The version 8.6 SBUV ozone data record: An overview

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[1] Under a NASA program to produce long-term data records from instruments on multiple satellites, data from a series of nine Solar Backscatter Ultraviolet (SBUV and SBUV/2) instruments have been reprocessed to create a coherent ozone time series. Data from the BUV instrument on Nimbus 4, SBUV on Nimbus 7, and SBUV/2 instruments on NOAA 9, 11, 14, 16, 17, 18, and 19 covering the period 1970–1972 and 1979–2011 were used to create a long-term data set. The goal is an ozone Earth Science Data Record—a consistent, calibrated ozone time series that can be used for trend analyses and other studies. In order to create this ozone data set, the radiances were adjusted and used to reprocess the entire data records for each of the nine instruments. Interinstrument comparisons during periods of overlap as well as comparisons with data from other satellite and ground-based instruments were used to evaluate the consistency of the record and make calibration adjustments as needed. Additional improvements in this version 8.6 processing included the use of the Brion, Daumont, and Malicet ozone cross sections, and a cloud-height climatology derived from Aura OMI measurements. Validation of the reprocessed ozone shows that total column ozone is consistent with the Brewer/Dobson network to within about 1% for the new time series. Comparisons with MLS, SAGE, sondes, and lidar show that ozone at individual levels in the stratosphere is generally consistent to within 5%.


1. Introduction

[2] Ozone is an important component of our atmosphere, both because it is the critical absorber of ultraviolet radiation and because it affects climate [McLinden and Fioletov, 2011]. The abundance of ozone directly affects the Earth’s biosphere since the total column amount of ozone overhead determines the amount of ultraviolet light that reaches the ground. Ozone absorbs solar ultraviolet radiation in the stratosphere, modifying the chemistry of the stratosphere and producing heat that modifies the dynamics of the stratosphere. For these reasons, stratospheric ozone is considered a key climate parameter. The decline in ozone resulting from the release of chlorofluorocarbons, particularly the development of the Antarctic ozone hole each year, has been a clear example of man’s effect on the global environment.

[3] An accurate time series of total column ozone and the ozone vertical distribution is needed to document the changes that have occurred. A continuing time series is needed to verify the expected recovery of ozone as a result of the Montreal Protocol and other measures that limited the release of ozone depleting substances [WMO, 2010; Randel and Wu, 2007; SPARC, 1998]. An ozone time series is also needed to verify the accuracy of the models that are being used to predict the expected behavior of ozone in the next 100 years [Park et al., 1999]. Because climate change and ozone change turn out to be intimately related, a good historical record is particularly important for model verification.

[4] The NASA program called MEaSUREs, an acronym for Making Earth System data records for Use in Research Environments, supports the creation of long-term data records from multiple satellite systems. Where NASA support has traditionally been aligned by instrument and spacecraft, MEaSUREs is a logical extension to provide continuing support by product. Take ozone as an example. As new ozone measuring instruments were launched, a dedicated instrument team calibrated each instrument as well as possible based on prelaunch laboratory calibrations and in-flight measurements. Comparisons with previous instruments and with ground-based measurements were done for validation purposes, but the calibration of each instrument was determined independently. MEaSUREs supports taking the measurements of one product, ozone in our case, and applying a coherent calibration to an ensemble of instruments measuring the same atmospheric parameter to create a unified, trend-quality time series.

2. Instruments in the Time Series

[5] In what we designate the version 8.6 processing, we have applied a coherent calibration to the radiances for a series of Solar Backscatter Ultraviolet (SBUV) instruments to create an ozone time series that can be used for trend analysis. (Here
we will use the term SBUV generically for BUV, SBUV, and the SBUV/2 instruments on NOAA spacecraft.) This version was designated 8.6 to distinguish it from the 8.5 version number used for the processing of Aura OMI data. We concentrated on the nine SBUV instruments—the Nimbus 4 BUV, the Nimbus 7 SBUV, and SBUV/2 instruments on NOAA 9, 11, 14, 16, 17, 18, and 19. The time period of coverage of these instruments is shown in Figure 1. (NOAA 19 data were added to the series recently.) Unfortunately, the BUV instrument had complete coverage only through mid-1972, when partial failure of the solar power array on Nimbus 4 led to increasingly degraded coverage. Otherwise, there is almost complete coverage from one or another SBUV instrument from late 1978 to the present.

