



Description of Integrated Ozone profile Data

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1. Executive summary

A methodology has been developed for the integration of profile ozone data from various sources in order to provide consistent ozone vertical distribution time series as well as tropospheric and stratospheric ozone partial columns at 4 NDACC stations. This methodology was developed for measurements performed in the stations forming the Alpine station (e.g. Haute-Provence Observatory OHP – France, Bern – Switzerland, Jungfraujoch – Switzerland). Ozone measurements from the lidar at OHP, the microwave spectrometer (MW) at Bern and the FTIR spectrometer at the Jungfraujoch station were used for this purpose. It was also developed for similar types of measurements performed at La Reunion Island (France), Izaña (Spain) and Ny Alesund (Norway).

The merged ozone data and related stratospheric and tropospheric ozone columns have been submitted on the following data server, where they can be downloaded using an anonymous logging: ftp://latmos.ipsl.fr/outgoing/NORS_WP6

Daily merged ozone profiles including stratospheric and tropospheric partial ozone columns as well as the monthly means of these products were delivered.

2. Introduction

The main objectives of D6.2 and D6.3 work packages were to develop a methodology for integrating ground-based ozone profile data from different types of measurements, in order to provide consistent and homogeneous ozone vertical distribution time series as well as tropospheric and stratospheric ozone partial columns at the 4 NDACC stations included in the NORS project.

The data considered in the work package are listed in the table below:

Ny Alesund 79°N, 12°E	Alpine station	Izana 28°N, 16°W	La Réunion 22°S, 56°E
FTIR 2003-2013	FTIR (Jungfraujoch 47°N, 8°E) 2003-2013	FTIR 2000-2012	FTIR 2004-2011
Lidar 2003-2013	Lidar (OHP (44°N, 6°E)) 2003-2013	Ozone sondes 2000-2012	Lidar 2004-2013
Microwave 2006-2013	Microwave (Bern, 47°N, 7°E) 2003-2013		Ozone sondes 2003-2013
Ozone sondes 2003-2013	Ozone sondes (OHP, 44°N, 6°E) 2003-2013 Ozone sondes (Payerne, 47°N, 7°E) 2003-2013		

Table 1: Data used for WP6

The FTIR, lidar and microwave techniques used for the measurement of ozone profiles have been described in detail in other NORS reports (e.g. based on the WP4, deliverables D4.2, D4.2). Measurements are based on passive or active (lidar) remote sensing techniques and are characterized by different temporal sampling, vertical resolution and error profile. Ozone

sonde measurements also used in this work are based on in situ sensing of ozone concentration by a balloon borne electrochemical sensor coupled to a Teflon air pump and interfaced to a meteorological radiosonde.

The construction of the merged ozone profile time series is based on the assumption that the bias between each measurement type at the various stations is mainly instrumental, except for the stations located in the Alpine area where geophysical bias linked to statistically different sampled air masses can also be found due to the distance between the stations.

3. Description of the methodology

Due to the different characteristics of the ozone profiles in terms of vertical resolution and validity domain, a compromise has to be made in order to integrate the data. For instance the vertical resolution of higher resolved measurements, e.g. from ozone sondes and lidar, has to be degraded using the averaging kernels of the passive remote sensing techniques (FTIR and microwave). Also the difference between FTIR and microwave measurements can be due to the use of different a priori profiles in the retrieval and this difference has to be corrected. After correction of these potential sources of bias, systematic differences can still persist. Satellite measurements can then be used in order to investigate the remaining biases and eventually correct them.

The various steps of the integration methodology can thus be summarized as follows:

- Evaluation of the validity domain and vertical resolution of the various data sets.
- Adjustment of vertical resolutions: smoothing of high resolved data.
- Check of bias due to a priori profile (for FTIR and microwave data) and correction.
- Check of remaining bias using satellite data and correction
- Check of geophysical bias (Alpine stations case)
- Data integration
- Calculation of stratospheric and tropospheric partial columns

3.1 Validity domain and vertical resolution of the data sets

The validity domain and vertical resolution of the measurements is summarized in Table 2

	Technique	Altitude range	Resolution (km)
Lidar	active remote sensing (UV)	10 – 45 km	0.5 – 5
Microwave	passive remote sensing	20 – 60 km	10 – 15
FTIR	passive remote sensing (IR)	4 – 42 km	7 – 15
Ozone sonde	in situ electrochemical sensor	0 – 35 km	0.3

Table 2: Validity domain and vertical resolution of measurement techniques considered in WP6

3.2 Data smoothing

Lidar and ozone sondes measurements are characterized by a higher vertical resolution compared to that of FTIR and microwave. In order to evaluate their systematic differences with respect to microwave and FTIR measurements, the profiles have to be smoothed using the following formula:

$$x_s = x_a + A(x_h - x_a) \quad (1)$$

where x_s is the smoothed lidar or ozone sonde profile, x_h is the initial lidar or ozone sonde profile and x_a and A are the FTIR or microwave a priori profile averaging kernel matrix, respectively.

Examples of microwave and FTIR averaging kernels are displayed in figure 1.

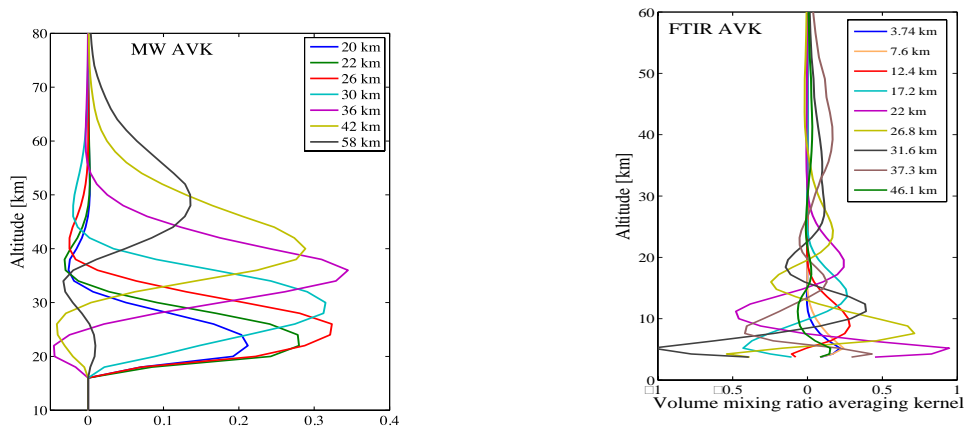


Figure 1: Averaging kernels for the microwave measurements performed in Bern (Switzerland) and FTIR measurements performed in Jungfraujoch (Switzerland).

In equation (1), x_h must cover the same altitude range as the averaging kernels. Therefore, the lidar or ozone sonde profiles have to be extended as a function of altitude. In the case of OHP for example, an ozone sonde climatology has been used to extend the lidar data from 15 km to the ground and a climatology based on SAGE II measurements selected in the vicinity of the station has been used (see figure 3).

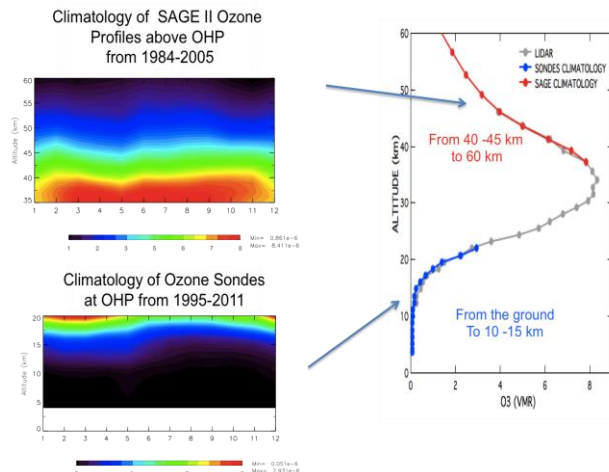


Figure 3: extension of lidar profile in order to apply the averaging kernels

For each station, SAGE II climatologies were used to extend the lidar or ozone sonde profiles in the upper ranges. Ozone sondes climatologies were used to extend lidar data to the ground (e.g. for NyAlesund lidar data).

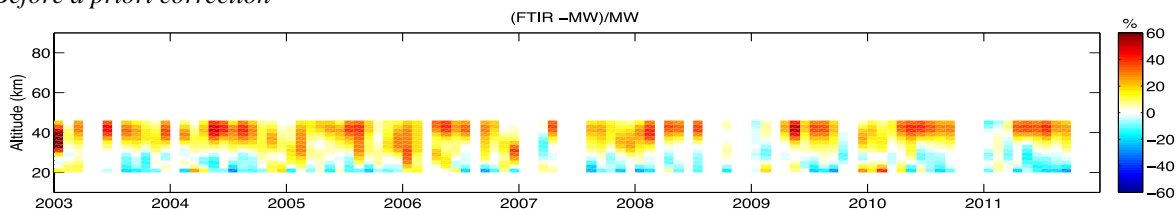
3.3 Bias evaluation

In order to evaluate the validity of the various data sets, their respective systematic differences for coincident data (± 12 h difference) have been investigated and compared to similar systematic difference with measurements performed by the AURA-MLS satellite instrument. The AURA-MLS measurements were selected within a domain of 4° in longitude and 3° in latitude around each station.

