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Technical Note: a combined SBUV and SAGE zonal-mean ozone data set

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Abstract

A stratospheric monthly, zonal-mean combined ozone data set based on Satellite Aerosol and Gas Experiment (SAGE) and Solar Backscatter UltraViolet (SBUV) data spanning 1978–2005 is presented. Drifts in individual SBUV instruments and inter-SBUV biases are corrected using SAGE I and II by calculating differences between coincident SAGE-SBUV measurements. In this way the daily, near-global coverage of SBUV(/2) is combined with the stability of SAGE to provide a homogeneous ozone record. The resultant data set shows, for example, a more realistic Quasi-Biennial Oscillation signal compared to the one derived from SBUV data alone. Furthermore, this methodology can be used to extend the present data set beyond the lifetime of SAGE II.

1 Introduction

Monitoring of stratospheric ozone remains an important endeavor for many reasons, chief among them being to clearly identify the recovery of stratospheric ozone in this post-Montreal Protocol era (Austin and Butchart, 2005) and to determine how climate change may be impacting stratospheric ozone, and visa-versa (Waugh et al., 2009). Such tasks require high quality, global, long-term ozone datasets.

While there have been a large number of satellite instruments measuring stratospheric ozone over the past thirty years, each is subject to its own instrument effects (noise, systematic errors) and sampling issues (vertical and horizontal sampling, resolution, repeat time). Knitting together these varied sources into a single, homogeneous data record suitable for trend studies is a daunting challenge.

Several such datasets exist including ones based on SAGE (Satellite Aerosol and Gas Experiment) I and II data (Randel and Wu, 1997), SBUV (Solar Backscatter Ultra-Violet) and SBUV2 data (Frith et al., 2004), and those based on multiple instruments (Hassler et al., 2008; Jones et al., 2009). In this work, a global stratospheric ozone data set it constructed based on two long-term satellite ozone data records: SBUV and SAGE. The aim of this work is to combine the coverage and data density of SBUV with the stability and precision of SAGE. There have been other attempts at combining data from the various SBUV and SBUV2 instruments, collectively referred to as SBUV(/2). A "merged ozone" data set (Frith et al., 2004) was constructed by adjusting the calibration of individual SBUVs based on comparisons during overlap periods. However, this algorithm does not completely remove biases in some individual SBUV/2 time series because the overlapping periods are not always long enough and biases are not always constant in time.

There are also limitations related to the SBUV algorithm itself. As discussed by Bhartia et al. (2004), the algorithm is capable of retrieving ozone content for relatively thick (6–8 km) layers at 30–50 km and very limited information about ozone content can be retrieved outside these limits. As a result, the amplitude of ozone fluctuations could be dampened if such fluctuations have a fine vertical structure. To illustrate this, the Quasi-Biennial Oscillation (QBO) signal in SAGE II and the SBUV merged-ozone (downloaded from http://hyperion.gsfc.nasa.gov/Data_services/merged/index.html) is examined in Fig. 1.

The QBO is a periodic oscillation of the zonal-mean wind in the tropical, lower-mid stratosphere with a period of about 28 months (Baldwin et al., 2001). It also manifests itself in other geophysical quantities, including ozone. Figure 1 shows the zonal, monthly-mean tropical (5° S to 5° N) ozone anomalies (monthly-mean with annual cycle removed). SAGE II data has been mapped onto SBUV layers (see below) so that equivalent quantities are being compared. The left panel, displaying SAGE II anomalies, shows the characteristic QBO downward propagation of the maxima and minima in the ozone anomaly with time (Randel and Wu, 1996). By contrast, while there is some oscillatory behavior in the merged-SBUV data, the amplitude is much smaller and the downward propagation is not properly captured as seen in the right panel.

2 Data sets

2.1 SBUV(/2)

The SBUV-family of instruments date back to 1978 when the original, SBUV, was launched on Nimbus 7. Operational versions, SBUV2, were launched in 1984 on NOAA 9 and later on NOAA 11, 14, 16, 17, 18, and 19. Collectively they cover the period from 1978 to present with minimal gaps. Figure 2 shows the temporal coverage of each.

SBUV(/2) measures sunlight scattered from the atmosphere and surface into the nadir via a scanning double monochrometer. Twelve discrete wavelengths from 252.0 to 339.8 nm are measured at a resolution of 1.1 nm. The ground swath is about 160 km × 160 km and provides daily, near-global coverage. Profiles are retrieved on a standard 21 layer grid such that there are 5 layers every decade of pressure. Hence each layer is roughly 3–3.5 km thick. Ozone data is reported for each layer as a partial column (in DU). The layers used in this study are given in Table 1 and span roughly 18–51 km. The SBUV(/2) vertical resolution is 6 km at an altitude of 40 km and increase above and below, with only one piece of vertical information below the number density peak (Bhartia, 2004). SBUV measures roughly 35 000 profiles per month. See Fig. 3 for coverage.

SBUV data version 8.0 (Bhartia et al., 2004), obtained from http://www.orbit.nesdis.noaa.gov, is used. The time periods for the individual SBUV(/2) instruments are given in Table 2. Only profiles that are measured at a solar zenith angle of 80° or smaller and assigned an error code of “0” are used. Furthermore, data in the aftermath of two major volcanic eruptions, El Chichon (1982) and Pinatubo (1991), are excluded as follows: for El Chichon all levels from 10° S to 30° N between March 1982 and February 1983, and for Pinatubo all levels from 20° S to 30° N between June 1991 and May 1992.

