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Interpreting SBUV smoothing errors: an example using the Quasi-Biennial Oscillation

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Abstract

The Solar Backscattered Ultraviolet (SBUV) observing system consists of a series of instruments that have been measuring both total ozone and the ozone profile since 1970. SBUV measures the profile in the upper stratosphere with a resolution that is adequate to resolve most of the important features of that region. In the lower stratosphere the limited vertical resolution of the SBUV system means that there are components of the profile variability that SBUV cannot measure. The smoothing error, as defined in the Optimal Estimation retrieval method, describes the components of the profile variability that the SBUV observing system cannot measure. In this paper we provide a simple visual interpretation of the SBUV smoothing error by comparing SBUV ozone anomalies in the lower tropical stratosphere associated with the Quasi Biennial Oscillation (QBO) to anomalies obtained from the Aura Microwave Limb Sounder (MLS). We describe a methodology for estimating the SBUV smoothing error for monthly zonal mean (mzm) profiles. We construct covariance matrices that describe the statistics of the inter-annual ozone variability using a 6-yr record of Aura MLS and ozonesonde data. We find that the smoothing error is of the order of 1 % between 10 hPa and 1 hPa, increasing up to 15–20 % in the troposphere and up to 5 % in the mesosphere. The smoothing error for total ozone columns is small, mostly less than 0.5 %. We demonstrate that by merging the partial ozone columns from several layers in the lower stratosphere/troposphere into one thick layer, we can minimize the smoothing error. We recommend using the following layer combinations to reduce the smoothing error to about 1 %: surface to 25 hPa (16 hPa) outside (inside) of the narrow equatorial zone 20° S–20° N.

1 Introduction

Measurements from the series of Solar Backscattered Ultraviolet (SBUV) instruments provide the longest record of satellite-based global ozone profiles, spanning the period from April 1970 through the present, except for a 5-yr gap in the 1970s (McPeters et al., 2012). The SBUV instruments measure solar radiance in the ultraviolet spectral range between 250 and 340 nm backscattered by the Earth's atmosphere and surface in the nadir direction. The SBUV series includes the Nimbus-4 BUV, Nimbus-7 SBUV, and seven SBUV(/2) instruments launched on NOAA operational satellites (NOAAs 09, 11, 14, 16, 17, 18, and 19). Data from all instruments have been reprocessed with the version 8.6 (v8.6) retrieval algorithm. In v8.6 the Optimal Estimation technique (Rodgers, 2000) is used to retrieve ozone profiles as ozone layer amounts (partial columns, DU) in 21 pressure layers. Consistency among SBUV instruments in v8.6 is achieved through radiance-level adjustments based on precise comparison of radiance measurements during the periods when instruments overlapped (DeLand et al., 2012). Despite the evolution in instrument design from the first BUV version to the modern SBUV(/2) model, the fundamental features of the measurement technique remain the same (Bhartia et al., 2012), lending further consistency to the SBUV long-term record compared to those based on measurements using different instrument types and making the SBUV data preferable for long-term trend analysis. However, an understanding of the characteristics of the SBUV retrieval algorithm and related uncertainties is essential for proper interpretation of the data. The goal of this paper is to demonstrate the benefits and limitations of the SBUV retrieval algorithm and provide clear recommendations for SBUV data users.

In Sect. 2 we visually illustrate the SBUV smoothing error due to the limited vertical resolution. We then describe the methodology used to estimate the smoothing error for the SBUV mzm ozone profiles. We also introduce and analyze parameters that compose the smoothing error. In Sect. 3 we analyze the patterns of the SBUV smoothing error and make recommendations for best use of the data. In the last section we summarize our results. Hereafter we will use "SBUV" to refer to all instruments.

2 Smoothing error

The primary source of error in the SBUV retrieval algorithm, particularly in the troposphere and lower stratosphere, is the smoothing error due to the limited vertical resolution of the SBUV observing system (Bhartia et al., 2012). The smoothing error represents the difference between the retrieved profile and the true profile due to vertical smoothing by the retrieval algorithm (Rodgers, 2000). When the vertical resolution is low, the retrieval algorithm relies on the a priori information. Therefore the smoothing error depends on the vertical resolution of the observing system, the accuracy of the a priori data, and the magnitude of the natural ozone variability (Rodgers, 2000). For the first time with the v8.6 dataset we include estimates of the smoothing error for the monthly zonal mean (mzm) SBUV data product, also newly available in v8.6.

2.1 QBO detection: a smoothing error example

A vivid example of the smoothing error is the misrepresentation of the Quasi-Biennial Oscillation (QBO) signal in the SBUV data in the lower tropical stratosphere (e.g. Hollandsworth et al., 1995). The QBO is a quasi-periodic oscillation between easterly and westerly regimes of the equatorial zonal wind, which in turn effects the distribution of chemical constituents, such as ozone, water vapor, and methane, due to induced circulation changes (e.g. Baldwin et al., 2011). The period of the QBO varies from 24 to 32 months with an average period of about 28 months. One of the pronounced features of the equatorial QBO is its downward vertical propagation with a rate of about 1 km month^{-1} (e.g. Baldwin et al., 2011).

Figure 1 shows time series of the deseasonalized mzm ozone anomalies obtained from NOAA17 SBUV/2 (black lines) and Aura Microwave Limb Sounder (MLS) (red lines) over the tropics (0–5° N) for several layers in the stratosphere. The deseasonalized anomalies are calculated by subtracting seasonal cycles from each data set independently to remove systematical biases between the observing systems. There is a clear QBO signal in both datasets between 100 and 6.4 hPa, but the phases of

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the QBO signals are shifted. SBUV "sees" the same phase of the QBO at all layers, while MLS shows a vertical downward propagation of the QBO signal over time. Also, the amplitude of the QBO signal derived from MLS is larger compared to that derived from SBUV. Neither data set shows a QBO above 6.4 hPa. The magenta lines in the panels of Fig. 1 show the MLS anomalies convolved by the SBUV averaging kernels. The convolved MLS anomalies agree well with the SBUV anomalies, meaning that the differences in the original profiles are due solely to the differing vertical resolutions. This is particularly evident in layers below 16 hPa. For the layers between 100 and 6.4 hPa, the convolved MLS now shows the same QBO phase lag as the SBUV measurements. The difference between the deseasonalized MLS and SBUV anomalies shows the portion of ozone variability that the SBUV observing system cannot measure, and this quantity can be understood as the SBUV smoothing error.