A first source of systematic difference between measurements types can be due to different a priori profiles, when MW and FTIR measurements are concerned. Indeed in the case of Alpine stations, Bern MW and Jungfraujoch FTIR measurements use different a priori profiles. Bern uses monthly climatologies based on ECMWF data in the lower range (up to 20 hPa) and MLS data in the higher range, while Jungfraujoch uses an annual climatology based on Payerne ozone sonde data and Bern MW data in the upper range. In order to improve the comparison, a priori profiles have to be adjusted. FTIR measurements have thus been corrected using the MW a priori profiles.

Figure 4 displays the comparison between FTIR and MW measurements comparison before and after a priori correction of FTIR measurements.

Before a priori correction



After a priori correction

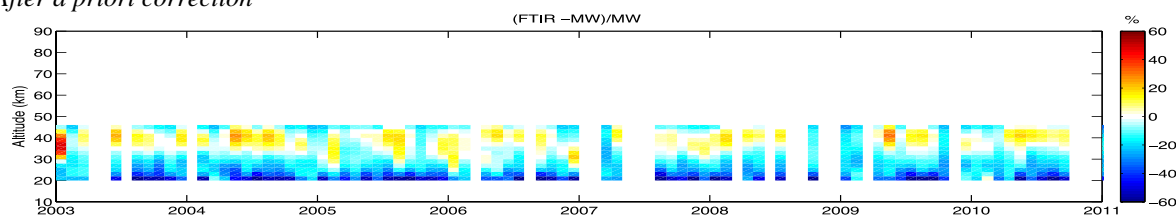


Figure 4: Comparison between Bern MW and Jungfraujoch FTIR measurements before and after a priori correction of FTIR measurements.

Systematic differences between lidar and MW data for coincident dates are also investigated. Figure 5 displays the bias between such data in the case of the Alpine stations.

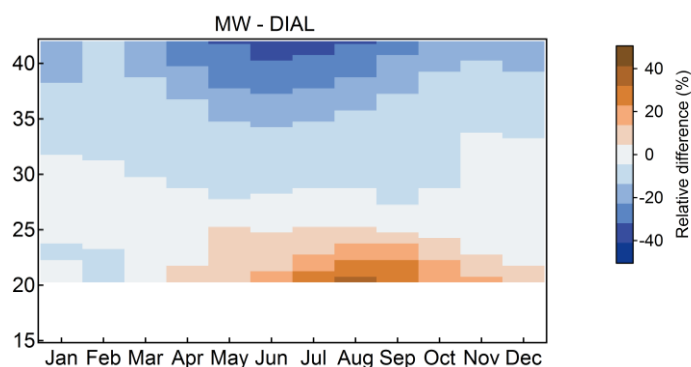


Figure 5 : Climatology of systematic differences between Bern MW and OHP DIAL data over the 2003-2013 period.

AURA-MLS data are then used in order to decide which data set is the most accurate (see figure 6). The respective systematic differences for coincident data (± 12 h difference) have been investigated and compared to similar systematic difference with measurements performed by the satellite instrument. These measurements were selected within a domain of 4° in longitude and 3° in latitude around each station

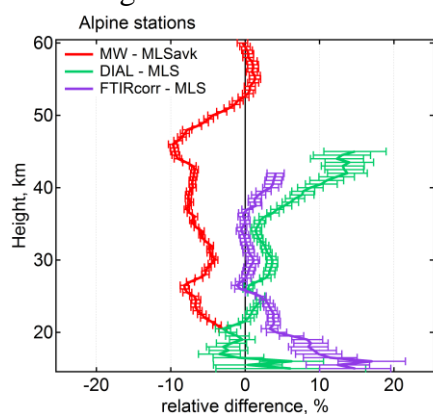


Figure 6a: Average bias between FTIR corrected for a priori and MLS coincident measurements (purple), lidar and MLS (green) and microwave and MLS (red) measurements in the case of the alpine stations.

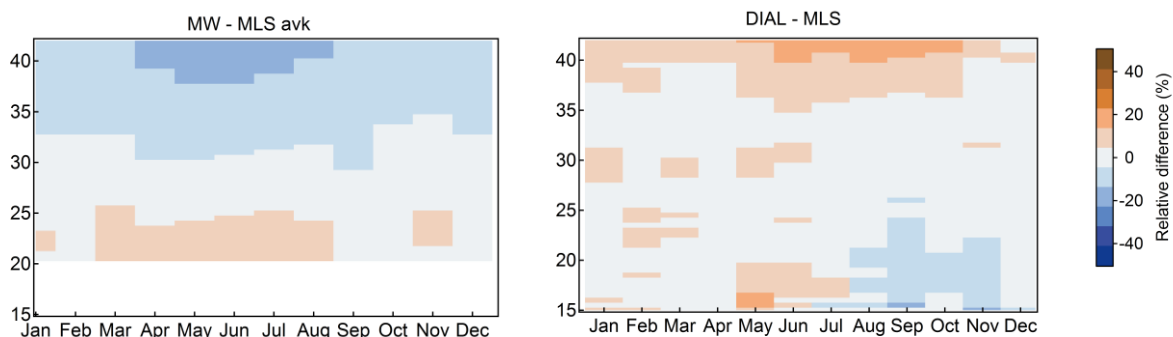


Figure 6b: left: climatological bias between Bern MW and MLS data smoothed with MW averaging kernels (AVK); right: climatological bias between OHP lidar and MLS data.

For the comparison between lidar and MLS data, no additional smoothing was applied since both measurement types are characterized by similar vertical resolution. Lidar data have a higher resolution in the lower range (below 30 km) and a lower resolution in the higher range (above 30 km). The bias between lidar and ECC data at OHP is also shown in Figure 7:

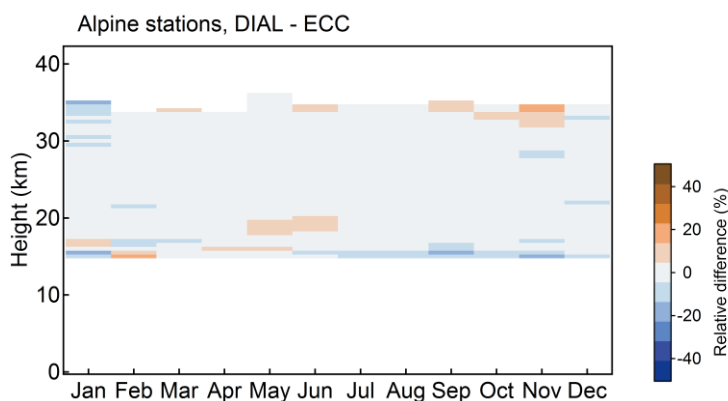


Figure 7: Climatological bias between coincident lidar and ECC ozone sonde data at OHP.

Since lidar data present a somewhat lower bias with respect to MLS data and very small bias with respect to ozone sonde data, MW data have been corrected from their bias with MLS. Figure 8 shows the bias between MW corrected data from their bias with MLS and DIAL data smoothed using MW averaging kernels.

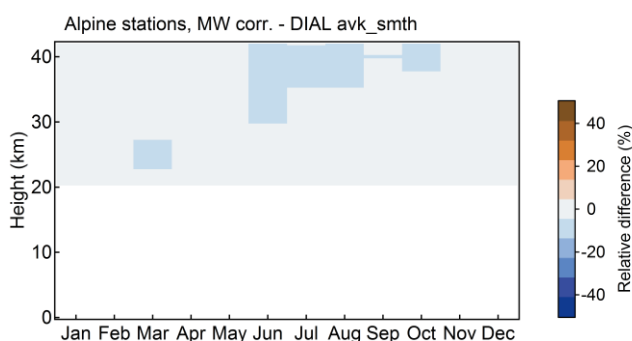


Figure 8: Bias between Bern MW corrected data and smoothed OHP lidar data

Regarding Jungfraujoch FTIR data, their bias with respect to lidar and ozone sonde data at OHP and Payerne was also investigated. As mentioned previously, FTIR data have been corrected using the a priori profile of MW. The FTIR climatological systematic difference (over the 2003 – 2013 period) with respect to OHP DIAL data (smoothed with MW AVK) and Payerne ozone sondes are displayed in Figure 9. Similar systematic differences with MW corrected data are shown in Figure 10.

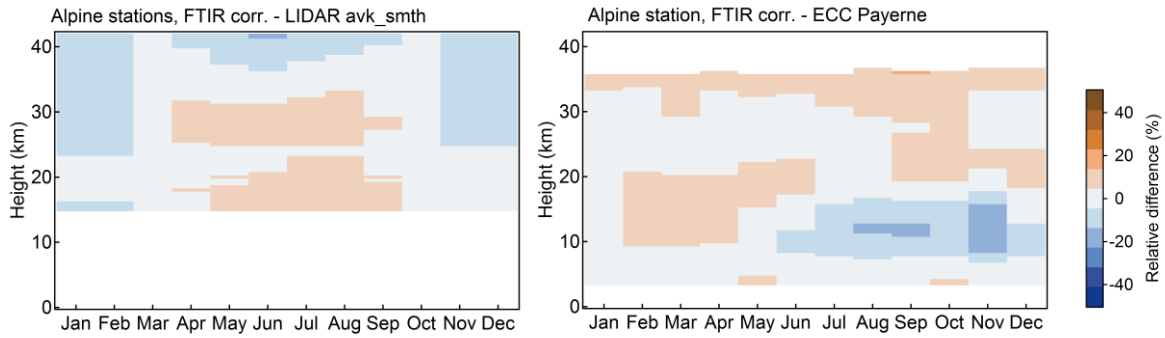


Figure 9: Systematic difference between a priori corrected FTIR data and (left) smoothed DIAL data, (right) Payerne ozone sondes.