2.2 SAGE I and II

The SAGE series of instruments utilize the technique of solar occultation in which the sun is tracked during a satellite sunrise or sunset event. The first, SAGE I, was a four channel (380, 450, 600, and 1000 nm) spectrometer collecting data from 1979 to 2001. SAGE II was a seven channel spectrometer (385, 448, 453, 525, 600, 940, and 1020 nm) that operated between 1984 and 2005. See Fig. 2 for temporal overlap with the SBUV(/2) instrument series. Inversion of SAGE radiometric data first requires the normalization of spectra to a high-tangent altitude reference. From this all interfering species are removed, including Rayleigh, aerosols, and NO_2, whose concentrations are inferred simultaneously. The final step is the conversion of slant path ozone extinctions to vertical profiles of concentrations.

The solar occultation technique offers the benefit of being insensitive to the absolute response of the instrument which makes it ideal for long-term monitoring. Its primary shortcoming is that only two profiles are obtained per orbit and latitudinal sampling is uneven. On average, SAGE II measured about 800 profiles per month, with some tropical and/or mid-latitudes not sampled in the summer and winter months. See Fig. 3 for coverage.

This study uses SAGE I version 7.0 and SAGE II version 6.2 (Wang et al., 2006). Each profile is given in number density on a 0.5 km standard grid, 0.5–70 km, and is accompanied by NCEP (National Centers for Environmental Prediction) temperature and pressure profiles. SAGE pointing is stable with an uncertainty of about 0.2 km (Chu et al., 1989). Validations studies indicate the SAGE I precision is roughly 10% and SAGE II is 5% (Cunnold et al., 1989). This is in agreement with a more recent study that found SAGE II precision to be 4–8% (Fioletov et al., 2006).

The SAGE data screening methodology employed by Hassler et al. (2008), based on suggestions by Wang et al. (1996) and Rind et al. (2005), was adopted here. Data was rejected for: (i) all profiles are excluded for times when the absolute value of the beta angle exceeds 60° until it returns to less than 40°; (ii) altitudes between 30 and 50 km from 23 June 1993 to 11 April 1994 whenever the error exceeds 10%; (iii) between 10.5 and 24.5 km if the mixing ratio exceeds 10 ppmv; (iv) altitudes above 25 km if the mixing ratio exceeds 100 ppmv; and (v) altitudes above 3 hPa if the mixing ratio exceeds 50 ppmv. In addition, an altitude shift as a function of latitude has been applied to SAGE I data according to the results of Wang et al. (1996), Fig. 3. This amounted to an upward shift of the profiles by 0.3±0.3 km. The only departure from the Hassler et al. (2008) screening is for volcanic eruptions where the criteria described for the SBUV is employed.

2.3 SAGE II sunrise-sunset bias

The coverage of SAGE II is such that frequently at tropical latitudes both sunrises and sunsets occur in the same month. On these occasions, sunrise/sunset (SR/SS) differences can be observed, beginning in layer 7 (∼37 km) and increasing with altitude up to a maximum of ∼10% in layer 10, with the largest differences occurring in the tropics. Wang et al. (1996) observed the same SR/SS bias, the cause of which is not completely understood but appears to be due to multiple factors, both geophysical and satellite-related. When the absolute value of the beta angle drops below 60° this bias appears. This motivated the beta angle screening criteria mentioned above, but it is unlikely that this completely eliminates this source of bias. Additionally, there is evidence that there may be errors in the satellite ephemeris in January. The diurnal tide may also explain 1–2% of the bias. While not considered important in Wang et al. (1996), it is suggested here that the diurnal cycle of ozone may also be contributing to the bias. Above 45 km the lifetime of odd-oxygen ($O+O_3$) lifetime is less than 1 day (Brasseur and Solomon, 1984) and as a consequence ozone at sunrise and sunset will differ, with the largest gradients in ozone occurring through sunrise and sunset when the sunlight available for photolysis rapidly varies. As occultation samples all altitudes down to the tangent height, and the SZA varies along this path, it seems likely that some component of the bias is diurnal-related.

To remove any SR/SS bias, a simple model is employed. For a SBUV-SAGE II pair, all coincident measurements (see below), at each latitude band and layer, the following model is fit:

$$X_{\text{SBUV}} = X_{\text{SAGE}}(a + b \ \ i), \tag{1}$$

where X is the partial column in the SBUV layer, a and b are constants, and i is an indicator function assigned a value of −1/2 for a sunrise and +1/2 for a sunset. SBUV data is reported in partial columns while SAGE data has been integrated over SBUV layers (see below). A linear regression is performed using all SAGE-SBUV coincidences to determine the values of a and b. The coefficient a can be interpreted as the constant SBUV-SAGE ratio, independent of SR/SS, and is close to unity while b/a represents the SR/SS bias. Evaluating b/a for each SBUV-SAGE II pair gave very consistent results for all individual SBUV instruments with typical standard deviations over the various SBUV-SAGE pairs of about 0.01. Thus it suffices to use a value of b/a averaged over all pairs, $(b/a)_{\text{avg}}$. The SR/SS corrected SAGE ozone is thus,

$$X_{\text{SAGE},c} = X_{\text{SAGE}}/[1 + (b/a)_{\text{avg}} \ \ i]. \tag{2}$$

The SBUV-SAGE II relative differences, together with their differences calculated after the correction was applied to the SAGE II profile, are shown in Fig. 4a for NOAA16, 2001–2006, layer 10, 0–5° N. The corrected time series shows less month-to-month variability. Following a failure of the azimuth gimbal system in July 2000, the number of SAGE II measurements was reduced by a factor of two with alternating periods of sunrise-only and sunset-only occultations. Thus, every month consisted of one or the other, as opposed to some months prior to 2001 that consisted of both, thereby increasing the overall impact of the bias.