We will now describe the methodology for estimating the smoothing error and introduce and analyze parameters that compose the smoothing error.

2.2 Mathematical definition of smoothing error

According to Rodgers (2000) smoothing error can be calculated as:

$$\mathbf{S}_{\text{serr}} = (\mathbf{A} - \mathbf{I}) \cdot \mathbf{C} \cdot (\mathbf{A} - \mathbf{I})^T, \tag{1}$$

where **I** is a unit matrix, **A** is a matrix that represents the sensitivity of the SBUV retrival $\hat{\boldsymbol{x}}$ to the true state $\boldsymbol{x}$: $\mathbf{A} = \partial \hat{\boldsymbol{x}} / \partial \boldsymbol{x}$; and **C** is the covariance matrix of an ensemble of true states about the mean state, calculated as

$$\mathbf{C} = \text{cov}\{(\boldsymbol{x} - \bar{\boldsymbol{x}})(\boldsymbol{x} - \bar{\boldsymbol{x}})^T\}. \tag{2}$$

In Eq. (2), $\boldsymbol{x}$ is a set of independent high-resolution ozone profiles that characterize the ozone variability.

In this representation, the resulting quantity $\mathbf{S}_{\text{serr}}$ is the smoothing error covariance matrix, which can be understood as an "error pattern" (Rodgers, 1990). $\mathbf{S}_{\text{serr}}$ is defined

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by two parameters: the SBUV **A** matrix and the covariance matrix **C**. In short, the **A** matrix provides information on the resolution that can be achieved by the retrieval, while the **C** matrix provides information on the magnitudes of the true ozone variability. Before analyzing the smoothing errors, we consider each of these parameters separately.

2.3 SBUV averaging kernels

The SBUV **A** matrix has dimensions of number of layers by number of layers, though the top layer is not included, so the dimensions are 20 by 20. The **A** matrix shows how information from measurements and a priori are utilized during the retrieval process. A column of the **A** matrix at a given layer l gives the response of the retrieval at each layer to a delta-function perturbation of ozone amount in layer l; a row of the **A** matrix at a given layer l indicates the sensitivity of the retrieved ozone at layer l to delta-function perturbations of ozone at each layer (Rodgers, 2000). Rows of the **A** matrices are called the averaging kernels (AK), while columns are referred to as the response functions. Hereafter, we will follow Rodgers terminology and use a term "AK" to refer to rows of the **A** matrix.

The shape of the AK for each layer describes the vertical resolution of the observing system at that layer. An idealized AK for a defined layer would have a Gaussian shape with an integrated value of about one, and a width within the boundary of the layer. Limitations of the resolution are indicated when the AK peak is very broad and displaced in altitude (Rodgers, 2000).

Figure 2 shows typical SBUV AK for the northern midlatitudes and tropics. The SBUV AK for layers between 16 and 1 hPa have sharp maxima at nominal altitudes. This means that the SBUV algorithm is capable of accurately retrieving layer ozone amounts in this vertical range. The AK for layers below 16 hPa (and above 1 hPa) have broad peaks, which are shifted upward (downward), showing that the retrievals are more sensitive to ozone changes at higher (lower) layers. In these vertical ranges, the SBUV retrievals contain less information about the true ozone changes at these layers, and the retrieval algorithm relies on the a priori. In the tropics the shapes of the AK for layers below 10 hPa differ from those at mid-latitudes (see Fig. 2). Peaks of the tropical AK for layers below 25 hPa are shifted upward with the maximum around 25 hPa, and the amplitudes of the AK are significantly reduced below 60 hPa. Thus, compared to mid-latitudes, the tropical retrievals are less sensitive to ozone changes in the lower stratosphere and troposphere and heavily rely on a priori information.

We note that the **A** matrix as described here is normalized by the a priori and applicable to profiles of fractional ozone change. The normalization is done as follows:

$$\mathbf{A}(i,j) = \mathbf{A}_{\mathrm{ik}}(i,j) \cdot \boldsymbol{x}_a(j)/\boldsymbol{x}_a(i) \tag{3}$$

where $\boldsymbol{x}_a$ is the SBUV a priori profile, and i and j are layer indices. The $\mathbf{A}_{\mathrm{ik}}$ matrix should be used when analyzing ozone profiles in SBUV native units of layer amount (DU/layer). Bhartia et al. (2012) refer to the rows of the $\mathbf{A}_{\mathrm{ik}}$ matrix as integrating kernels.

The number of independent pieces of information available from measurements is given by the diagonal elements of the **A** matrix, known as Degrees of Freedom for Signal (DFS) (Rodgers, 2000). Note that the diagonal elements of **A** and $\mathbf{A}_{\mathrm{ik}}$ are the same. The sum of all diagonal elements of the **A** matrix – the total DFS – varies from 3.7 to 6.9 out of the 6–9 wavelengths used in the retrieval algorithm depending on the solar zenith angle (SZA). The retrieval algorithm uses only 6 wavelengths for small SZA and 9 wavelengths for high SZA (Bhartia et al., 2012). As a result the DFS is larger for higher SZA.