3. The Version 8.6 Processing

Before the initiation of the MEaSUREs ozone project, merged ozone data sets (MODs) were created by making basic ozone adjustments, instrument by instrument. The first version of a total ozone Earth Science Data Record archived through MEaSUREs used this approach [Stolarski and Frith, 2006] to merge SBUV and TOMS total ozone data. The more advanced approach is to go back to the original data sets and apply calibration corrections to the measured radiances in order to guarantee that data from the different instruments are consistent. This is the more accurate approach because radiance calibration errors propagate nonlinearly to retrieved ozone, producing latitudinally and seasonally dependent errors in ozone. Establishing a consistent calibration for the series of SBUV instruments was a large effort and could only be done by working with the original instrument teams. While all nine instruments had the same basic design, there were instrument-specific errors such as detector hysteresis, stray light errors, and grating drive errors, that had to be corrected. These corrections were all reviewed to be sure that they were consistently applied.

The v8.6 designation indicates that the version 8 algorithm has been used with a new calibration implementation. The ozone retrieval is done using the version 8 ozone algorithm [Bhartia et al., 2004], an implementation of the Rodgers [1976] optimal estimation approach. A paper by Deland et al. [2012] gives the details of how the different instruments were analyzed to derive instrument calibrations that are consistent from instrument to instrument and over the 41 year time series, while Bhartia et al. [2012] describes the algorithm that has been applied to the SBUV series with a particular emphasis on characterizing the sources of errors that are relevant for deriving trends from monthly mean anomalies and in estimating biases between different types of ozone sensors.

3.1. The Orbit Drift Problem

The most significant problem in creating a unified calibration sequence was orbit drift in the NOAA satellites. A sun synchronous orbit is one in which the satellite is in a near-polar orbit that precesses such that the satellite crosses the equator at the same local time each orbit. Such an orbit provides an instrument with nearly global coverage each day. As shown in Figure 2, the early NOAA satellites were in orbits which slowly drifted—from an early afternoon equator crossing time, to late afternoon, across the terminator and into a morning orbit—in only a few years. The problem with orbit drift is that the error in retrieved ozone produced by a calibration error or instrument error increases significantly for observations near the terminator [Bhartia et al., 2012]. Thus, orbit drift will cause calibration error to create an apparent time-dependent ozone change that could be interpreted as an ozone trend.

![Figure 1](image1.png)

Figure 1. Data from nine instruments were reprocessed. Periods of ascending (afternoon equator crossing time) orbit are distinguished from descending (morning) orbit data periods. Use of near-terminator data is not recommended.

![Figure 2](image2.png)

Figure 2. The local time at which each instrument in the time series crosses the equator each orbit varies due to orbit drift.
[10] A secondary problem caused by orbit drift is that ozone in the upper stratosphere and mesosphere varies with time of day [Parrish et al., 2011]. In this region, ozone measured by a morning satellite will not be the same as that measured by an afternoon satellite. Because of these problems, creation of a unified ozone time series by combining measurements from the overlap period of different satellites was greatly complicated. We found that it was not sufficient to do zonal mean overlap comparisons. Fortunately, satellites in different polar orbits usually have geographic coincidences at high latitudes that can be used to determine the relative calibration. The orbit of a satellite in a near-earth orbit as it enters the descending part of its orbit in the summer hemisphere can cross the orbit of a satellite in a near-terminator orbit. Carefully matching observations from the two satellites that were taking observations at nearly the same time alleviates both the diurnal variation problem and the fact that a calibration error produces a larger ozone error at larger solar zenith angles. This allows us to isolate the error due to calibration difference.