The magnitude of the bias coefficient, $(b/a)_{\text{avg}}$, is shown in Fig. 4b as a function of latitude and layer. Below layer 7 the magnitude of b did not differ significantly from zero and so no correction was applied. The magnitude is seen to increase with altitude reaching a maximum of about −0.1 in the tropics for layer 10. Above and poleward of this the magnitude decreases.

This correction was applied only to SAGE II data. Due to power issues, SAGE I measured sunrises and sunsets only during the first six months of operation; the remaining 2+ years were strictly sunsets. Analysis of the six months of sunrise + sunset data reveals no significant SR/SS bias, consistent with the results of Wang et al. (1996), who also found no significant bias between SAGE SR and SS measurements and SBUV data. The reason for this is not known. Outside of the first six months, any correction applied would amount to a constant scaling of the original data. As there is no apparent bias between the end of the SAGE I data record and the beginning of the SAGE II record, it seems reasonable to leave the SAGE I data as is.

3 SAGE-corrected SBUV ozone data set

As stated above, the SBUV(/2) data set offers global coverage spanning thirty years (1978-present). Yet differences between the individual instruments reveal unexplained biases making it unsuitable for trend analysis without some kind of bias correction. Figure 5 shows an example of these differences for layer 8 at mid-latitudes. Plotted are monthly, zonal mean ozone anomalies, expressed as a fraction of the removed annual cycle, for each SBUV(/2) instrument. Jumps of 5–10% are evident. Other latitude/layers reveal even larger discrepancies.

The biases between the individual SBUV data sets can be removed with the help of SAGE data. The SAGE I and II data sets span the first 25 years of the SBUV data record, with a 3 years long gap between them. Using the difference between SAGE monthly, zonal means and the individual SBUV monthly, zonal means directly might remove the inter-SBUV biases but would introduce sampling biases due to the greatly reduced data density of SAGE. SBUV data will populate a particular month and latitude-band equally, but SAGE may not, as is clear from Fig. 3. In more extreme cases SAGE might move through a latitude band in a single day or just graze the edge of a latitude band.

In order to avoid the introduction of a sampling bias, an intermediate step is required:

the comparison of SAGE and SBUV zonal means where only coincident data are used. It is necessary to map SAGE data, reported on a standard 0.5 km vertical grid (0.5–70 km), onto SBUV layers. Each SBUV layers is approximately 3 km thick and so will contain multiple SAGE levels. Pressure at each SAGE level, supplied in the data file, is interpolated to the mid-points between the standard SAGE grid (0.75–69.75 km). The number density is taken as a constant between the mid-point levels and used to calculate the partial ozone column between these two levels. Based on this method the partial column for each 0.5 km SAGE layer is computed. The partial column over each SBUV layer is then determined by summing over all SAGE layers it contains. For SAGE layers that span two SBUV layers, it is split between them according to the fraction overlap, in pressure.

SAGE-SBUV coincidences are determined for each combination of SAGE and SBUV instrument that overlap in time. The coincidence criteria adopted are same-day and within 1000 km. This ensures that the large majority of SAGE observations have a coincidence with SBUV. If more than one SBUV observation met these criteria then the one closest in distance was used. Only SBUV and SAGE data that passed their respective screening criteria are retained. In addition, for a given SBUV-SAGE instrument pair, the distribution of monthly-mean differences for a particular latitude and layer were examined. Months in which this difference was outside of the mean ±5-sigma were excluded. Such differences are typically caused by errors in SAGE profiles. For example, in at least one case the cause of the anomalously large difference appeared to be an altitude shift of the SAGE II profiles by about 500 m that lasted ~3 days. Overall, very few monthly-means were removed based on this 5-sigma criteria, significantly less than 0.1%.

Zonal, monthly-means were calculated over 5°-wide latitude bands, centred at −87.5°, −82.5°,..., 87.5°, for:

i. SBUV, all data

ii. SBUV, considering only SAGE-SBUV coincidences

iii. SAGE (diurnal bias removed), considering only SAGE-SBUV coincidences.

The means were computed for each SBUV(/2) and for each SAGE-SBUV pair that overlapped in time.

The Nimbus 7 data set (1978–1990) was used to calculate an annual cycle which was then subtracted from each time series (i, ii, and iii, above), yielding ozone anomalies. The bias correction for a given SBUV is taken as the difference between the coincident SAGE and SBUV anomaly time series (SAGE minus SBUV). A three-month running mean of this correction is found. Of the three months being averaged over, if one or two months are missing, the mean is calculated over the month(s) for which data is present. This smoothed-correction is then applied to each time series of SBUV monthly-mean anomalies.

The steps outlined above are shown in Fig. 6 using SBUV2 from NOAA 9 (40–45° N, layer 8) as an example. Panel (a) shows the three initial time series and panel (b) with their annual cycles removed. The correction, smoothed and unsmoothed, is shown in panel (c). The original, from panel (a), and corrected data are shown in panel (d), after the addition of the annual cycle. Note the correction is not constant in time and so simply shifting the data to match another SBUV(/2) would introduce spurious trends.