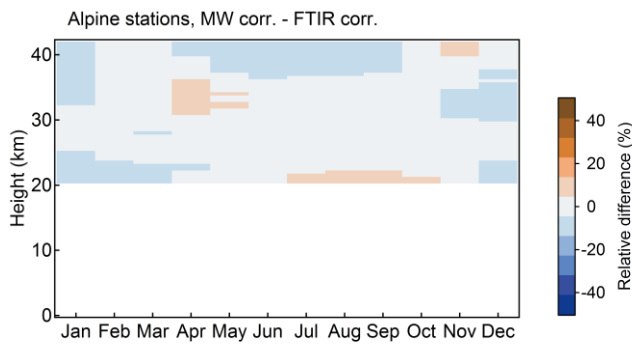


Figure 10: Systematic difference between a priori corrected FTIR data and MW corrected data

3.4 Data integration

After the corrections presented in the previous section, e.g. a priori profile correction in the case of FTIR and MLS bias correction in the case of MW, the various data sets show systematic differences in the range of $\pm 10\%$, which makes them suitable for merging.

Merged ozone profile data are computed from the error weighted average of the individual coincident daily ozone profiles corrected from eventual instrumental and geophysical bias. A general formula for the computation of merged ozone data is the following:

$$O_3(z) = \sum_{i=1}^n w_i(z) B_i(z) G_i(z) O_{3i}(z) \quad (2)$$

where $O_3(z)$ is the merged ozone profile, $w_i(z)$ is the weight linked to the error of the measurements, $B_i(z)$ corresponds to the correction for eventual instrumental bias, $G_i(z)$ is the correction for geophysical bias, $O_{3i}(z)$ are the individual eventually smoothed ozone profile sources and n is the number of individual profiles taken into account. The weight related to the error of the measurements is computed as follows:

$$w_i(z) = \frac{\varepsilon_i^{-1}(z)}{\sum_{i=1}^n \varepsilon_i^{-1}(z)} \quad \text{where } \varepsilon_i(z) \text{ is the error profile of the individual ozone measurements.}$$

Figure 11, which displays the vertical distribution of average estimated error for each measurement type considered in the Alpine stations case shows how the error related weight will affect the contribution of each measurement in the merged ozone profile, as a function of altitude.

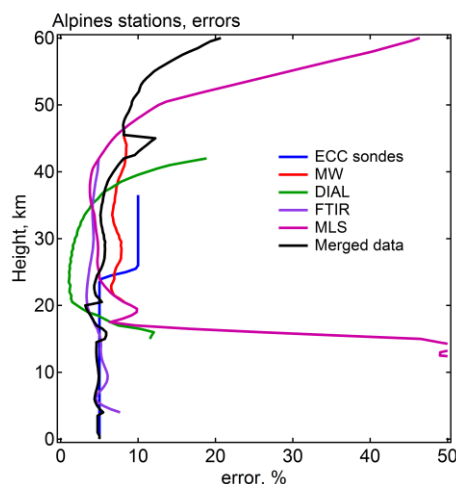


Figure 11: Vertical distribution of average estimated error for measurements performed in the Alpine stations and for MLS measurements performed in the vicinity of these stations.

Examples of merge ozone profile for the Alpine stations case is displayed in figure 12:

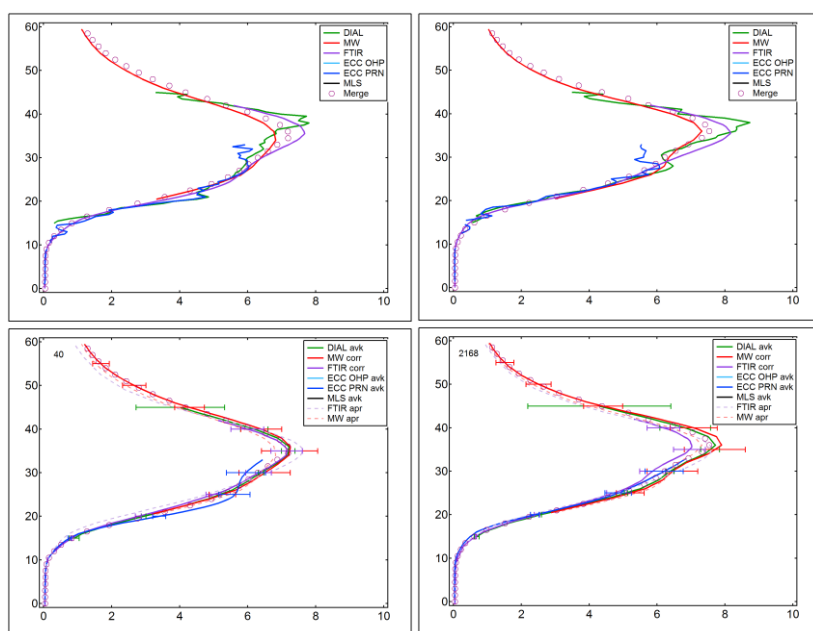


Figure 12: Example of merged ozone profile (violet open circle) compared to the various individual profiles.

3.5 Calculation of stratospheric and tropospheric partial columns

Once the merged ozone profiles are computed, the stratospheric and tropospheric partial columns can be computed by integrating the tropospheric and stratospheric part of the merged vertical profile after determination of the tropopause altitude.

For each station, the tropopause altitude is computed using the standard WMO definition, which defines the tropopause as “the lowest level at which the lapse-rate decreases to 2°C/km or less, provided that the average lapse-rate between this level and all higher levels within 2 km does not exceed 2°C/km.

4. Results

This section presents the results of integration for the various stations considered in the study. Daily merged ozone data have been computed for each day when an ozone profile measurement from one of the instrument considered in this work is available. A file has been produced for each merge ozone profile, containing the merge ozone profile, its error as a function of the altitude, the tropopause altitude and the stratospheric and tropospheric partial columns. Monthly average merged ozone data sets have also been produced.

4.1 Alpine Stations

As mentioned in the introduction, the Alpine stations considered here are Haute-Provence Observatory (OHP – France), Bern and Jungfraujoch (Switzerland). The latter stations are located at a distance as the crow flies of 60 km, while OHP is located at about 350 – 370 km from both other stations. Table 3 displays the number of measurements from the different instruments over the 2003-2013 period. The number of coincident measurements with at least two measurements types and three measurement types are also shown.

	FTIR Jungfraujoch	Microwave Bern	Lidar OHP	Ozone sondes		MLS
				OHP	Payerne	
Number of measurements	1169	3798	1299	448	1521	992
Number of coincidences ≥ 2	1389					
Number of coincidences ≥ 3	863					

Table 3: Number of ozone profile measurements considered from ozone profile integration in the Alpine stations

4.1.1 Geophysical bias

In the case of the Alpine stations, because of the distance between OHP and the other sites, possible geophysical bias has been investigated. This bias is evaluated using coincident measurements from AURA-MLS in the vicinity of the various sites.

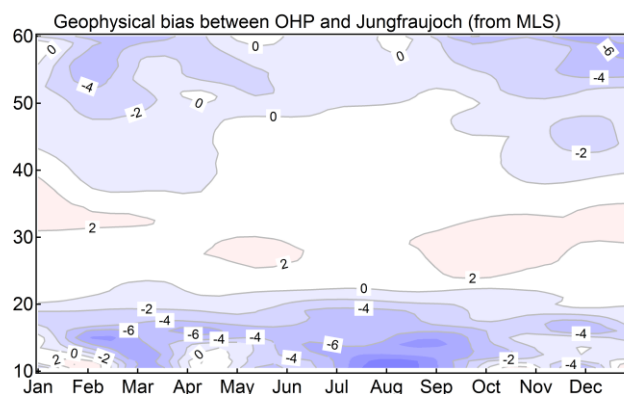


Figure 13: Difference between coincident MLS ozone measurements obtained at OHP and Jungfraujoch.

Results showed that the difference between MLS measurements obtained at OHP and both other Alpine stations is generally very small above 20 km. Below 20 km, MLS measurements uncertainty increases rapidly, which could explain the larger biases observed.

In order to better understand the measurement difference below 20 km, the systematic difference between OHP and Payerne ozone sondes measurements on coincident days was analysed. Results of the climatological difference are displayed in figure 14, which shows biases not exceeding 10 %. Largest biases are observed in July around 10 km altitude.

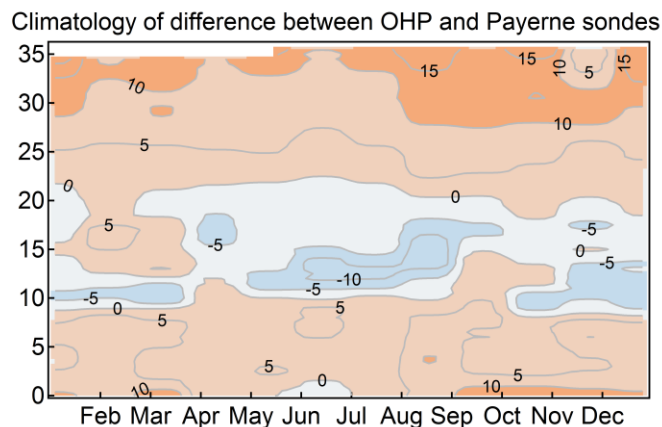


Figure 14: Climatological differences between Payerne and OHP ozone sondes measurements on coincident days.