3.2. Calibration Adjustment

[11] Establishing a consistent calibration across the different instruments was the most important factor in creating this data set. In previous data processing, there was no requirement that ozone from successive instruments agree exactly; rather, each instrument was viewed as an independent standard. The base calibration for each instrument was determined from prelaunch laboratory measurements and initial on-orbit measurements of an on-board mercury lamp and solar irradiance measurements. A variety of “soft” calibration techniques were used to maintain the calibration over the life of the instrument. These included pair justification, in which wavelength-dependent degradation is corrected through the requirement that the same ozone be derived for all wavelength pairs, and scene stabilization, in which the average reflectivity of the Antarctic ice sheets or minimum ocean reflectivity is assumed to be constant over long time periods [Deland et al., 2012]. In the 1990s, the SSBUV instrument was flown on the space shuttle specifically to track the calibration of the NOAA SBUVs. While such comparisons did not provide the precision hoped for, such comparisons spanning the decade did establish a baseline calibration reference.

[12] For the v8.6 reprocessing, we carefully reanalyzed the time-dependent calibration of each instrument in light of current understanding. Radiance adjustments for each instrument were determined through the comparison techniques just described. In setting the overall absolute calibration scale, the NOAA 17 instrument was chosen as the reference instrument because of its excellent prelaunch calibration traceable to laboratory standards. The process by which overlap and proxy comparisons were used to set the calibration of the series of SBUV instruments is explained in detail by Deland et al. [2012].

[13] At the conclusion of this process, the quality of the calibration for the different instruments was not uniform. The recent instruments, on NOAA 16, 17, and 18, are the best calibrated and most consistent. Because of orbit drift, data gaps, and residual instrument problems, the NOAA 9, 11, and 14 instruments have the greatest uncertainty. The Nimbus 7 instrument was in a very stable orbit but may have a small residual calibration drift over its ten year life, especially seen in the southern hemisphere. The original BUV instrument on Nimbus 4 has good data coverage only through 1972, when failure of the solar power array sharply reduced the observation duty cycle. Because of the lack of overlap with Nimbus 7 and the greater uncertainty of the ground observations in the early 1970s, BUV has the greatest uncertainty in setting its absolute scale.

3.3. Other Improvements in Version 8.6

[14] In addition to the revised calibration for each instrument, there were three significant improvements implemented for the v8.6 processing—new ozone cross sections were used, a new cloud-height climatology was used, and an updated ozone climatology was used for the a priori. Previously, data from the SBUV series of instruments were processed using the ozone cross sections measured by Bass and Paur [1984]. Here we use the ozone cross sections measured by Brion, Daumont, and Malicet [Brion et al., 1993; Malicet et al., 1995]. The new cross sections correct small errors in the temperature dependence and wavelength registration of the previous cross sections and are more accurate longward of 330 nm where the Bass and Paur measurement uncertainty was higher. The effect of the new ozone cross sections on SBUV retrievals is small, decreasing total column ozone by about half a percent at low and midlatitudes.

[15] The cloud-height climatology used previously was based upon the International Satellite Cloud Climatology Project in which cloud-heights are derived from measurements in the infrared. When Joiner and Vasilkov [2006] implemented a Raman-based cloud-height retrieval for the OMI instrument on Aura, they found that the ultraviolet wavelengths used for ozone retrieval penetrate much further into clouds than do infrared wavelengths and are much less sensitive to cirrus. Consequently, a cloud-height climatology derived from four years of OMI cloud-height retrievals was used as much more appropriate for UV ozone retrievals. The effect of the new cloud climatology on total column ozone can be as high as 5% for areas of local heavy cloud cover, but the effect on trends or on zonal average ozone is small.

[16] The ozone climatology used as the algorithm a priori has been updated. In preparation for the v8.6 processing, McPeters and Labow [2012] revised the ozone profile climatology used previously. The new climatology was formed by combining data from Aura MLS (2004–2010) with data from balloon sondes (1988–2010). The Microwave Limb Sounder (MLS) instrument on Aura has much better latitude coverage than the SAGE II data used previously and measures ozone daily from the upper troposphere to the lower mesosphere. The additional balloon data now available, especially from new stations in the tropics, provided a much more accurate tropospheric ozone climatology.