Figure 7 shows the corrections at 40–45° S and 40—45° N, layer 8, that need to be applied to each SBUV(/2). The gap between SAGE I and II is taken as constant in time as there is no relative bias between the two due to the correction applied to SAGE I data (Wang et al., 1996). The same constant was also used to fill the gaps in the SBUV-SAGE I differences record since there are periods where the number of SAGE I profiles is not enough to estimate the SBUV-SAGE I bias within a 3-month window.

Corrected SBUV ozone anomalies are shown in Fig. 8, and can be compared with the original data in Fig. 5. For periods of overlap there are virtually no inter-SBUV differences. The final data set is obtained by taking the average over all instruments for these overlap periods. This is referred to as the SAGE-corrected SBUV ozone data. Latitude-time slices of the SAGE-corrected SBUV data set for layers 4 and 8 are shown in Fig. 9 were deviations in percent from the annual cycle (estimated for the period 1978–1990) are plotted. Figure 9 shows no major gaps in data (except for the two volcanic eruption periods and a gap due to a SAGE record interruption in 2000(?). The tro panels show on overall ozone decline from the early 1980s to the late 1990s over middle and high latitudes. The QBO signal is also evident from the plot. Calculating the zonal-monthly mean anomalies in the tropics now reveals a high level of consistency in the SAGE-corrected SBUV ozone QBO signal with the SAGE II QBO signal from Fig. 1. This is shown in Fig. 10.

4 Regression analysis

A statistical regression analysis of the SAGE-corrected SBUV ozone data set was performed to estimate long-term ozone changes and compare them with the available long-term trend estimates for SBUV and SAGE data (WMO, 2007). The ozone time series for each latitude band and layer were fit with a regression model including seasonal cycle, equivalent effective stratospheric chlorine (EESC), solar cycle, and QBO, as explanatory variables (WMO, 2007 and references therein) . The EESC term is a measure of the stratospheric halogen burden and is used in the regression analysis to isolate long-term ozone changes associated with the amount of ozone depleting chlorine and bromine in the stratosphere. The EESC function used here increases nearly linearly from 1979 to its maximum in 1997 and thus the EESC fit to ozone can be expressed as decadal ozone change in percent during that time (Stolarski et al., 2006; WMO, 2007). The QBO time series are based on observed equatorial winds at 30 hPa and 50 hPa and the solar cycle term is the standard F10.7 radio flux. The regression model includes a constant and an annual harmonic term for the regression coefficients of the EESC and QBO function.

Figure 11a shows the meridional cross section of zonal mean ozone trends derived from the ozone projection onto the EESC term for the combined data set presented in this study. The long term changes of ozone profiles show a maximum in the region above 40 km reaching –10% per decade around 60° S. The negative trend decreases towards the equator where it shows values between 0 and −2% and is statistically not significant. In the NH upper stratosphere a negative trend of up to −6% can be found. Between 35 and 25 km the trend is small with values around 2% for all latitude bands. For comparison Fig. 11b and c show zonal mean ozone trends for SAGE (I+II) and SBUV(/2), respectively. The estimates for SAGE (I+II) and SBUV(/2) ozone trends are derived from regression onto EESC and taken from WMO, (2007, their Figs. 3–7). The magnitude of the trend for the combined data set is similar to that for the SBUV data set, although the vertical structure of the latter is smoothed due to its vertical resolution. There is also some difference in trend values in the tropical upper stratosphere (layers 9–11); however trend uncertainties are also large there. These uncertainties are partially related to ozone values in 2001–2005 when the number of SAGE II measurements was reduced substantially. It should be also mentioned that it is possible that long-term temperature trends in the upper stratosphere are not correctly reproduced in the NCEP data set (Randel at al., 2009), which was used to convert SAGE data on the altitude grid to the SBUV pressure-based levels. If so, this may have an impact on the estimated ozone trends derived from the SAGE-corrected SBUV data set. Assessing this will require additional investigation.

5 Summary

A stratospheric monthly, zonal-mean ozone data set based on Satellite Aerosol and Gas Experiment (SAGE) and Solar Backscatter UltraViolet (SBUV) data spanning 1978–2005 was presented. Drifts in individual SBUV instruments and inter-SBUV biases are corrected using SAGE I and II by calculating differences considering SAGE-SBUV coincidences. In this way the daily, near-global coverage of SBUV(/2) is combined with the stability of SAGE to provide a homogeneous ozone record. The resultant SAGE-corrected SBUV data set shows a realistic Quasi-Biennial Oscillation signal in contrast to other SBUV data sets. In addition, a regression analysis produced trend estimates consistent with other current estimates.

The SAGE-corrected SBUV data set presented is limited by the end of the SAGE II operations. However, with multiple SBUVs still in operation this method can be used to extend the time series using solar occultation instruments such as FTS or MAESTRO on the ACE satellite to provide the bias correction.

The SAGE-corrected SBUV data set is available for download at ftp://es-ee.tor.ec.gc.ca/pub/SAGE_corrected_SBUV.

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Table 1. SBUV (v8) layer definitions. Layer 1, not used in this study, is 1013–63.9 hPa.