The small values of the biases displayed in figure 13 and 14 indicate that the geophysical bias between the OHP and other Alpine stations is very small and similar to the estimated error of the various measurements. **As a consequence, no geophysical bias correction was applied to the individual data before the merging.**

4.1.2 Integrated ozone profiles

As mentioned in the previous sections, the integrated data for the Alpine stations, are constructed from the error weighted average of the following individual profiles:

- Smoothed OHP lidar data using Bern MW averaging kernels
- Corrected Bern MW data from their bias with MLS data
- Corrected Jungfraujoch FTIR data using MW a priori profiles
- Smoothed OHP ozone sonde data using Jungfraujoch FTIR averaging kernels
- Smoothed Payerne ozone sonde data using Jungfraujoch FTIR averaging kernels

The monthly average ozone profiles based on the merged ozone data sets are displayed in figure 15a. Corresponding MLS monthly averages are displayed in figure 15b.

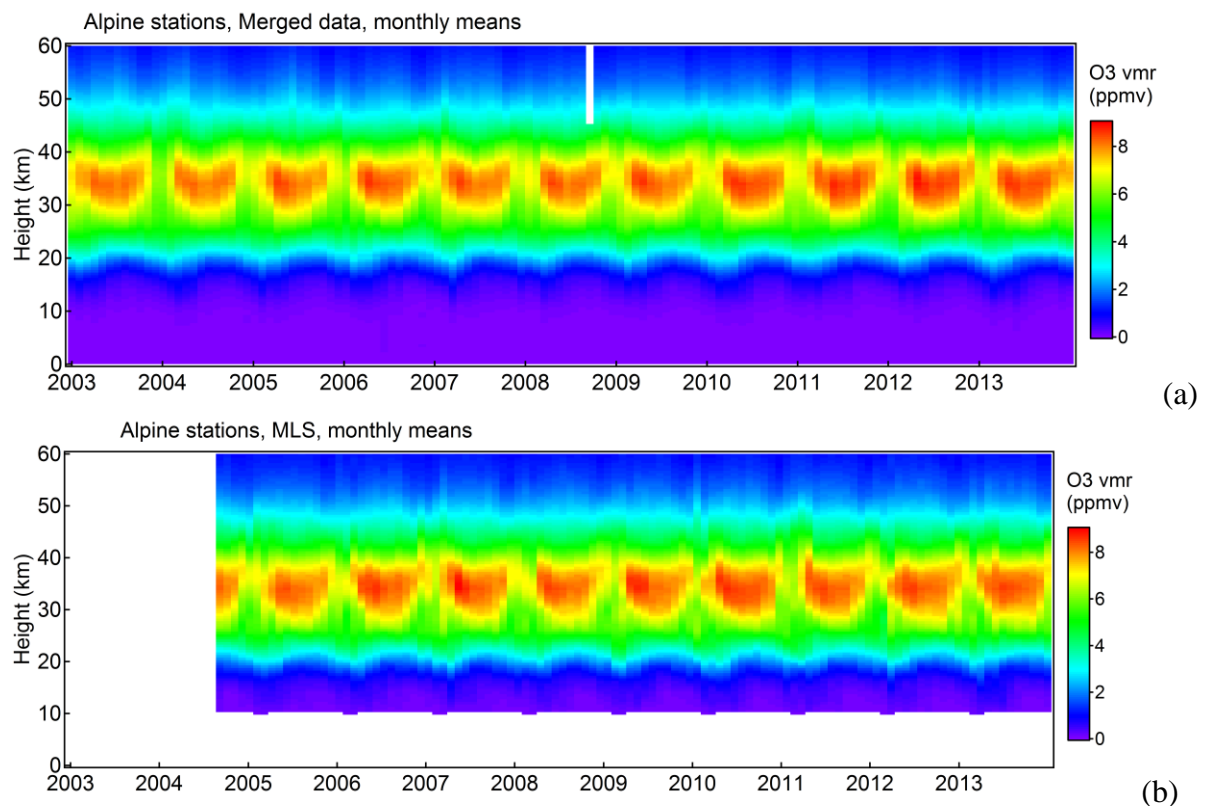


Figure 15: Monthly average ozone profiles from the merged data set (a) and MLS (b)

Corresponding ozone anomalies, e.g. monthly average ozone data minus the climatological average are displayed as a function of altitude in figure 16:

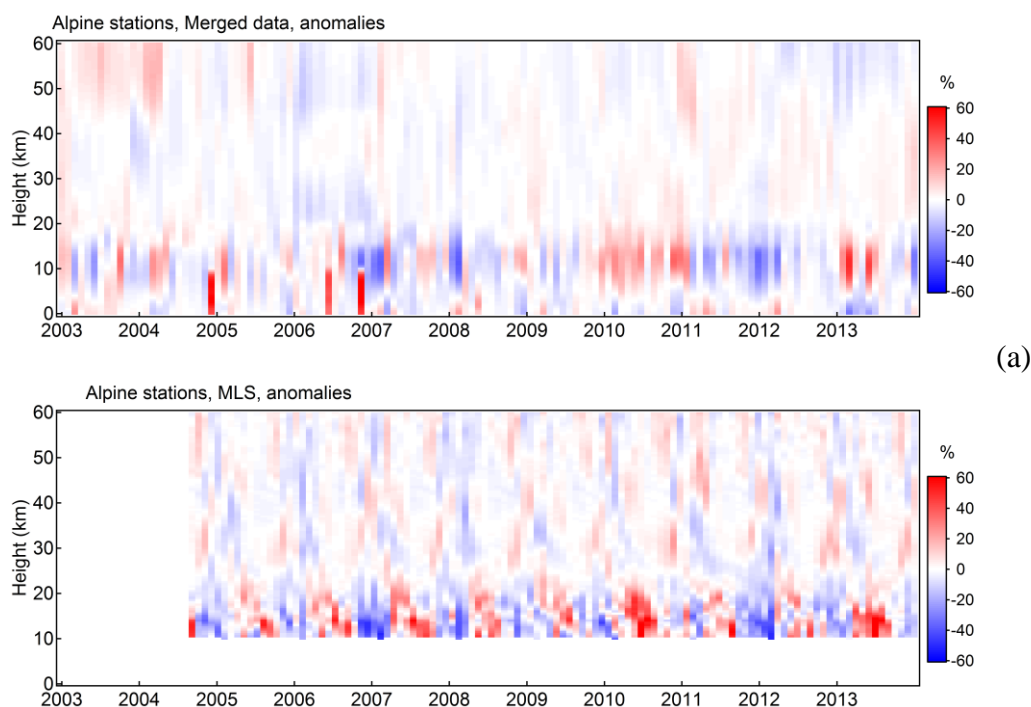


Figure 16: Monthly average ozone anomalies from the merged data set (a) and MLS (b)

For a better view of how the merged ozone data set compares with the various data sets, anomalies of the merged data set integrated over 3 altitude ranges is displayed in figure 17, together with the anomalies of individual data sets.

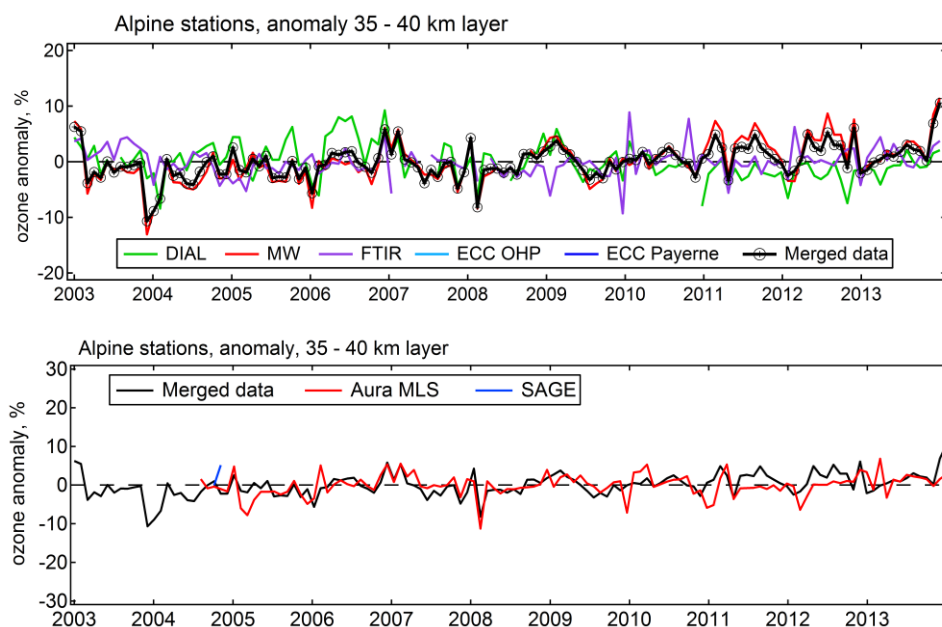


Figure 17a: Monthly average ozone anomalies from the merged data set integrated over 5 km in the 35-40 km altitude range, compared to ozone anomalies of individual data sets and of MLS measurements