3.4. Effect of Version 8.6 Processing: Change From Version 8.0

[17] Version 8.0 data represented the best effort calibration of each instrument, based on prelaunch calibrations and ongoing soft calibration data. Version 8.6 has the benefit of access to the full time series for each instrument and the calibration techniques of Deland et al. [2012] described in section 3.2. The result is significant change in the ozone time series. Figure 3 shows the percent difference between version 8.6 ozone data and data previously archived as version 8.0. Daily zonal mean ozone differences are plotted in Figure 3.
for one latitude, 45°N, for total column ozone, for upper stratospheric ozone (at 2 hPa), and for lower stratospheric ozone (at 20 hPa). Tests show that cross section change by itself reduces SBUV total ozone by 0.5% at low latitudes to 1% at high latitudes. The net effect of the cross section change, climatology change, and the new cloud climatology is mostly in the 1% to 2% range for zonal average data. The ozone changes we see in Figure 3 of up to 10% (depending on instrument and latitude) are mostly caused by the calibration changes we have applied.

At mid- to high latitudes, the effect of a calibration change will vary with solar zenith angle, leading to the large seasonal variations of the differences seen in Figure 3. A similar plot for low latitudes has much smaller seasonal variation but similar offsets. Because the calibration change versus wavelength varies from instrument to instrument, the resulting ozone change varies with altitude. For the NOAA 9 instrument, the calibration changes had a large seasonal effect on lower stratospheric ozone and a small effect on upper stratospheric ozone. For NOAA 14 through 18, the effect was larger in the upper stratosphere than in the lower stratosphere. For the NOAA 18 instrument, there was a large absolute shift of about 6% for both lower and upper stratospheric ozone.

4. The Data: Long-Term Ozone Change

The goal of the v8.6 reprocessing was to create an accurate data set of uniformly calibrated and consistently processed ozone data that could be used to create an ozone time series for trend analysis and other studies. The initial release of these data was in the form of monthly zonal means for each instrument for 5° zones, from 80°S to 80°N. The monthly average profiles were released in ASCII format in two forms, as layer ozone amounts (DU/layer) for 21 layers from the surface to 0.1 hPa, and as ozone mixing ratios (ppmv) for 15 pressure levels from 0.5 hPa down to 50 hPa. This was followed by release of the individual profiles with averaging kernels in HDF format. While the profiles are given for relatively fine 3.2 km layers, the actual vertical resolution of an SBUV retrieval varies from about 6 km resolution in the middle and upper stratosphere to about 15 km in the troposphere. The information content of these profiles is discussed by Kramarova et al. [2013a].

4.1. Total Ozone Stability

Detailed comparisons of total column ozone with the Dobson/Brewer network are given by Labow et al. [2013]. But possibly the best verification of the long-term stability of the v8.6 ozone series over four decades is a comparison with the World Standard Dobson instrument I83 as shown in Figure 4. While this comparison with the World Standard Dobson I83 is of total column ozone only, it represents a fairly strong constraint on ozone in the lower and middle stratosphere. Total column ozone measurements for this instrument have been maintained to a precision of ±0.5% since 1962 [Komhyr et al., 1989]. Dobson I83 has made regular observations at Mauna Loa Observatory, Hawaii (19.5°N, 156°W) since 1972, usually in the summer. Since an SBUV ozone measurement is nadir-only and the orbits are spaced 26° apart, the lack of spatial coincidence increases the uncertainty of the comparisons of SBUV with I83. The SBUV overpass observation for a given day's Dobson measurement consists of the distance weighted average of SBUV observations from the two closest orbits. The difference between ozone measured by
SBUV and I83 Dobson ozone averaged for the season, typically June, July, and August, is plotted in Figure 4. The $2\sigma$ standard error for each year's observations is also plotted. Figure 4 shows that, relative to I83, the 40 year SBUV series for total column ozone is consistent to within ±0.88%. The average bias, 0.85%, is mostly due to the use of different ozone cross sections and is not a concern for trend analysis.

Notice that in 2008, the NOAA 16 comparison was over 1% different from NOAA 17 and NOAA 18. NOAA 16 was in a near-terminator orbit at this time, and for reasons noted by Bhartia et al. [2012], we do not recommend the use of the near-terminator data because of its increased sensitivity to error.

Unfortunately, the BUV comparison in 1972 had a fairly high uncertainty, ±2.1%, because there were comparisons for only 9 days that year. Within that uncertainty, total column ozone measured by BUV in 1972 is consistent with ozone from the other eight instruments.