SBUV layer number	Pressure limits (hPa)	Approximate altitude (km)
2	63.9–40.3	21
3	40.3–25.5	24
4	25.5–16.1	27
5	16.1–10.1	30
6	10.1–6.39	33
7	6.39–4.03	37
8	4.03–2.55	40
9	2.55–1.61	43
10	1.61–1.01	46
11	1.01–0.64	49

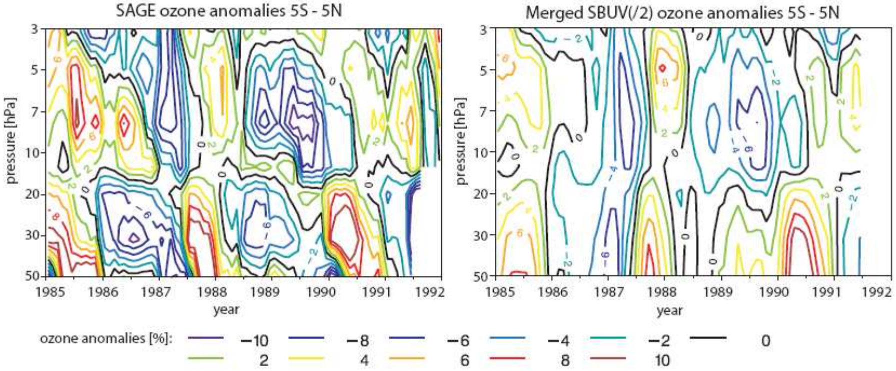

Fig. 1. Quasi-biennial signals in **(a)** SAGE II data and **(b)** merged SBUV data. Plotted are monthly, zonal-mean ozone anomalies in the tropics (5° S–5° N). Anomalies were calculated as percent deviations from the 1978–1990 means.

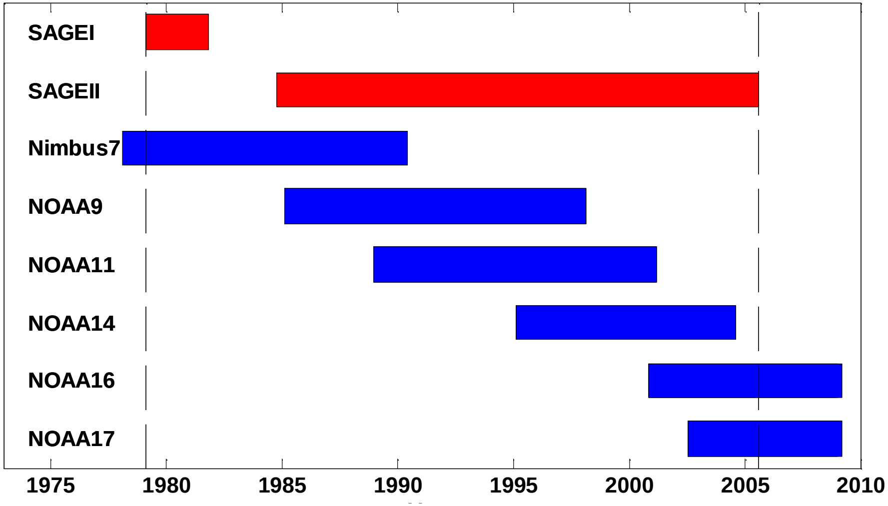

Fig. 2. Satellite instruments used in this study, and their temporal coverage. Dashed vertical lines indicate period of overlap used to create SAGE-corrected SBUV dataset (red – SAGE instruments, blue – SBUV(/2) instruments).

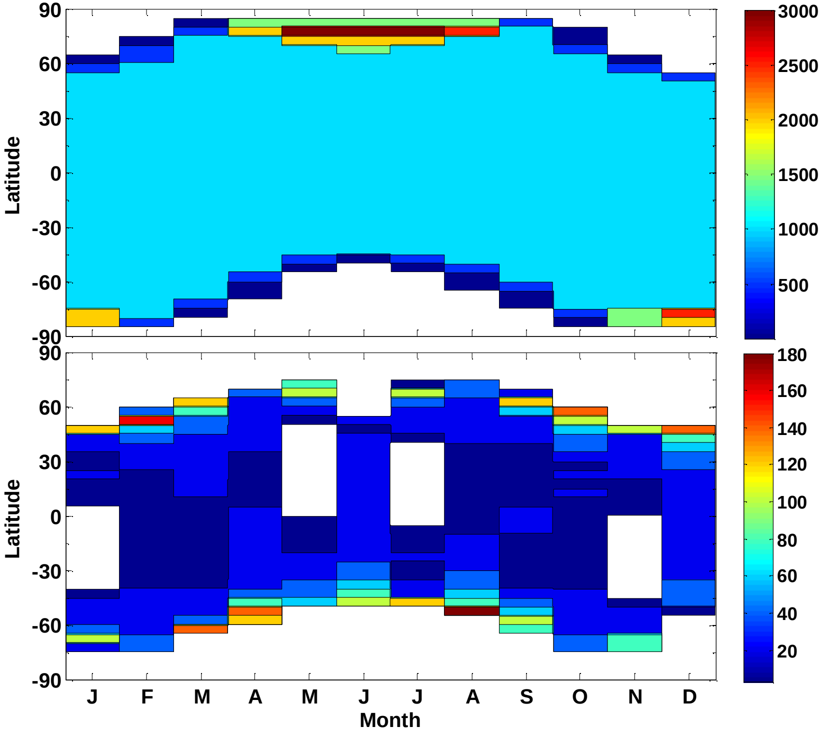

Fig. 3. Comparison of NOAA14/SBUV2 (top) and SAGE II (bottom) data density. Shown is the number of profiles in each month and latitude bin for 1997. White indicates months/latitudes with no data.