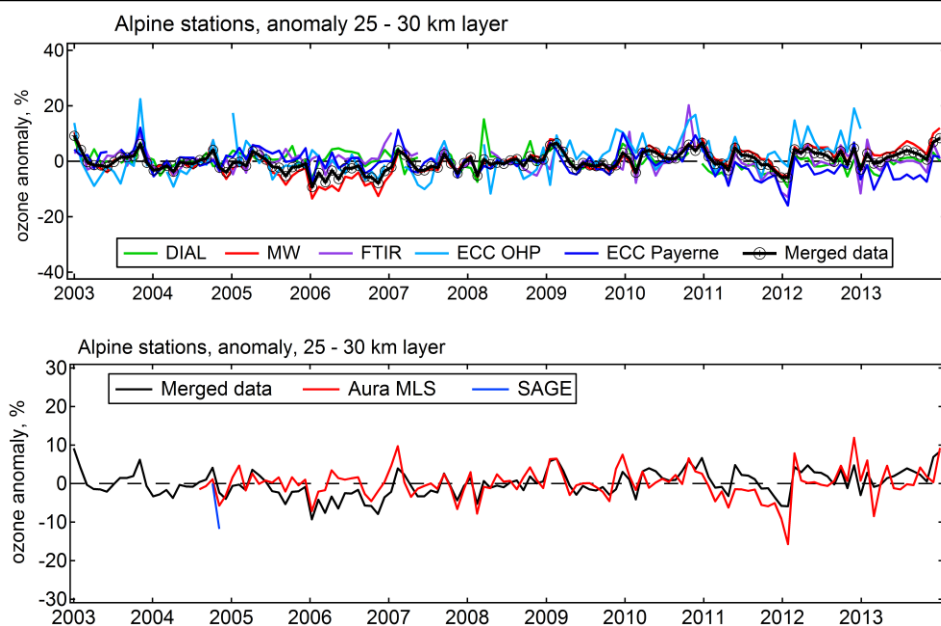


Figure 17b: Monthly average ozone anomalies from the merged data set integrated over 5 km in the 25-30 km altitude range, compared to ozone anomalies of individual data sets and of MLS measurements

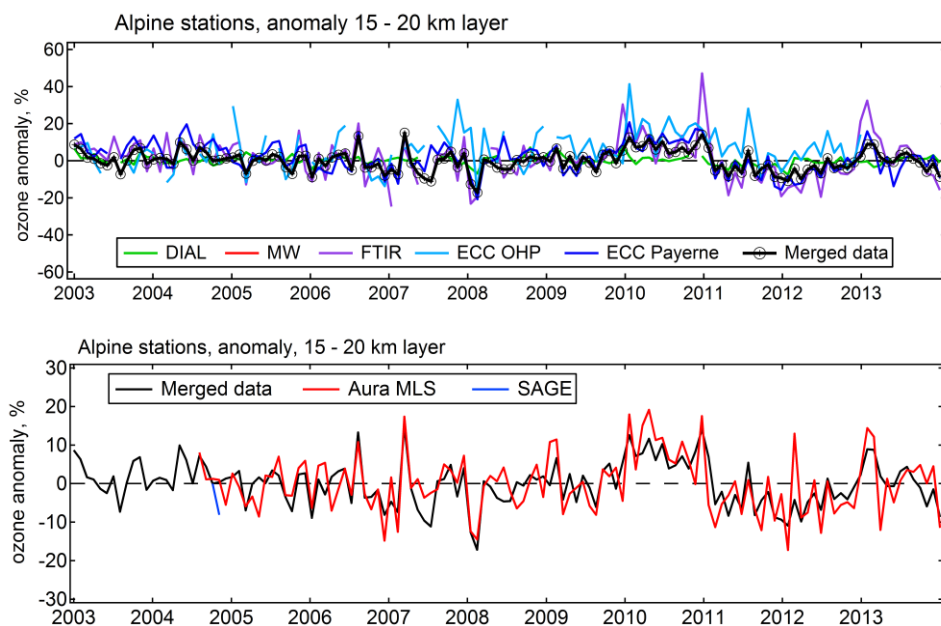


Figure 17c: Monthly average ozone anomalies from the merged data set integrated over 5 km in the 15-20 km altitude range, compared to ozone anomalies of individual data sets and of MLS measurements

4.1.3 Partial and total ozone columns

The stratospheric and tropospheric partial ozone columns derived from the merged data and the calculation of the tropopause altitude are shown in figure 18:

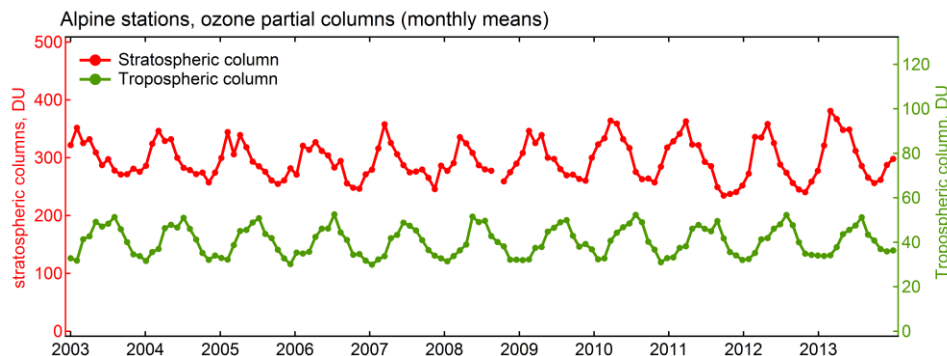


Figure 18: Temporal evolution of monthly averaged stratospheric and tropospheric partial ozone columns derived from the merged data at the Alpine stations

In addition, the total ozone columns, which were derived from the integration of the merged ozone profiles have been compared to the SAOZ UV-Visible total ozone data at OHP (figure 19). The comparison shows a good agreement between both data sets.

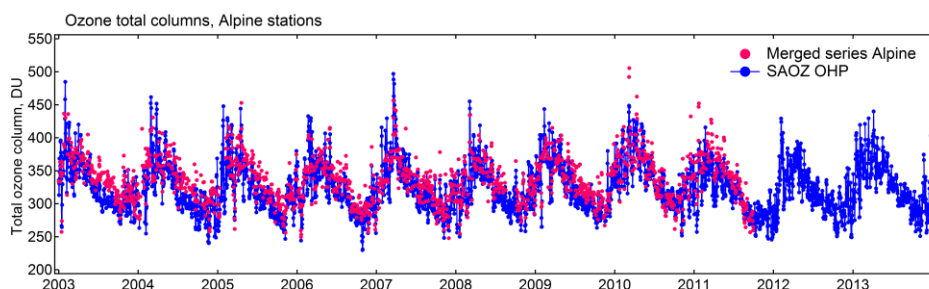


Figure 19: Comparison of total ozone columns derived from the merged ozone data and total ozone columns observed at OHP with the SAOZ UV-Visible spectrometer.

4.2 NyAlesund

For the measurements performed at the NyAlesund station, the same methodology was applied to integrate the various individual ozone profiles. The integrated data for the NyAlesund station, are constructed from the error weighted average of the following individual profiles:

- Smoothed ozone lidar data using MW averaging kernels
- Corrected MW data from their bias with MLS data
- FTIR data
- Smoothed ozone sonde data using FTIR averaging kernels

Measurements considered are listed in table 4.

	FTIR	Microwave	Lidar	Ozone sondes	MLS
Number of measurements	83	1216	129	811	694
Number of coincidences ≥ 2	310				
Number of coincidences ≥ 3	17				

Table 4: Number of ozone profile measurements considered from ozone profile integration in At NyAlesund over the 2003-2013 period.

The vertical distribution of average estimated error for each measurement type considered for data integration at NyAlesund is displayed in figure 20.

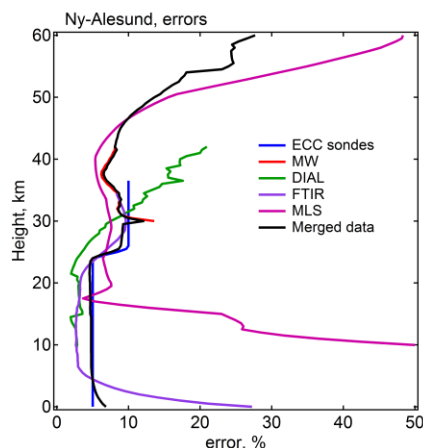


Figure 20: Vertical distribution of average estimated error for measurements performed in the Alpine stations and for MLS measurements performed in the vicinity of these stations.

4.2.1 Integrated ozone profiles

The monthly average ozone profiles based on the merged ozone data sets are displayed in figure 21a. Corresponding MLS monthly averages are displayed in figure 21b.