### 4.2. Global Average Ozone Variation

As an example of the results of the v8.6 reprocessing, Figure 5 shows global average area weighted ozone, 60°S – 60°N, for each of the SBUV instruments. The lower panel shows total column ozone for each instrument, while the upper panel shows the same data plotted as a percent change from the 1979/1980 monthly averages. A percent deviation plot removes the large annual variation in order to reveal the small (sub-one percent) long-term changes. This plot shows that there has been about a 4% decline in global average total column ozone since 1980, with about half of the decline occurring by 1985. There is no obvious ozone increase in the last decade, but a multivariate analysis would be needed to extract an accurate trend from these data. An important point to notice is that during overlap periods when ozone is being measured by more than one instrument, the measurements are consistent to within about 1%.

The accuracy of the long-term total column ozone time series is very high. Labow et al. [2013] have compared the instruments in the series to average ozone from a set of 33 northern hemisphere ground systems that have operated almost continuously since 1978. They find that over that period satellite ozone agrees with ground-based ozone to better than 1%. Uncertainty of the BUV comparisons (1970–1975) is higher, but the accuracy of both the ground systems and the satellite is questionable in that period.

### 4.3. Comparison With European Merged Ozone Data

A long-term merged total ozone data set has been produced using data from three European instruments—GOME, SCIAMACHY, and GOME2. Data from GOME
[Burrows et al., 1999] from the period July 1995 through May 2003 are used unadjusted. SCIAMACHY nadir data [Bovensmann et al., 1999] from the period August 2002 to the present have been adjusted to match the GOME data. Data from GOME2 from March 2007 to the present have also been adjusted to be consistent with GOME and SCIAMACHY. In each case, WFDOAS retrievals [Coldewey-Egbers et al., 2005] have been used to derive total column ozone. The data are available via http://www.iup.uni-bremen.de/gome/wfdoas/merged/wfdoas_merged.html.

[26] Global average ozone (60°S–60°N) from the GSG (GOME-SCIAMACHY-GOME2) merged data set is plotted in the bottom panel of Figure 6 along with the v8.6 ozone from seven SBUV instruments, while the percent difference of the v8.6 data is plotted in the top panel. Agreement is mostly within 2%. The differences for NOAA 11 SBUV/2 show a strong seasonal variation. Over the period 1996 – 2008, the two time series show the same time dependence if the NOAA 11 data are discounted. Beginning in 2008, there appears to be a time dependence in the difference. The v8.6 data for 2008–2012 averages 0.9% lower than GSG, where the 1996–2007 data are only 0.2% lower.

4.4. Ozone Profile Variation

[27] Figure 7 shows examples of ozone change as a function of altitude for the equator and for a 10° zone centered at 45°N. Total column ozone and ozone in two altitude regions, one in the upper stratosphere and one in the lower stratosphere, are shown for each latitude zone. As before, we have plotted the deviations from the 1979/1980 averages in order to better show small long-term changes in ozone.

[28] The lowest ozone seen at 45°N was about 18 months after the eruption of Mt. Pinatubo in June of 1991. The drop in total column ozone at 45°N since 1979/1980 is very similar to that in global average ozone, a decline of 3.7% averaged over the 2000–2010 period. In the equatorial zone (5°N to 5°S), the decline is much smaller, only 1.5% averaged over the same period. This implies that most of the decline in global ozone is occurring outside the tropics. The large variation seen in equatorial total column ozone is mostly due to the well known quasi-biennial oscillation (QBO). The decline in ozone in the upper stratosphere since 1979/1980 is much larger, amounting to 13.6% at the 2 hPa level at 45°N, and 7.9% even at the equator.

[29] The consistency of ozone derived for different instruments is one indicator of the quality of the reprocessed data and the success of our instrument-to-instrument calibration. As stated earlier, the total column ozone retrievals are very robust and mostly agree to better than 1%. At 45°N, for example, during the 19 month period when there were measurements from SBUV instruments on Nimbus 7, NOAA 9, and NOAA 11, the average standard deviation of total ozone differences from the three instruments was 0.5%. During the 67 month period when there were measurements from NOAA 16, NOAA 17, and NOAA 18, the standard deviation of the differences was also 0.5%.