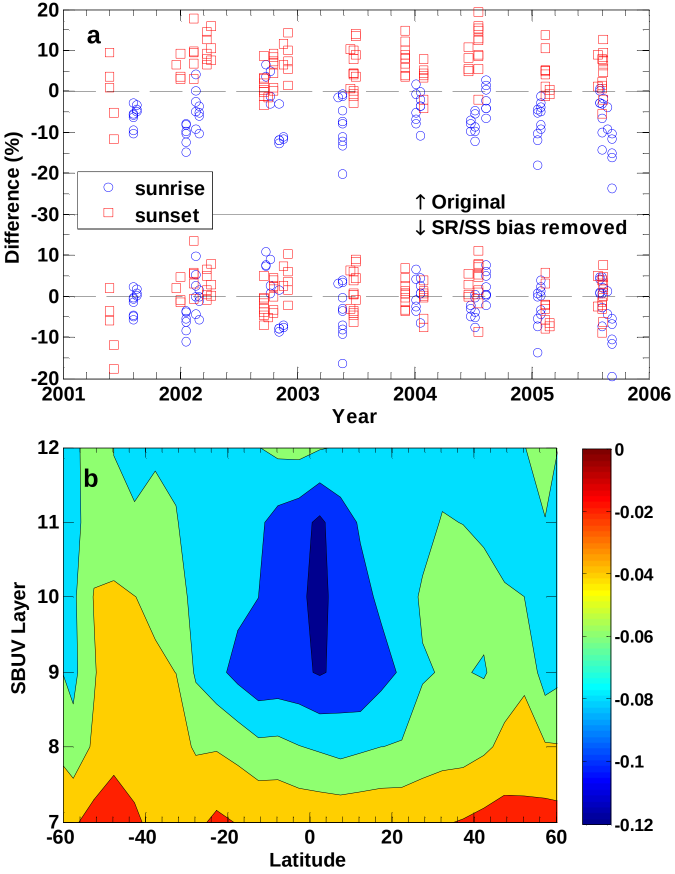

Fig. 4. **(a)** Relative difference between SAGE II and NOAA16/SBUV2 ozone partial columns in layer 10 at 0–5° N before and after the sunrise/sunset (SR/SS) bias was removed. **(b)** SR/SS bias, $(b/a)_{\mathrm{avg}}$, coefficient as determined using Eq. (1).

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Interactive Discussion

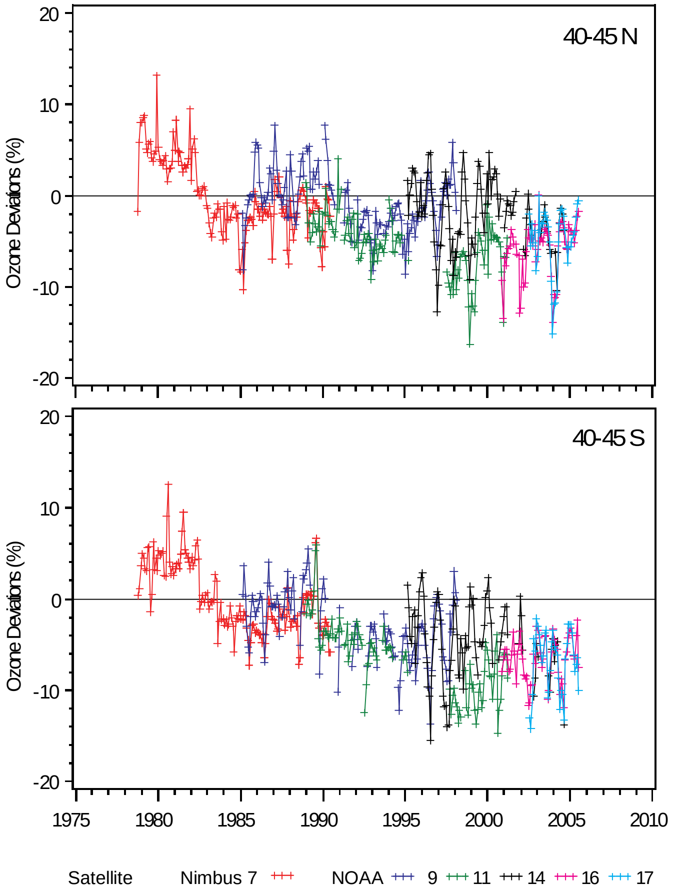

Fig. 5. Time series of SBUV(/2) zonal mean ozone deviations in layer 8 (~40 km) at 40–45° N (top) and 40–45° S (bottom) for Nimbus 7, and NOAA 9, 11, 14, 16, and 17 instruments. Ozone deviation is defined as the anomaly/mean.