Each diagonal element of the **A** matrix in turn indicates the DFS for the individual layer. Figure 3 shows the layer DFS for the northern mid-latitudes in winter and summer (blue and green lines, respectively) and for the tropics (red line). Peaks of the layer DFS occur between 25 and 1 hPa, where the layer DFS are about 0.5. The total DFS is larger in northern mid-latitudes in winter (5.5) and slightly decreases in summer (5.0). The increase of total DFS in winter is due to the higher SZAs and resulting increased vertical resolution in the upper layers. The layer DFS also increases in the upper layers when the satellite approaches the terminator and SZA rapidly increases. In the tropics, SZA does not significantly change with season, and the **A** matrices are similar for all

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seasons. The shapes of the layer DFS in the tropics and mid-latitudes in summer (red and green lines on Fig. 3) are very similar above 25 hPa, but below 40 hPa the tropical layer DFS abruptly decreases.

Since the diagonal elements d_s of the **A** matrix show the DFS per layer, one can estimate the vertical resolution as the number of layers per degree of freedom $1/d_s$ (Rodgers, 2000). The AK show that the vertical resolution of the SBUV algorithm is about 6 km near 3 hPa, decreasing to 15 km in the troposphere (Bhartia et al., 2012).

2.4 Ozone mzm covariance matrix

The second parameter that defines the smoothing error is the covariance matrix, which is used to represent the statistics of ozone variability. We are computing the smoothing error for SBUV mzm profiles, and therefore we need to construct appropriate covariance matrices that will characterize typical year-to-year variability of the ozone mzm profiles for each latitude bin.

Aura MLS profiles provide the high vertical and spatial resolution needed to obtain the statistics of ozone variability (e.g. Froidevaux et al., 2008). In the troposphere, we extend MLS profiles by merging them with ozone sonde mzm profiles, obtained from the ensemble of 49 stations listed in Table 1. We construct MLS mzm time series over the 6-yr period from January 2005 to December 2010 for each 5-degree zonal bin using version 3.3 daytime-only MLS profiles with SZAs less than 83°. Additional filtering is applied according to recommendations outlined in the MLS Version 3.3 users guide (Livesey et al., 2011). We distribute sonde data by latitude bins according to the recommendations provided by McPeters and Labow (2012) to account for limited sampling in some latitude bins. Data from many sonde stations were not available during the Aura MLS period, so we instead used sonde data over the 6-yr period from January 2000 to December 2005. The sonde mzm time series were smoothed using a 3-month moving average to reduce noise. Both MLS and sonde profiles were preliminary converted into ozone partial columns at SBUV pressure layers.

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We merge Aura MLS and sonde mzm profiles in the altitude range between 160 and 40 hPa (layers 5–7) using a proportional 75/50/25 % weighting for lower/mid/upper parts of the range. Since the SBUV technique depends on backscattered solar radiation, measurements at high-latitudes are not possible in winter months. Thus we estimate the statistics of the ozone variability at high latitudes using data only in months when SBUV ozone measurements exist (see Table 2). The covariance matrices for each 5-degree latitude bin have been calculated by employing Eq. (2), and are included in the SBUV mzm data files.

The resulting covariance matrix **C** is a matrix with dimensions of number of layers by number of layers (20 by 20; top layer not included), with the diagonal elements equal to the squares of the standard deviations of mzm profiles. Figure 4 shows the square roots of the diagonal elements of the covariance matrices for three different latitude bins as a percent from the a priori. Standard deviations vary between 2–15 %, increasing in the troposphere and lower stratosphere. However, in the lower tropical stratosphere between 100 and 10 hPa standard deviations are larger compared to mid- and high-latitudes due to the QBO.

Off-diagonal elements of **C** reveal correlations among the layers. If the correlation between any two layers is high, the corresponding off-diagonal elements will also be large, and vice versa. We do not analyze off-diagonal elements of **C** here, as they are difficult to visualize. In addition, a simple sensitivity test in which the smoothing error was calculated with the off-diagonal elements of covariance matrices set to zero showed that the off-diagonal elements had a very small effect on the smoothing error values. Nevertheless off-diagonal elements of the covariance matrices are included in our computation of the smoothing error matrix.

3 Application of smoothing error concept to SBUV data analysis

It is not easy to analyze and understand errors represented in terms of the smoothing error covariance matrix (see Eq. 1). To simplify the analysis, we ignore inter-level

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correlation and assume that the square roots of the diagonal elements of $\mathbf{S}_{serr}$ represent the smoothing errors for individual layers. We also calculated eigenvectors of $\mathbf{S}_{serr}$ and found that diagonal elements provide a reasonable estimation of the layer smoothing errors. However, the smoothing error for total ozone is calculated as a square root of a sum of all elements of $\mathbf{S}_{serr}$ (including off-diagonal). In the mzm SBUV files we report the smoothing error as a percent (%) from the retrieved layer ozone amount.

3.1 Profile and total ozone smoothing error

Figure 5 shows profiles of the smoothing error at 45–50° N in winter and summer (blue and green lines, respectively) and at 0–5° N (red line). In the stratosphere between 10 and 1 hPa, where the SBUV vertical resolution is the highest, the smoothing errors are of the order of 1–2 %. Larger smoothing errors (as large as 15–20 %) occur in the troposphere. Errors also increase up to 5 % in the mesosphere above 1 hPa.

In the mid-latitudes the layer smoothing errors vary with season due to seasonal changes of the AK. It is important to remember that the covariance matrix is a function of latitude only. Thus, all temporal changes in the smoothing errors are defined by the temporal changes in the AK. Overall, there is a very good correspondence between seasonal changes of the layer DFS and smoothing error (Figs. 3 and 5). At those layers where the DFS is larger the corresponding smoothing errors are smaller and vice versa.

In the tropical stratosphere below 10 hPa the layer smoothing errors are notably greater compared to the mid- and high-latitudes. We previously noted a decrease of the tropical layer DFS below 40 hPa. However, the smoothing error increases in the tropics primarily because of the larger inter-annual ozone variability in the tropical lower stratosphere associated with the QBO (see Fig. 4).