[30] In contrast, the profile retrievals are much more sensitive to calibration and instrument problems. The instruments on NOAA 9, 11, and 14 were particularly a problem. Again using consistency as a metric, the average standard deviation of 2 hPa ozone differences for Nimbus 7 and NOAA 9 and 11 overlap period was 2.3%, while the standard deviation during the NOAA 16, 17, and 18 overlap period was 1.3%, only about half as large. These are not random differences. Examination of the 2 hPa plot for 45°N in Figure 7 reveals that this increased standard deviation is due in part to the different time dependence of the NOAA 9 data. Similar differences are seen for the NOAA 11 and 14 instruments at the 20 hPa level at the equator. Proper evaluation of these differences in data quality will be important when a unified ozone time series is being created from these individual data records.

Figure 6. Global average ozone from the GOME-SCIAMACHY-GOME2 (GSG) merged ozone data set is shown in the bottom panel, while the percent difference of v8.6 individual time series from GSG is shown in the top panel.
5. Data Availability

[31] The v8.6 reprocessed SBUV data described here are available as either monthly zonal means or as individual measured profiles in HDF5 format. These are the fully detailed data, including averaging kernels. All the data have been archived at the Goddard DISC and are available via http://disc.sci.gsfc.nasa.gov/measures. The data can be found under “Measures Projects,” as project “Creating a Long-term Multi-Sensor Ozone Data record.”

[32] In addition, data in simple ASCII format are available from our anonymous ftp site. This site includes monthly zonal means data, overpass data for each instrument, and individual profiles in compressed (results only) format. The site is: ftp://toms.gsfc.nasa.gov/pub/sbuv.

6. Discussion and Conclusions

[33] We have produced a 40 year record of ozone from a series of nine recalibrated SBUV instruments. The calibration of each instrument was examined and adjusted as needed based on interinstrument comparisons during periods of overlap as well as reference to data from other instruments such as MLS, SAGE II, and ground-based measurements. The goal was an ozone time series with a coherent calibration spanning multiple instruments. Based on validation against external instruments and consistency during periods of overlap, we believe that the total column ozone record is accurate to within about one percent [Labow et al., 2013], and the profile ozone is accurate to 2% to 5%, depending on the instrument [Kramarova et al., 2013b].

Figure 7. Ozone change since 1979/1980 for the upper stratosphere (2 hPa), the lower stratosphere (20 hPa), and total column ozone. Ozone for the 45°N zone is shown in the upper plots, while equatorial ozone is shown in the lower plots.
The most stable instruments were those on NOAA 16, 17, and 18, and on Nimbus 7. The calibrations of the instruments on NOAA 9, 11, and 14 are the most uncertain because of orbit drift and instrument problems. The Nimbus 4 BUV instrument was difficult to put on the same scale as the succeeding instruments because of the lack of overlap and lack of good corroborating measurements. Comparison with a GOME–SCIAMACHY–GOME2 global ozone time series shows agreement to a few tenths of a percent from 1996 to 2008, and average differences of about a percent from 2008 to 2012.

The limited vertical resolution of the SBUV retrieval, about 6 km in the middle and upper stratosphere, decreasing to approximately 15 km in the troposphere, imposes a limit on the science that can be addressed with these data. A very clear example is QBO analysis. Because the timing of the QBO varies fairly rapidly with altitude, the low vertical resolution of the SBUV data can produce a significant mixing of this altitude response. This resulted in obvious differences in comparisons with MLS, which has vertical resolution high enough to resolve the QBO vertical structure. Kramarova et al. (2013a) show that comparison is properly done by applying an averaging kernel when comparing an SBUV profile with profiles from a higher-resolution data set.

Now that the production group has created the best effort data set for the individual instruments, the final step is to carefully evaluate the data from individual instruments and produce a single “best” MOD covering the period from 1970 to the present. Because of the varying quality and instrument problems, choices must be made on which data to include in creating the MOD data set. Following the guidelines of the MEaSUREs program, evaluation of the v8.6 data and creation of the MOD data set will be done independently.

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References