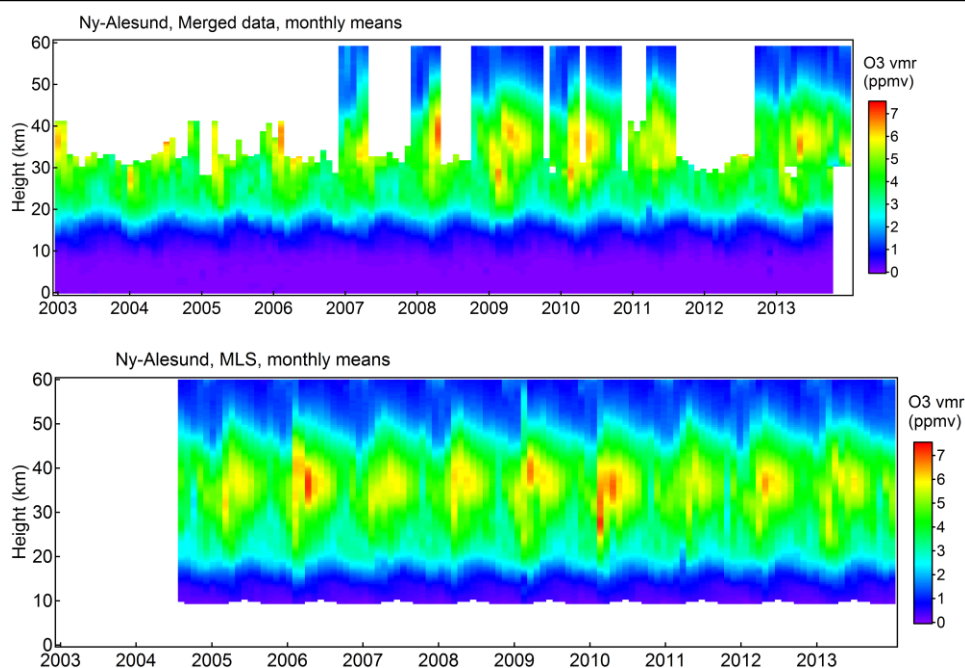


Figure 21: Monthly average ozone profiles from the merged data set (a) and MLS (b)

Corresponding ozone anomalies, e.g. monthly average ozone data minus the climatological average are displayed as a function of altitude in figure 22:

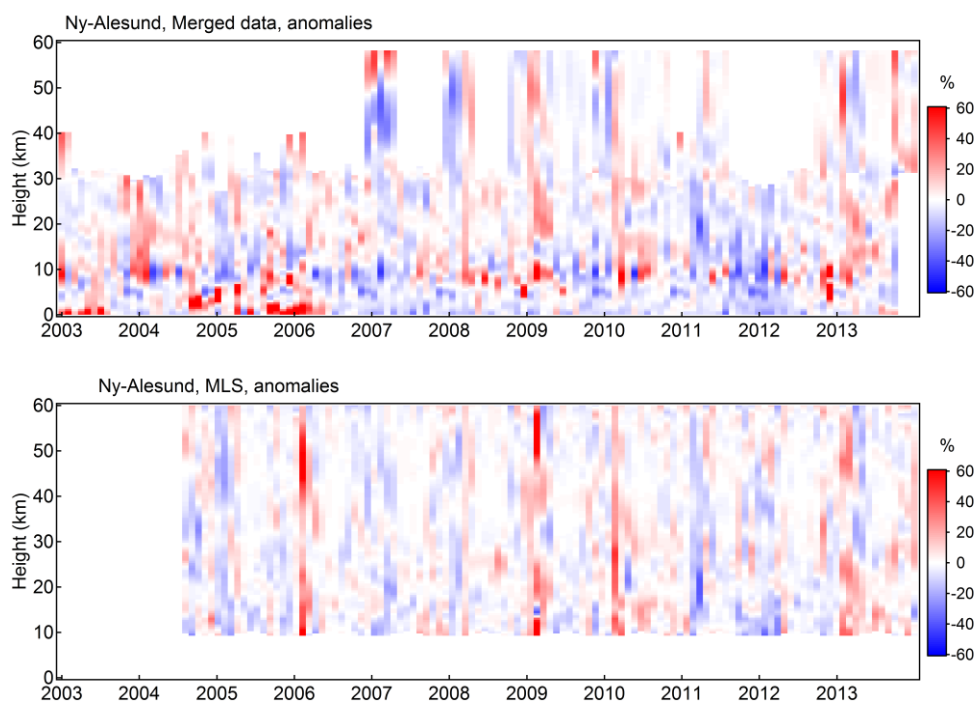


Figure 22: Monthly average ozone anomalies from the merged data set (a) and MLS (b)

For a better view of how the merged ozone data set compares with the various data sets, anomalies of the merged data set integrated over 3 altitude ranges is displayed in figure 23, together with the anomalies of individual data sets.

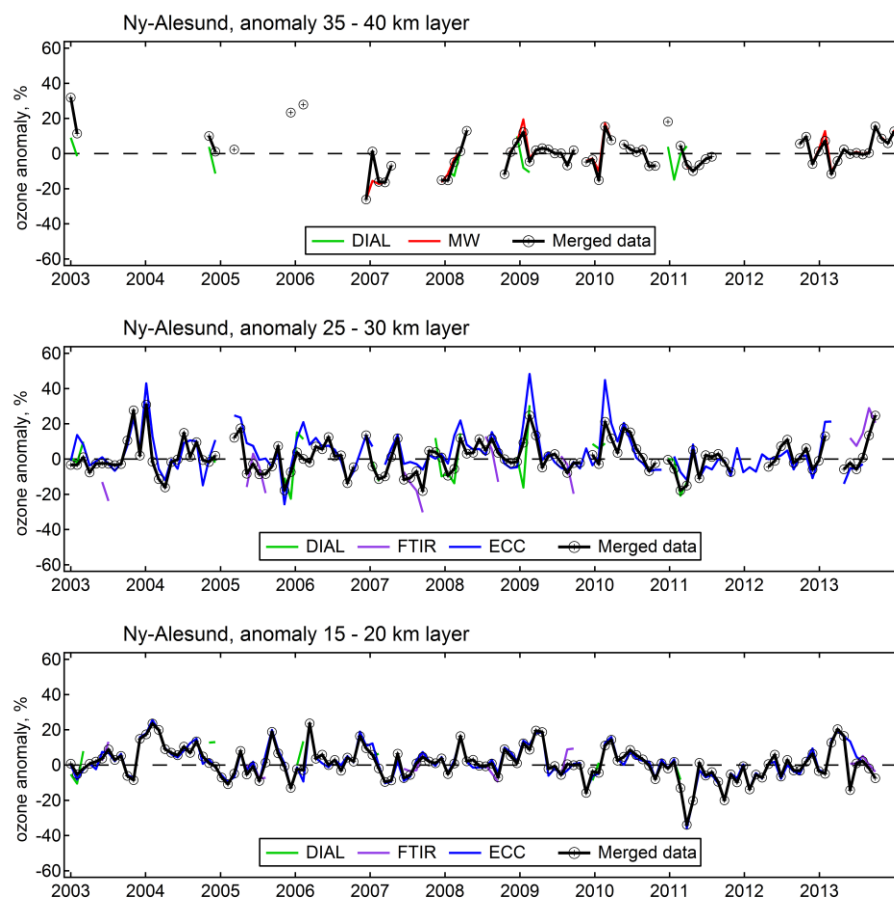


Figure 23: Monthly average ozone anomalies from the merged data set integrated over 5 km in 3 altitude ranges, compared to ozone anomalies of individual data sets

Figure 24 displays the ozone anomalies of the merged data set together with those derived from MLS measurements integrated over 3 altitude ranges.

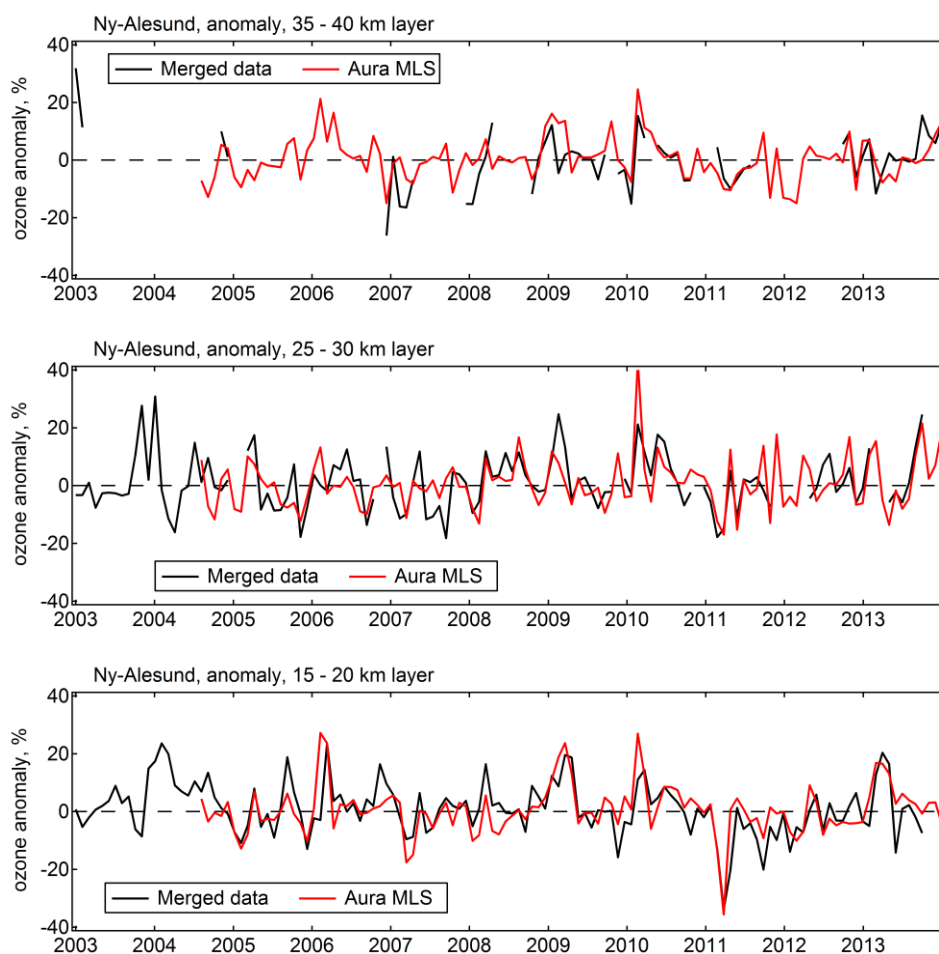


Figure 24: Monthly average ozone anomalies from the merged data set integrated over 5 km in 3 altitude ranges, compared to ozone anomalies of AURA-MLS