Figure 6 shows time series of the total ozone smoothing error at 0–5° N and 45–50° N. Smoothing errors for the total ozone vary between 0.2–1.2 %. The off-diagonal elements of the $\mathbf{A}$ matrix play a significant role in defining the error range for total ozone. The total ozone errors notably increase when the satellites approach the terminator and SZA increases. It might seem contradictory, since the total DFS increase with increasing SZA, implying that we have more information from measurements. But the increase in total DFS is related to increased sensitivity in the upper layers, not in the lower layers, which dominate total ozone. In the lower layers the diagonal elements of **A** change little with the SZA, while the off-diagonal elements of **A** in turn are very sensitive to SZA changes and decrease as SZA increases. Thus, as a result the total ozone smoothing error increases with increasing SZA.

We confirmed these results by running a sensitivity test in which the smoothing error was calculated with the off-diagonal elements of **A** set to zero. The changes to the layer smoothing error were small, but the total ozone smoothing errors increased by a factor of 5–10 (up to 2–6 %) when off-diagonal elements of **A** were ignored.

3.2 Recommendations for reducing the smoothing error

As we demonstrated, the smoothing error in the lower stratosphere and troposphere can be significant and caution should be taken when comparing SBUV ozone profiles with highly resolved profiles. One approach to such comparisons is to convolve a highly resolved profile with the SBUV AK (or integrated kernels) as shown in Fig. 1. We use $\mathbf{A}_{ik}$ here because we are comparing ozone partial column profiles (see Sect. 2.3 and Eq. 3). The profile with finer vertical resolution should be degraded first onto the SBUV vertical scale and then convolved using the SBUV $\mathbf{A}_{ik}$ matrix (Rodgers, 2000):

$$\boldsymbol{x}_{\text{smoothed}} = \boldsymbol{x}_a + \mathbf{A}_{\text{ik}} \cdot (\boldsymbol{x}_{\text{hr}} - \boldsymbol{x}_a) \quad (4)$$

where $\boldsymbol{x}_{\text{hr}}$ is the highly resolved profile converted to partial ozone columns and degraded to the SBUV scale.

However, it is not clear how to convolve a highly resolved profile that covers only a part of the atmosphere. For example, lidar instruments typically measure ozone only between 20 and 50 km, while the SBUV $\mathbf{A}_{ik}$ is supposed to be applied to the entire profile from the surface to top of the atmosphere. Liu et al. (2010) use MLS partial ozone columns complemented with Ozone Monitoring Instrument (OMI) retrievals below 215 hPa to convolve MLS ozone profiles with OMI AK. But different observing system have different sensitivities and vertical resolutions, and this approach might "project" the uncertainties of one observing system onto the other. Alternatively, the missing part of the profile could be assumed to be equal to the a priori, and then the term in brackets in Eq. (4) will be equal to zero in the vertical range where measurements are missing.

We tested these two approaches to convolving Aura MLS profiles (which cover the vertical range between 250 and 0.1 hPa) with the SBUV $\mathbf{A}_{ik}$. In the first approach we complemented MLS profiles below 250 hPa by the SBUV retrievals, and in the second approach we used the SBUV a priori profiles. We found that the difference between the two convolved profiles is fairly small (less 0.5 %) in the vertical range between 25 and 1 hPa, where the SBUV vertical resolution is the highest. At the same time, between 250 and 25 hPa, where the SBUV vertical resolution is limited, the difference between two approaches can be up to ±3 %. We found even larger differences (up to ±10 %) between the two approaches when we convolved lidar profiles. These differences reflect an additional source of uncertainty in the convolved profile. Further, the physical interpretation of comparisons with the convolved profiles is a challenge.

To avoid these complications, we propose merging several layers in the lower stratosphere/troposphere, where the smoothing errors are large, into a single thick combined layer. By merging several SBUV layers we can increase the DFS for the combined layer and decrease the corresponding smoothing error. Our previous analysis of the AK (see Fig. 2) indicates a limitation of the retrievals below 25 hPa (below 16 hPa) outside the tropics (in the tropics). Thus we test the resulting smoothing error when combining layers below these thresholds. Because the amplitudes of the AK are significantly reduced for layers below 250 hPa, we also test the layer combinations from 250 to 25 hPa (or 16 hPa) outside of the tropics (in the tropics). These layer combinations would be useful for comparisons with Aura MLS profiles that do not measure to the ground.

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The smoothing error for a merged layer $S_{\mathrm{serr}}^{k_o,k_n}$ can be estimated by using the following expression:

$$S_{\mathrm{serr}}^{k_o,k_n} = \sqrt{\sum_{i=k_0}^{i=k_n}\sum_{j=k_0}^{j=k_n} \mathbf{S}_{\mathrm{serr}}(i,j)} \tag{5}$$

where k_0 and k_n are indices for the bottom and top layers included into the merged layer.

Figure 7 shows the smoothing error as a function of latitude for several layer combinations. It is very important to note that even when the smoothing error for any individual layer in the troposphere/lower stratosphere is large, the smoothing error for the combined layer is substantially less. The smoothing errors are larger in the tropics and at high latitudes in winter.

In the narrow tropical zone between 20° S and 20° N, the smoothing errors are about 2–3 % for the surface – 25 and 250–25 hPa layers (see Fig. 7a and c). The smoothing error drops to about 1 % in the tropics when all layers up to 16 hPa are combined (see Fig. 7b and d). If we require the smoothing error for the combined layer to be ∼ 1 % or less (1σ interval), this condition is satisfied for the layer combinations from the surface (or from 250 hPa) to 25 hPa outside of the tropics. In the narrow tropical zone between 20° S and 20° N the upper boundary for the combined layers should be extended up to 16 hPa. With caution, users might choose other layer combinations depending on the scientific objectives of the study.

Comparisons with independent measurements in the defined broad layers support the theoretical results presented above. Comparisons of SBUV ozone amounts in the lower stratosphere/troposphere layer with Aura MLS (Kramarova et al., 2013) showed that the standard deviations in the tropics decreased from 3–4 % for the 250–25 hPa layer to 1 % for the 250–16 hPa layer. Labow et al. (2012) show ±5 % agreement between ozone amounts in the surface to 25 hPa layer measured by the SBUV and several ozone sonde stations over a 40-yr time period.