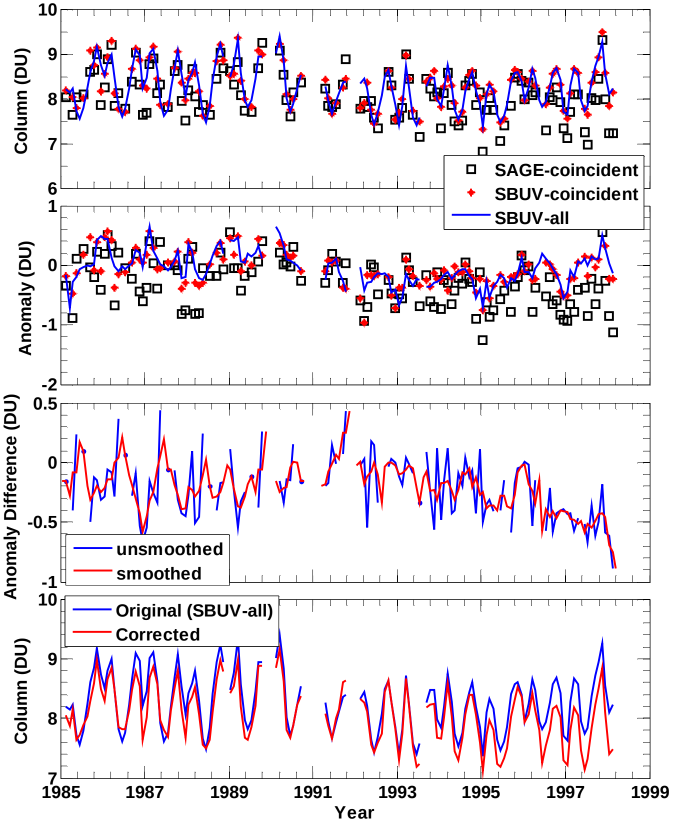

Fig. 6. Steps in the removal of the SBUV bias illustrated for NOAA 9, 40–45° N, layer 8: **(a)** monthly, zonal-mean ozone for SAGE data (coincident with SBUV), SBUV (coincident with SAGE II), and SBUV; **(b)** as (a) after the removal of the annual cycle, **(c)** difference between SAGE II and SBUV coincident means, before and after application of a 3-month running mean; **(d)** original, from panel (a), and corrected SBUV time series after the annual cycle has been added.

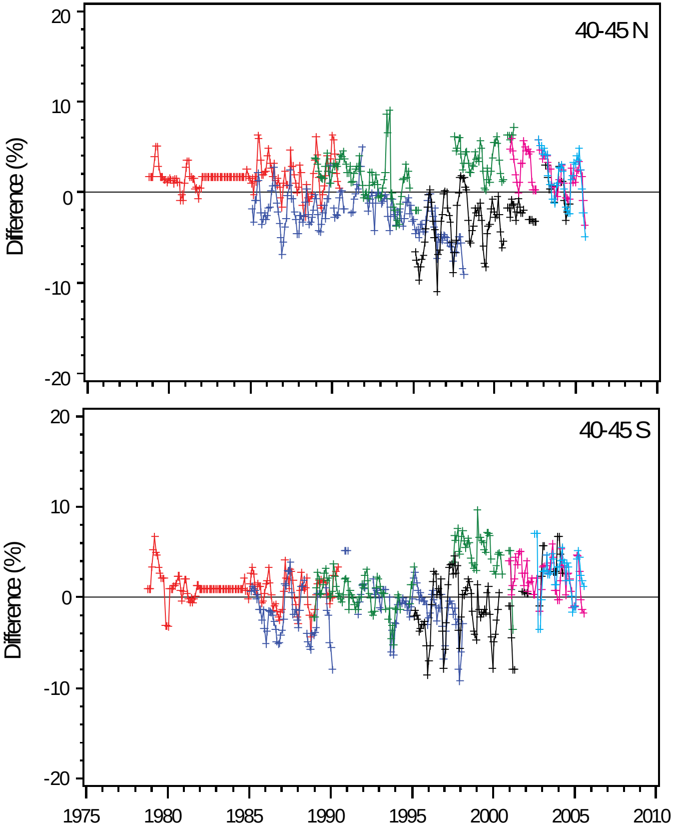

Fig. 7. Differences between SAGE and SBUV(/2) monthly, zonal-means (considering only coincident data) in layer 8 (∼40 km) at 40–45° N and 40–45° S for Nimbus 7, and NOAA 9, 11, 14, 16, and 17 instruments.

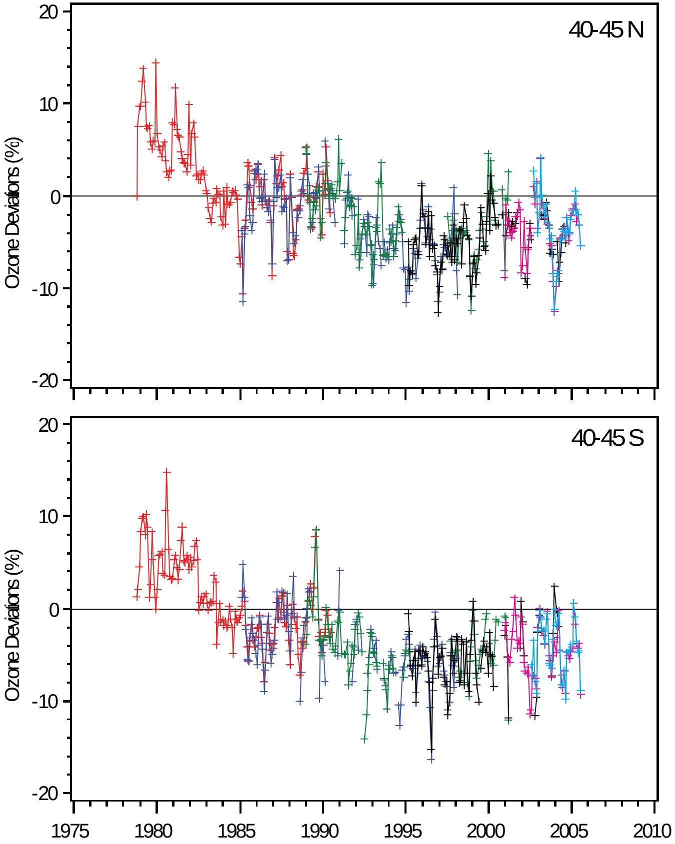

Fig. 8. Time series of SAGE-corrected SBUV(/2) zonal mean ozone deviations (considering only coincident data) in layer 8 (~40 km) at 40–45° N and 40–45° S for Nimbus 7, and NOAA 9, 11, 14, 16, and 17 instruments. Ozone deviation is defined as the anomaly/mean.