4.2.2 Partial and total ozone columns

The stratospheric and tropospheric partial ozone columns derived from the merged data and the calculation of the tropopause altitude are shown in figure 25:

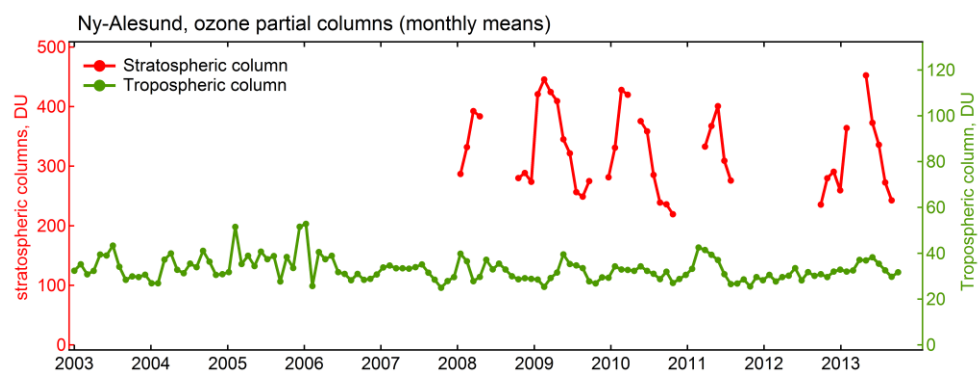


Figure 25: Temporal evolution of monthly averaged stratospheric and tropospheric partial ozone columns derived from the merged ozone data at NyAlesund

4.3 Izaña

At Izaña, there are only two long-term ozone profile data series available: measurements from the FTIR spectrometer performed by IMK (Germany) and ozone sondes measurements performed by AEMET.

	FTIR	Ozonesondes
Number of measurements	1210	631
Number of coincident dates	362	

Table 5: Number of ozone profile measurements considered from ozone profile integration at Izaña over the period 2003-2013

4.3.1 Integrated ozone profiles

The merged ozone profiles time series were constructed from the weighted average of FTIR data and smoothed ozone sonde data using FTIR averaging kernels.

Figures 26 and 27 show respectively the monthly averaged merged ozone profile time series and their anomalies with respect to climatological monthly means.

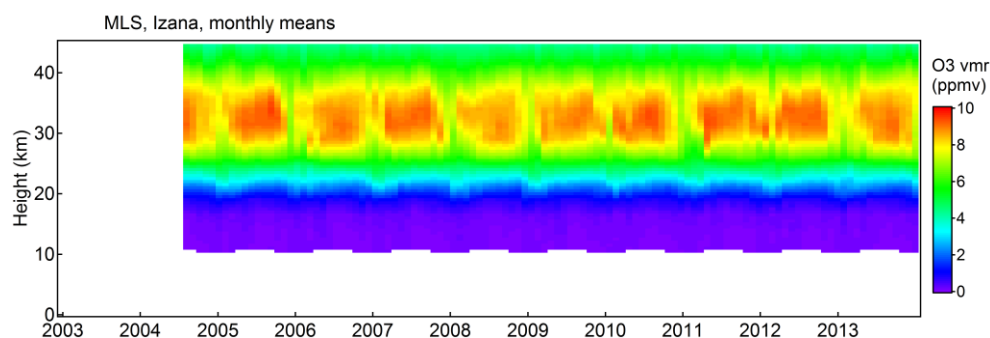


Figure 26: monthly averaged merged ozone profile time series at Izaña

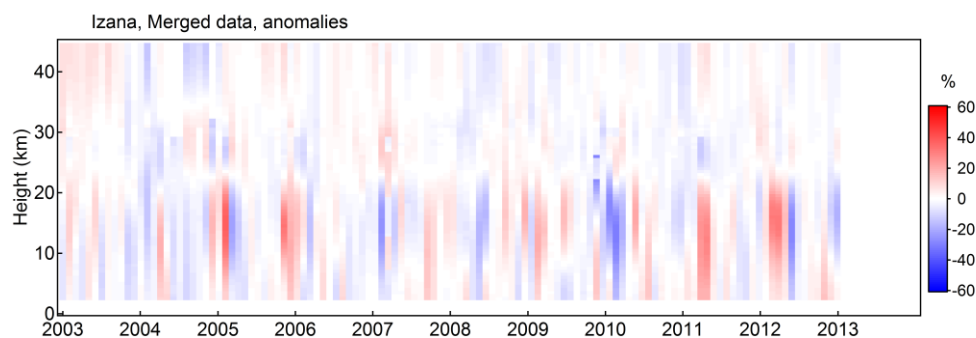


Figure 27: Monthly average ozone anomalies from the merged data set

Figure 28 displays the ozone anomalies of the merged data set together with those derived from AURA-MLS and SAGE II measurements integrated over 3 altitude ranges.

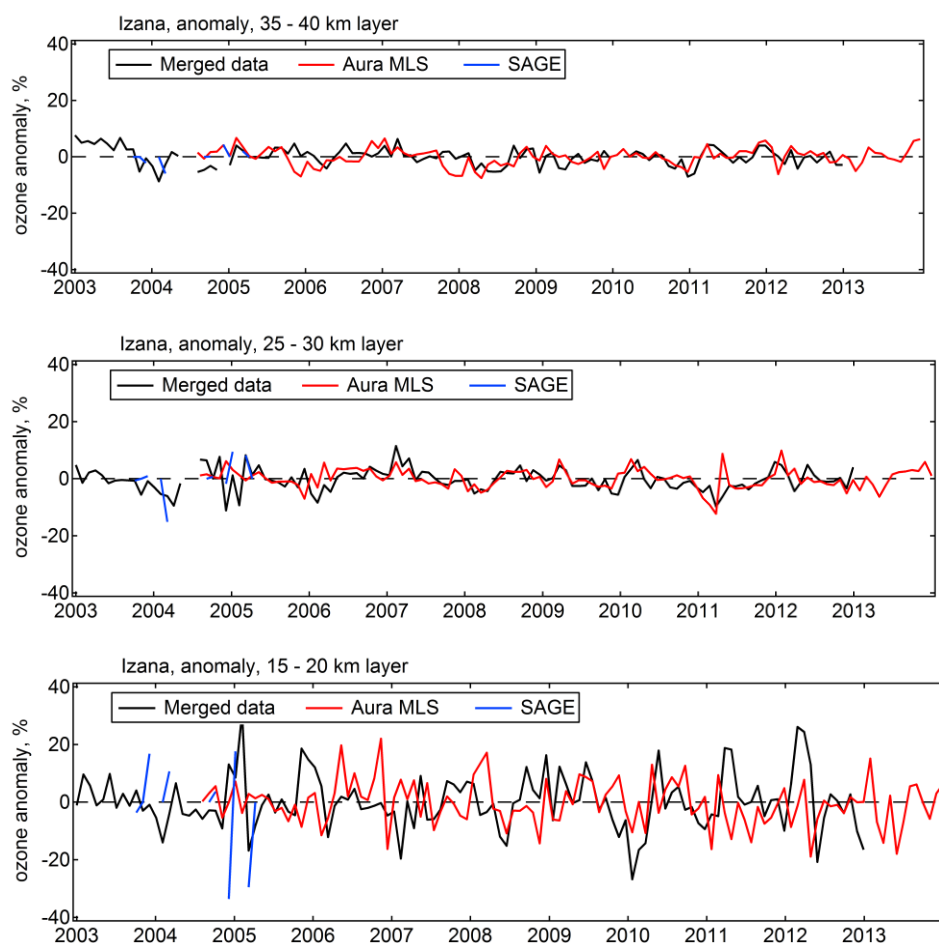


Figure 28: Monthly average ozone anomalies from the merged data set integrated over 5 km in three altitude ranges compared to ozone anomalies of AURA-MLS and SAGE II

4.4 La Réunion Island

At La Reunion Island, there are three long-term ozone profile data series available: measurements from the FTIR spectrometer performed by BIRA, ozone sondes and lidar measurements performed by LACy.

	FTIR	Lidar	Ozonesondes
Number of measurements	468	13	335
Number of coincident dates	48		

Table 6: Number of ozone profile measurements considered from ozone profile integration at La Reunion Island over the period 2003-2013

Due to the small number of lidar data during the period (the instrument suffered major breakdown and was completely refurbished for new operation from 2013), only ozone sondes and FTIR data were considered. Investigation of the systematic difference between FTIR data and coincident MLS data and between sondes data and coincident MLS data show that the FTIR profiles are generally larger than the other measurements and have to be corrected. Figure 29 shows the comparison of (1) coincident MLS and FTIR ozone profile data and (2) coincident MLS and ozone sonde ozone profile data, with the sondes and MLS data smoothed using the FTIR averaging kernels.