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3.3 OBO detection: interpretation of the SBUV smoothing error

In this section we will discuss a simple interpretation of the SBUV smoothing error by considering again the QBO ozone anomalies in the lower tropical stratosphere. Figure 8 shows the time series of the mzm seasonal anomalies for three individual layers and the combined layer (250–16 hPa) in the equatorial stratosphere. Red lines show the SBUV anomalies and black lines represent Aura MLS anomalies. The shadowed pink areas indicate the 2-σ range of the calculated SBUV layer smoothing error. At each layer the amplitudes of the ozone anomalies associated with the QBO are of the same order as the SBUV smoothing errors. Thus, the smoothing error can be understood as the limit (or range) of the SBUV sensitivity – if the amplitude of ozone anomalies at a particular layer is less than the corresponding layer smoothing error, the observing system cannot retrieve these anomalies. It is also important to note that the differences between MLS and SBUV anomalies are within the 2-sigma smoothing error bars. This means the instruments are measuring the same ozone profile and the difference between the two retrieval results is indeed due to the SBUV smoothing error. However, when we merge the recommended layers, the SBUV integrated ozone column contains the QBO signal with a proper amplitude and phase (Fig. 8d), and the smoothing error is substantially less than the amplitude of the QBO.

This example uses the tropics to demonstrate the limitation of the SBUV algorithm. Due to its coarse vertical resolution, the SBUV measures a signal from a broad vertical range, and the retrieval algorithm relies on the a priori profiles to distribute the measured signal among individual layers. The SBUV algorithm uses seasonal a priori profiles, which do not contain information about the QBO. The quasi-periodic nature of the QBO and its downward vertical propagation over time make it hard to capture QBO features in a seasonal climatology. The combination of all these factors results in the incorrect vertical distribution of the QBO signal measured by the SBUV and misrepresentation of the amplitude and phase of ozone anomalies at individual layers in the lower tropical stratosphere.

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4 Conclusions

In this study we presented a methodology for estimating the smoothing error for the SBUV ozone monthly zonal mean profiles. The smoothing error represents the error in the vertical profile due to the limited vertical resolution of the observing system. The smoothing error depends on two parameters – the SBUV averaging kernels that characterize the retrieval algorithm and its vertical resolution, and the covariance matrix that describes the natural variability of ozone fields. To estimate the smoothing error for the monthly zonal mean profiles, we constructed covariance matrices that characterize the inter-annual ozone variability for each latitude bin by using Aura MLS and sonde monthly zonal mean profiles over a 6-yr time period.

Between the 10 and 1 hPa layers the smoothing error is about 1 %. Outside of this vertical range the smoothing errors increase to as high as 15–20 % in the troposphere. The smoothing errors for total ozone are much smaller, mostly less than 0.5 %. The smoothing errors for the SBUV monthly mean time series over any particular location (for example, overpasses over ground-based stations) can be considered to be the same order of magnitude as the monthly zonal mean errors for the corresponding latitude bin.

The smoothing effect should be taken into account when analyzing SBUV ozone data at individual layers. When several ozone layers are merged together in the lower stratosphere and troposphere, the Degrees of Freedom for Signal of the thick layer increases and the corresponding smoothing error decreases. We recommend using the following layer combinations to get the most information from the SBUV data and to reduce the smoothing error to 1 % or less: surface to 25 hPa or 250 to 25 hPa everywhere outside of the narrow tropical zone from 20° S to 20° N. In these tropical latitudes we recommend merging all layers up to 16 hPa.

We found that the amplitude of the QBO ozone anomalies at any individual layer in the lower tropical stratosphere are of the same order as the SBUV layer smoothing error, meaning that the observing system cannot properly retrieve the signal at individual layers. The smoothing error can be understood as the limit (or range) of the SBUV sensitivity. If the amplitude of ozone anomalies at a particular layer is less than the corresponding layer smoothing error, the observing system cannot properly retrieve these anomalies. This explains why the SBUV algorithm produces an incorrect phase and amplitude of the QBO ozone anomalies at any individual layer and misses the vertical downward propagation of the QBO signal. However, we showed that the SBUV accurately captures the QBO signal in the thick 250–16 hPa layer in terms of both the amplitude and phase.

The implication of this study is that the SBUV observing system can be used to derive long time series of ozone measurements if one carefully considers the limitations of the retrieved ozone profiles imposed by the limitations of the vertical resolution of the measurements in the lower stratosphere and troposphere. We have suggested combinations of the traditionally derived layer amounts that lower the smoothing error and give an adequate representation of the ozone profiles measured by SBUV instruments. Use of these layer combinations are recommended for the proper interpretation of the SBUV data, including the ozone trend analysis and model comparisons. Accordingly, the merged ozone dataset from the SBUV instrument series for trend analysis studies will be released in the recommended layer combinations.

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Table 1. List of ozone sonde stations used to estimate inter-annual ozone variability for smoothing error calculations.

Latitude bin	Station	Latitude	Longitude	Number of profiles
90–80° S	South Pole	−89.9	24.8	347
80–70° S	Neumayer	−70.7	11.86	425
70–60° S	Davis	−68.6	79.9	61
	Marambio	−64.2	−56.7	121
	Syowa	−69	39.58	397
60–50° S	Macquarie	−54.5	158.9	248
40–50° S	Lauder	−45	169.6	337
40–30° S	Laverton	−37.8	144.7	257
30–20° S	Irene	−25.2	28.18	170
	Reunion	−21	55.48	175
20–10° S	Reunion	−21	55.48	175
	Samoa	−14.2	−170	205
	Fiji	−17.4	−149	154
10–0° S	Ascension Island	−7.58	−14.2	259
	Java	−7.5	112.6	191
	Nairobi	−1.27	36.8	343
	Natal	−5.42	−35.3	241
	Sancristobel	−0.92	−89.6	216
0–10° N	Cotonou	6.21	2.23	39
	Kuala-Lumpur	2.73	101.7	148
	Paramaribo	5.81	−55.2	261
	Trivandum	8.29	76.95	45
10–20° N	Hilo	19.72	−155	313
	Poona	18.53	73.85	25
20–30° N	Hanoi	21.02	105.8	23
	Hilo	19.72	−155	313
	Kagoshima	31.55	130.5	246
	Naha	26.2	127.6	245

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Table 1. Continued.

