences between SBUV retrievals and MLS. The difference with SABER cannot be explained as diurnal variation since this is an average of mid-day observations. This represents a real difference between the MLS and SABER ozone retrievals.
4.4 Comparison with the LLM Climatology

We have argued that the ML climatology is more accurate than the previous climatology for the reasons detailed in this paper. Figure 8 shows the percent difference between annual average ML ozone and annual average LLM ozone as a function of latitude and altitude. The largest differences are seen in the troposphere in the 0° to 20°N latitude zone, a region that was severely under-sampled by sondes when LLM was created. We now have 2600 sondes from six stations in this zone that show more tropospheric ozone than in the previous LLM average based on only two stations. There is a general small increase (less than 5%) in ozone in the 35 to 48 km region that represents an MLS versus SAGE difference. The decrease in ozone at high southern latitudes near 20 km comes mostly from better sampling of the ozone hole region by MLS in September and October. Overall, a very crude average of all altitudes and latitudes shows that ML ozone is only about 0.5% lower than LLM ozone.

5. Data Availability

The new ML climatology is easily available online from the Goddard anonymous ftp account: ftp://toms.gsfc.nasa.gov. The data are in the directory pub/ML_climatology. The ML climatology is available as ASCII tables of ozone mixing ratios (ML_ppmv_table.dat), the associated standard deviations (ML_ppmv_stats.dat), and a table of ozone layer amounts (MLdu_table.dat). A table of ozone layer amounts in umkehr layers instead of Z* layers is also included (ML_umkehr.dat). An Excel spreadsheet includes the climatology in all forms (ML_climo.xlsx).
6. Conclusions

The ML climatology captures the significant variations in both stratospheric and
tropospheric ozone as a function of latitude and season. We have used this climatology in the
version 8.6 processing of data from a series of eight SBUV instruments. Total column ozone
from the climatology agrees with that from the OMI usually to within 3%, and on average agrees
to about one percent. The large number of new sonde profiles and sonde stations has greatly
improved the accuracy of the tropospheric climatology, especially in the tropics. This is
significant for total column ozone retrievals because a good a priori is needed to account for the
poor penetration of UV in the lower troposphere.

The Aura MLS ozone data used in the climatology give excellent coverage even at high
latitudes, and because MLS ozone can be used down to the 200 hPa level, the effect of the
limited number of sonde stations in many latitude zones is reduced for the middle troposphere
part of the climatology. This climatology does not explicitly include the wave 1 variation of
ozone in the tropics in the middle and lower troposphere but accounts for it in the average.

Acknowledgments. The Aura MLS data were obtained from the MLS team via the Aura
Validation Data Center, while balloon sonde data were obtained from the WOUDC in Canada
and from the SHADOZ team at GSFC. We have a deep appreciation for the great effort that goes
into producing and maintaining long term data sets. We thank the MLS team and the many
people who launch ozone sondes around the world. This work was supported under NASA’s
MEaSUREs program for the creation of long term multi-instrument data sets.
References


Figure Captions

Figure 1. A comparison showing the MLS profiles and sonde average profiles used to create the climatology for two latitudes / months: 0°-10°N in June on left and 70°-80°S in October on right. The altitude region in which sonde and MLS profiles are blended is shown as the hatched area.

Figure 2. The climatology as annual average ozone partial pressure profiles shown for southern latitudes (on left) and northern latitudes (on right).

Figure 3. The month to month variation of the climatology shown for the 70°-80°S zone (on left) and for the 40°-50°N zone (on right).

Figure 4. The ozone (solid lines) and standard deviations (dashed lines) for March and for August for the 30°-40°N zone.

Figure 5. Total column ozone from the climatology compared with that from the OMI instrument (2005-2008) on Aura. Percent difference versus month and latitude is plotted.

Figure 6. Tropospheric ozone from five sonde stations in the 0°-10°S latitude zone for September 2001 compared with the September climatology.

Figure 7. Ozone in the upper stratosphere and lower mesosphere measured by SAGE II, SABER, and SBUV in March in the 40°-50°N zone compared with the March climatology.

Figure 8. A plot of the difference between the new ML climatology and the previous LLM climatology. Percent difference in annual average ozone as a function of latitude and altitude is shown.
### Table 1. ECC sonde stations used in climatology including total number of sondes in average.

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<th>Station</th>
<th>latitude</th>
<th>longitude</th>
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</tr>
<tr>
<td></td>
<td>Tahiti/Fiji</td>
<td>-17.5</td>
<td>164</td>
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<tr>
<td></td>
<td>Reunion</td>
<td>-20.0</td>
<td>55</td>
<td>399</td>
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<tr>
<td><strong>20°-30° S</strong></td>
<td>Reunion</td>
<td>-20.0</td>
<td>55</td>
<td>399</td>
</tr>
<tr>
<td></td>
<td>Irene</td>
<td>-25.2</td>
<td>28</td>
<td>371</td>
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<tr>
<td><strong>30°-40° S</strong></td>
<td>Laverton</td>
<td>-37.9</td>
<td>145</td>
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<tr>
<td><strong>40°-50° S</strong></td>
<td>Lauder</td>
<td>-45.0</td>
<td>170</td>
<td>1265</td>
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<tr>
<td><strong>50°-60° S</strong></td>
<td>Macquarie</td>
<td>-54.5</td>
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<tr>
<td><strong>60°-70° S</strong></td>
<td>Marambio</td>
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<td>-57</td>
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<td>Location</td>
<td>Temperature</td>
<td>Precipitation</td>
<td>Year Period</td>
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<tr>
<td>70°-80° S</td>
<td>Neumayer</td>
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<td>McMurdno</td>
<td>-77.9</td>
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<td>417</td>
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<td>80°-90° S</td>
<td>S. Pole</td>
<td>-89.9</td>
<td>-25</td>
<td>922</td>
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</table>

Notes:
* Greenland = Thule (68.7N, 69W) + Scoresbysund (70.5N, 22W)
** Canada = Yarmouth (43.9N, 66W) + Kelowna (49.9N, 119W) + Egbert (44.2N, 80W)
*** Pan-costa = Paramaribo (5.8N, 55W) + Alajuela/Heredia (10.0N, 84W) + Panama (7.8N, 80W)