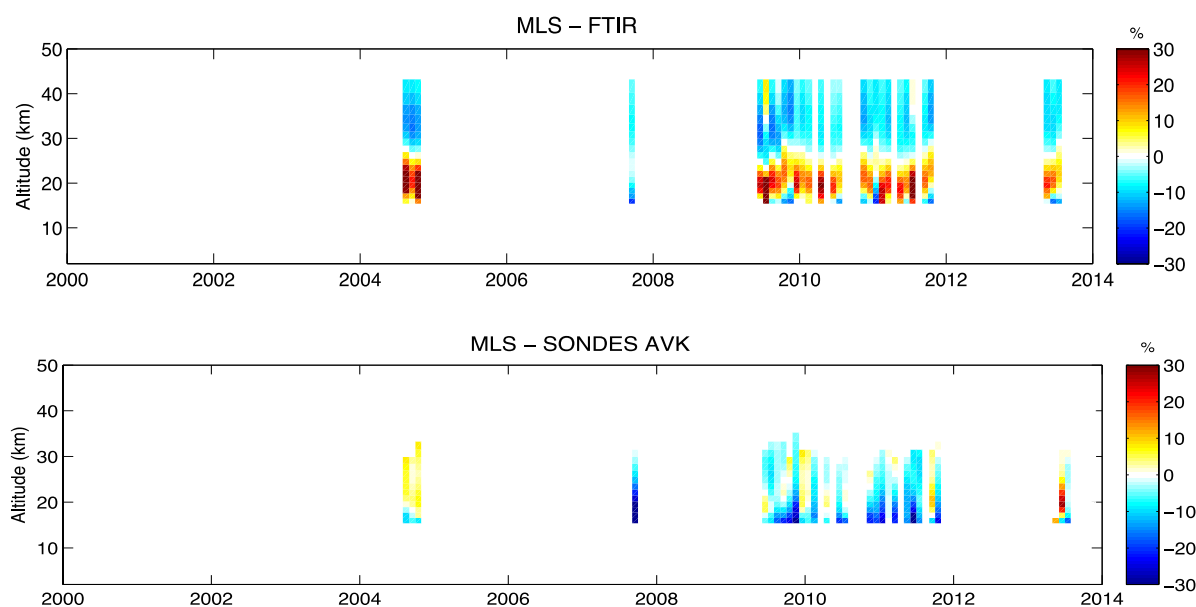


Figure 29: Monthly average bias between coincident MLS and FTIR ozone profile data (top panel) and between MLS and ozone sondes data (lower panel)

4.4.1 Integrated ozone profiles

The merged ozone profiles time series were constructed from the weighted average of FTIR data and smoothed ozone sonde data using FTIR averaging kernels. The FTIR data were corrected from their bias with AURA-MLS.

Figures 30 and 31 show respectively the monthly averaged merged ozone profile time series and their anomalies with respect to climatological monthly means.

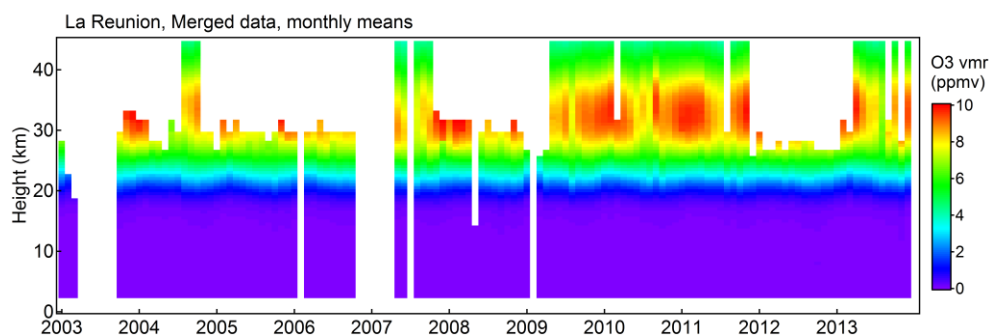


Figure 30: monthly averaged merged ozone profile time series at La Réunion

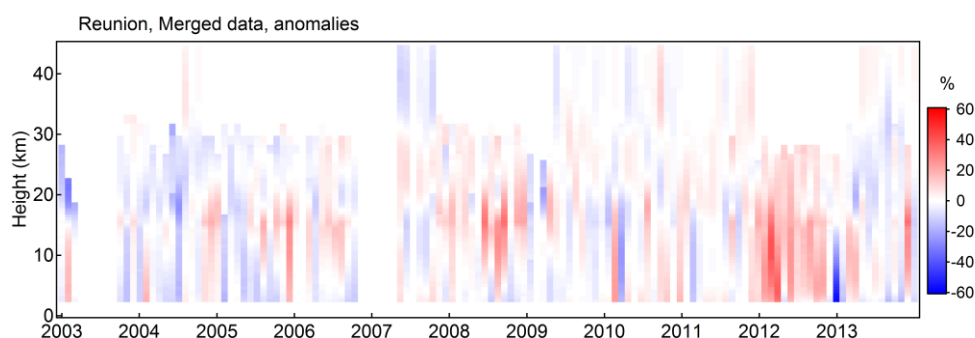


Figure 31: Monthly average ozone anomalies from the merged data set

Figure 32 displays the ozone anomalies of the merged data set together with those derived from AURA-MLS and SAGE II measurements integrated over 3 altitude ranges.

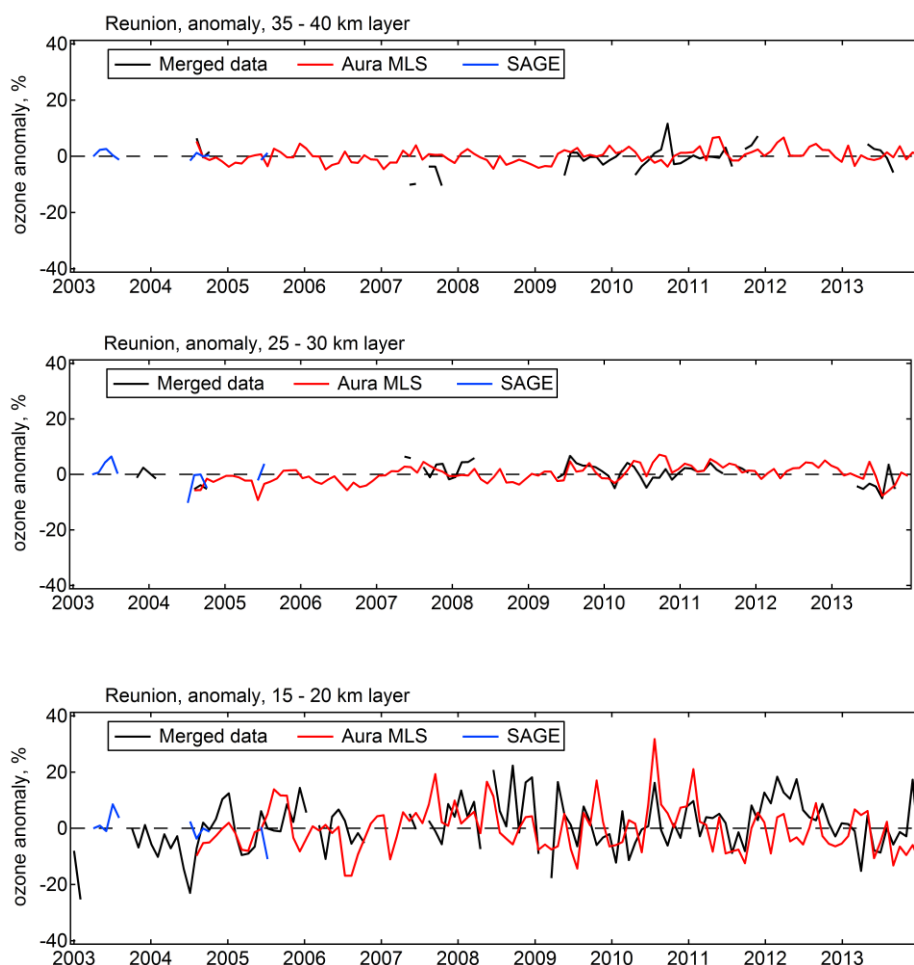


Figure 32: Monthly average ozone anomalies from the merged data set integrated over 5 km in three altitude ranges compared to ozone anomalies of AURA-MLS and SAGE II

Finally, the total ozone columns, which were derived from the integration of the merged ozone profiles have been compared to the SAOZ UV-Visible total ozone data at OHP (Figure 33). The comparison shows a general good agreement between both data sets.

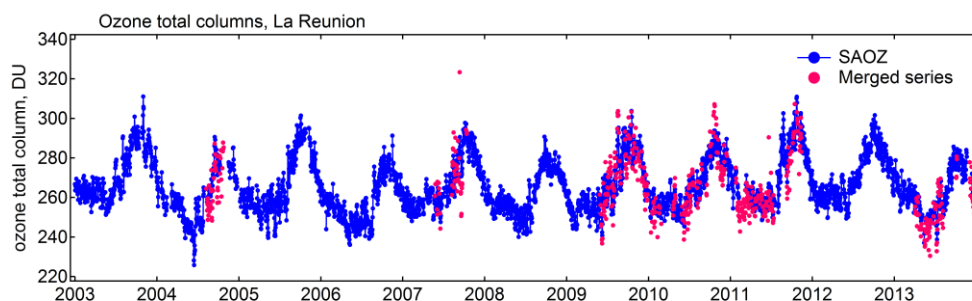


Figure 33: Comparison of total ozone columns derived from the merged ozone data and total ozone columns observed at OHP with the SAOZ UV-Visible spectrometer.