Latitude bin	Station	Latitude	Longitude	Number of profiles
30–40° N	Boulder	40.02	−105	291
	Huntsville	34.72	−86.6	228
	Madrid	40.46	−3.65	152
	Tateno	36.05	140.1	333
	Wallops	37.93	−75.4	241
40–50° N	Canada (Yarmouth, Kelowna)	−7.58	−14.2	138
	Hohenpeisenberg	47.8	11.02	755
	Payerne	46.8	6.95	904
	Sapporo	43.05	141.3	275
50–60° N	Edmonton	53.55	−114	269
	Goose	53.32	−60.3	266
	Lindenberg	52.21	14.12	288
	Uccle	50.8	4.35	823
60–70° N	Churchill	58.75	−94	221
	Lerwick	60.13	−1.18	233
	Sodankyla	67.39	26.65	409
70–80° N	Ny Alesund	78.93	11.88	521
	Resolute	74.72	−94.9	148
	Scoresbysund	70.49	−21.9	188
	Thule	76.53	−68.7	66
80–90° N	Alert	82.5	−62.3	300

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Table 2. Months of the year for high latitude regions when the SBUV measurements are not possible (or very limited) due to high SZA (polar night conditions). Note, between 60° S and 60° N the SBUV obtains measurements over the whole year.

Latitude bins	80–75° S	70–75° S	65–70° S	60–65° S	60–65° N	65–70° N	70–75° N	75–80° N
Missed Months	Apr–Sep	May–Aug	May–Jul	Jun–Jul	Dec	Nov–Jan	Nov–Feb	Oct–Feb
# of missed month	6	4	3	2	1	3	4	5

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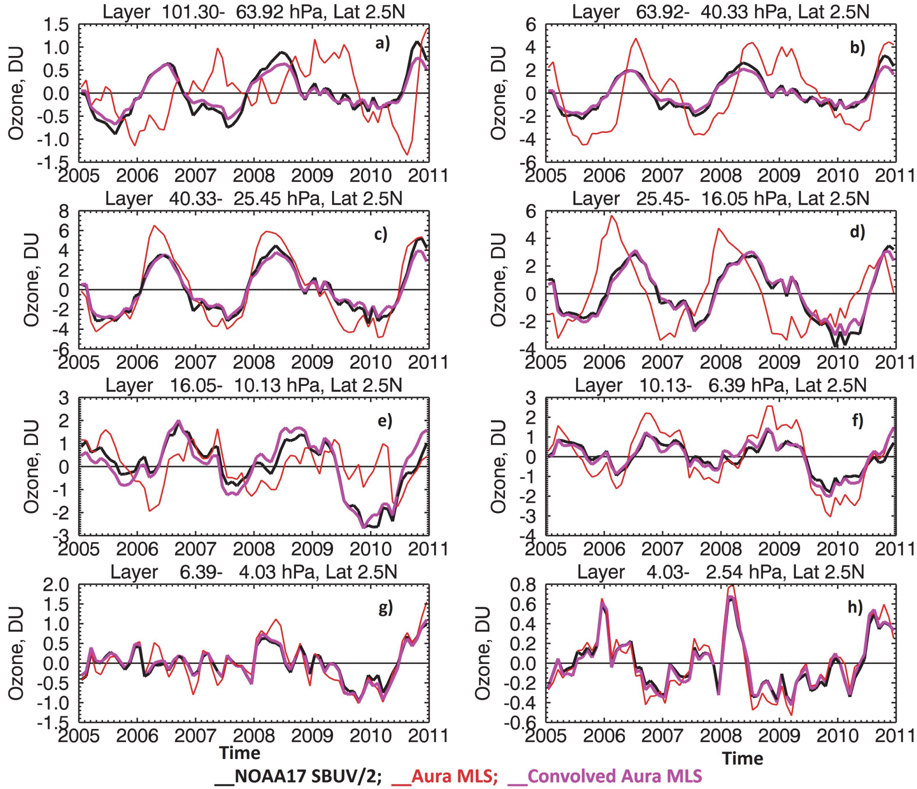

Fig. 1. Deseasonalized time series of the ozone mzm columns in the lower tropical stratosphere (0–5° N). Black lines correspond to SBUV anomalies, red lines show MLS anomalies and magenta lines indicate convolved MLS anomalies.

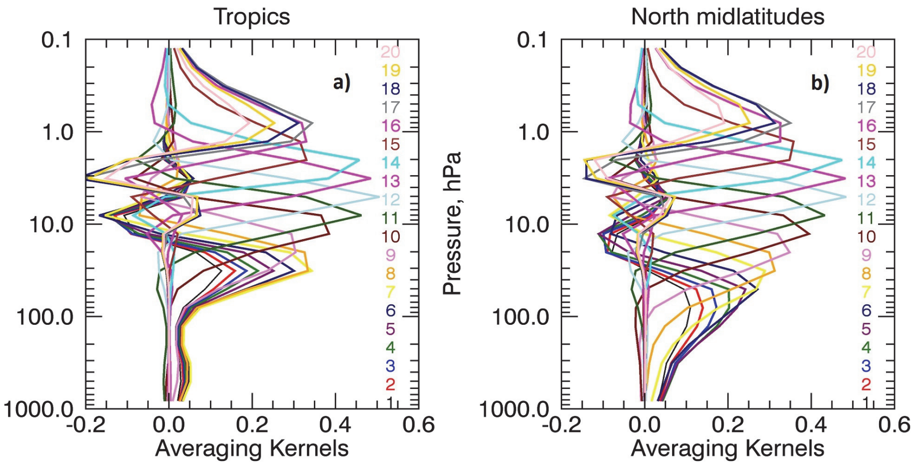

Fig. 2. Typical SBUV Averaging Kernels for **(a)** the tropics and **(b)** northern middle latitudes. Different colors correspond to individual layers, and layer numbers are indicated on the right.