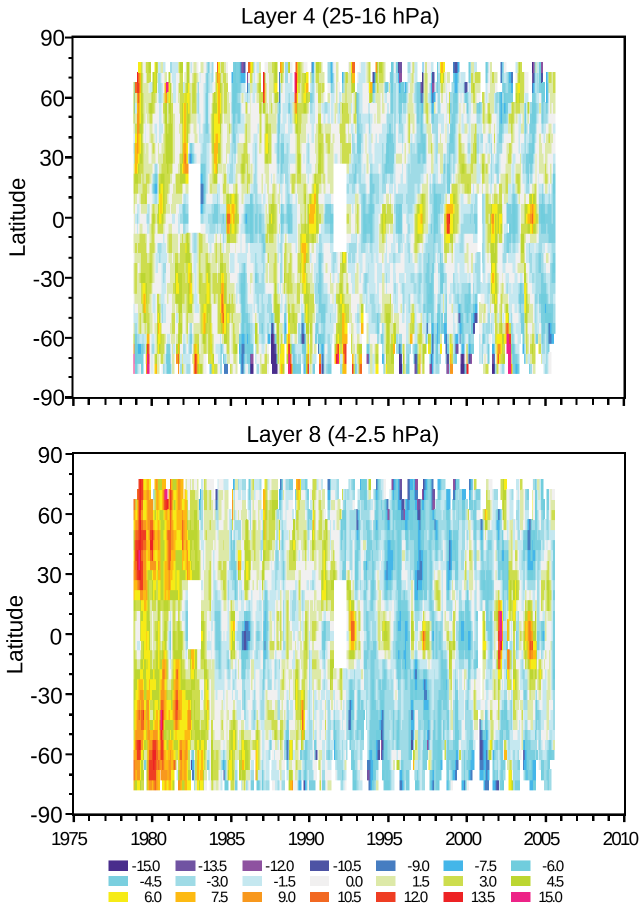

Fig. 9. Latitude-time slices of SAGE-corrected SBUV ozone residuals. Deviations in percent from the annual cycle (estimated for the period 1978–1990) are plotted. Layer 4 (top) and layer 8 (bottom) are shown.

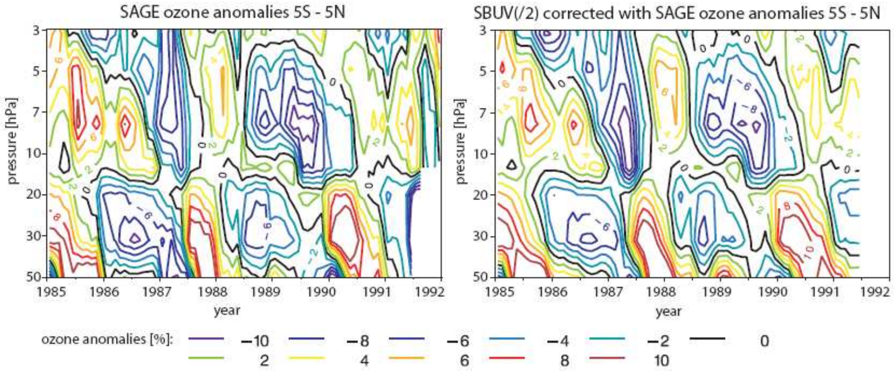

Fig. 10. Quasi-biennial signals in **(a)** SAGE II data and **(b)** SAGE-corrected SBUV data. Plotted are monthly, zonal-mean ozone anomalies in the tropics (5° S–5° N).

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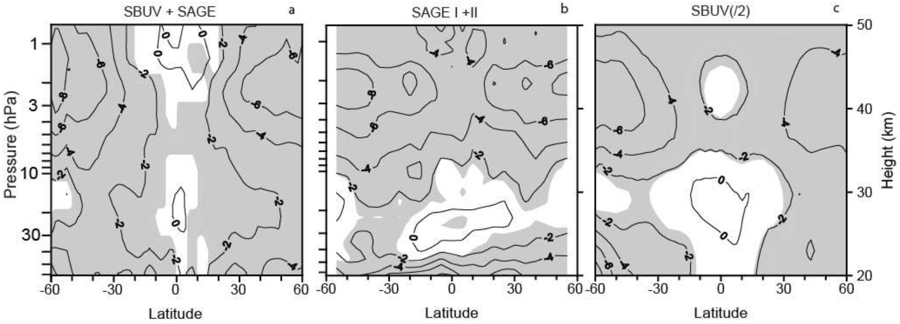

Fig. 11. Annual ozone trends in percent per decade as a function of latitude and altitude/pressure for the period 1978–2005 derived from regression analysis for **(a)** the SAGE-corrected SBUV (this work), **(b)** SAGE I+II, and **(c)** merged SBUV(/2). Shadings indicate that the changes are statistically significant at the 2σ level.