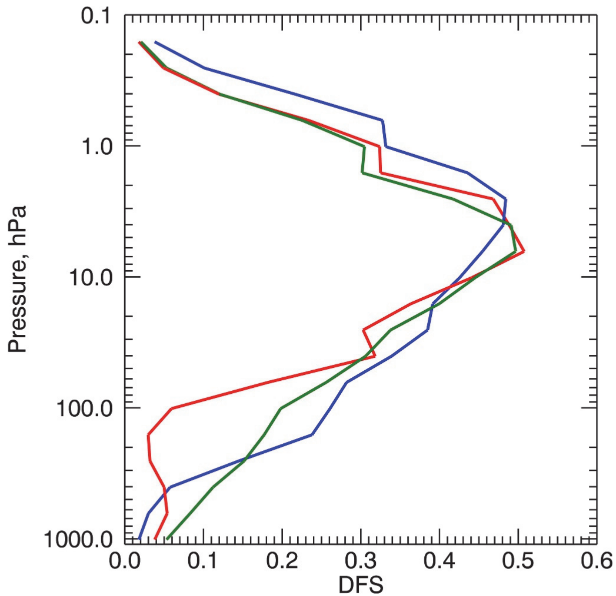

Fig. 3. DFS as a function of altitude for mid-latitudes in summer (green line), in winter (blue line) and for the tropics (red line).

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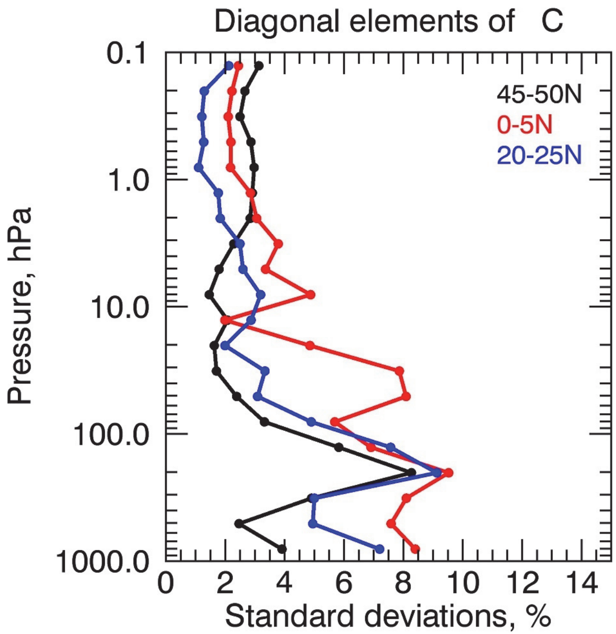

Fig. 4. Vertical profiles of the square roots of diagonal elements of the covariance matrix for three latitude bins as percent relative to the a priori. These quantities are equal to the standard deviations of the mzm profiles.

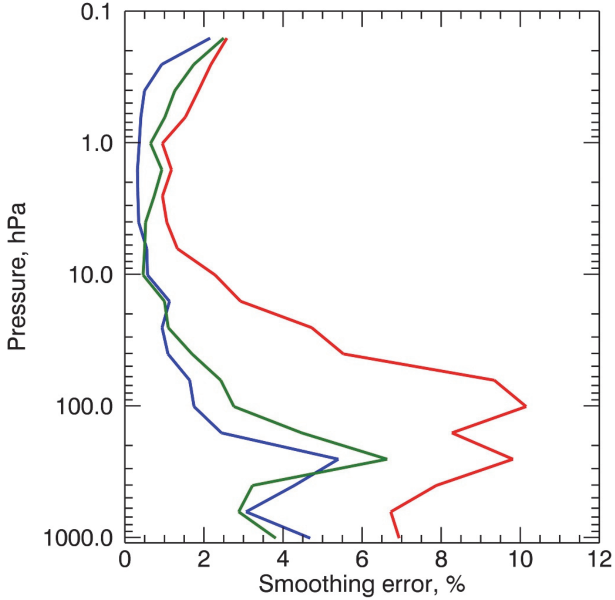

Fig. 5. SBUV smoothing error (%) as a function of altitude for mid-latitudes in summer (green line), in winter (blue line) and for the tropics (red line).

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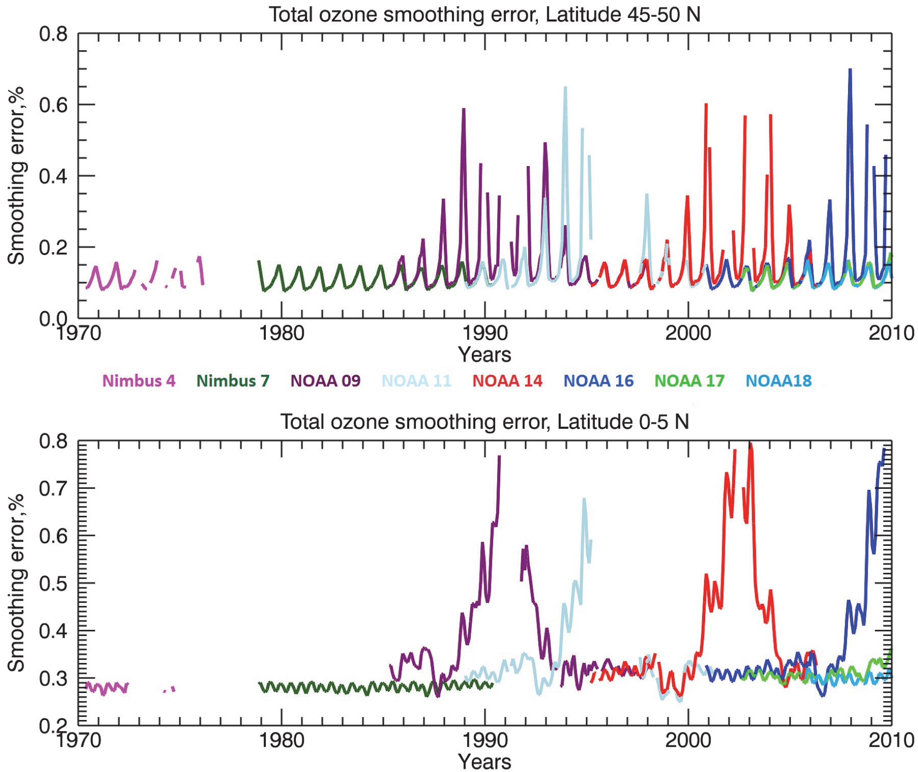

Fig. 6. Time series of the SBUV smoothing error for mzm total ozone column. **(a)** for 40–45° N latitude zone and **(b)** for 0–5° N latitude zone. Different colors correspond to individual SBUV instruments.

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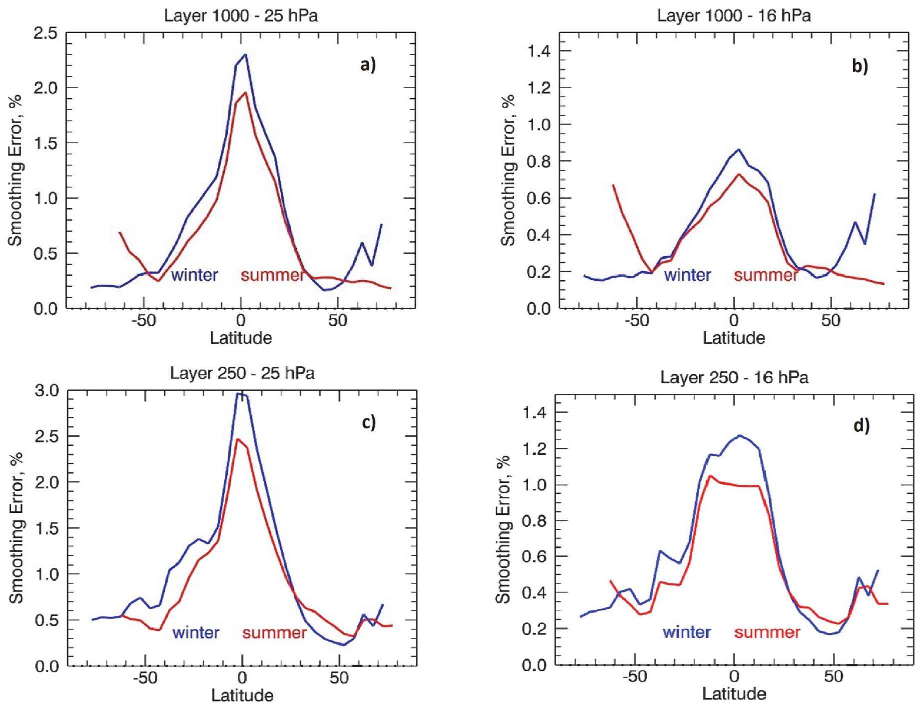

Fig. 7. Smoothing error as a function of latitude for different combinations of layers in the lower stratosphere/troposphere: **(a)** surface – 25 hPa; **(b)** surface – 16 hPa; **(c)** 250 hPa – 25 hPa; and **(d)** 250 hPa – 16 hPa. Blue lines show errors in winter months (DJF) and red lines errors in summer months (JJA).

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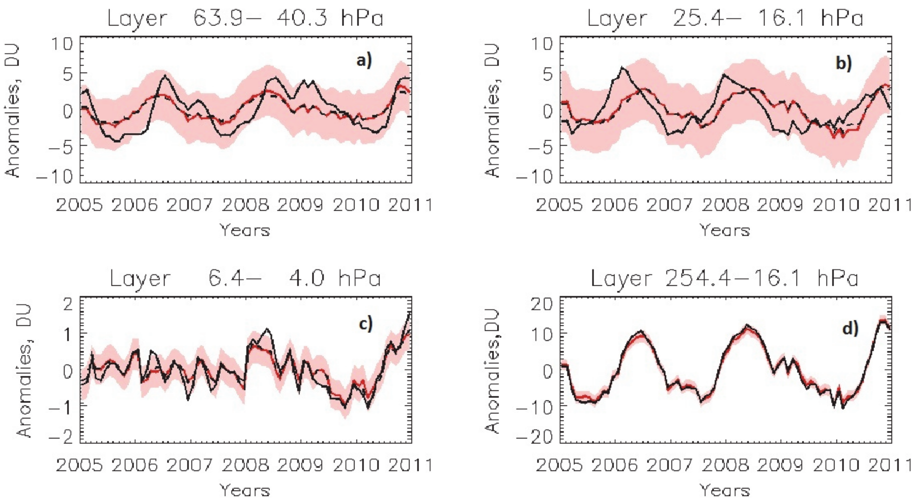

Fig. 8. Time series of the deseasonalized ozone anomalies obtained from SBUV and Aura MLS for several layers in the tropical stratosphere: **(a)** 63–40 hPa layer; **(b)** 25–16 hPa layer; **(c)** 6–4 hPa layer; and **(d)** 254–16 hPa layer. Red lines show SBUV anomalies along with the corresponding smoothing errors (shadowed pink areas indicate 2σ-range). Black lines show MLS anomalies, and black dashed lines indicate convolved MLS anomalies.

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