Umkehr Ozone Profile Analysis and Satellite Validation

WP-2190 | Final report

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1 Introduction

High quality and vertical resolution profiles of ozone that cover the troposphere, UTLS and the stratosphere, have been obtained by Brewer and Dobson spectrophotometers in a special viewing mode called *Umkehr*. Within the second phase of the European Space Agency IDEAS+ framework further efforts have been made to improve the operational Umkehr analysis algorithm and provide homogenized dataset optimized for the validation of the ozone profile observations by space-born sensors such as S5P/TROPOMI and GOME2 on the MetOp platforms. Within this phase of the project the improved Umkehr retrieval methods have been applied to Umkehr ozone profile measurements for a total of 9 ground-based stations (4 Brewer and 5 Dobson), and we updated the timeseries of the ground-based stations until the end of 2022.

In the following sections, the Umkehr observations retrieval methodology and the new improvements are briefly described. The particular settings used in each type of instrument, Brewer and Dobson so as to perform Umkehr measurements are given, and the homogenization methodology of the measurements is separately described, with emphasis on the recent activities related to the Arosa Dobson record. The results section comprises of the final updated time series of Umkehr observations for 4 Brewer and 5 Dobson stations, the description of the validation methodology, and the comparisons of the optimized Umkehr profiles to GOME-2 and TROPOMI satellite measurements. Case studies for Thessaloniki, Greece, Hradec Kralove (Czech Republic) (Brewer), Lauder, New Zealand and Boulder USA (Dobson) are shown, while a detailed summary of the validation statistics are presented for all stations and 4 atmospheric layers.

1.1 The Umkehr observations

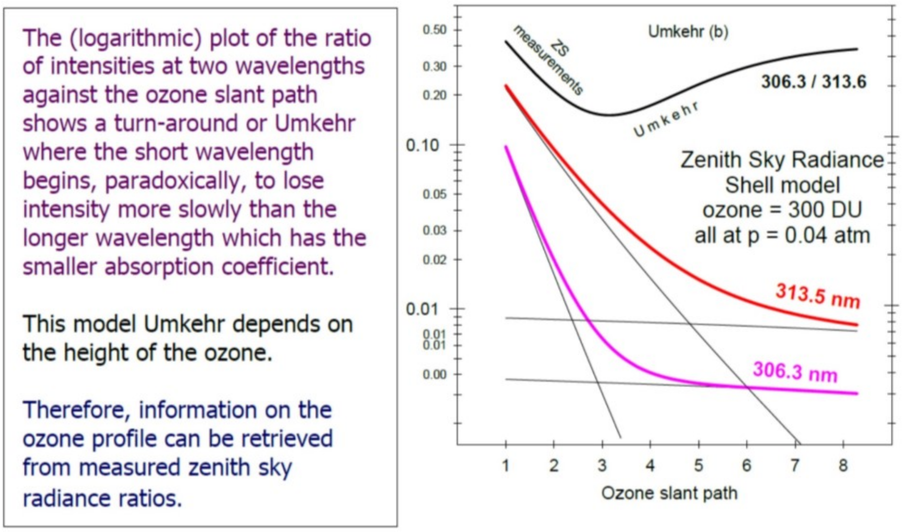
The Umkehr technique is an inexpensive way to retrieve the ozone profile in a coarse resolution from ground-based Dobson or Brewer spectrophotometers, which have a very long record of Umkehr measurements.

This method is based on measuring the difference in zenith sky intensities selected from two spectral regions over a range of solar zenith angles (SZA). When the ratio of the observed radiances is plotted against the SZA, the so-called Umkehr curve demonstrates an inflection point at about 86° SZA, shown in Figure 1-1 & Figure 1-2, which grants the observation its name since Umkehr stands for reversal or “change” in German (Petropavlovskikh et al., 2022).

Brewer and Dobson spectrophotometers record the zenith sky intensity at two different UV wavelengths (“short” and “long”), with the shorter to be more strongly absorbed by ozone. These two pairs are 311/332 nm for Dobson and 310/326 nm for Brewer observations while the SZA range is between 60°-90° SZA. The These intensities, called the N-Values, are calculated by the simplified formula:

$$N(\theta) = 100 \times log\left(\frac{I\prime(\theta)}{I(\theta)}\right) \qquad \textit{(Eq. 1)}$$

where I′ is the intensity at the “long” and I at the “short” wavelength and are interpolated at 12 nominal SZAs: 60°, 65°, 70°, 74°, 77°, 80°, 83°, 85°, 86.5°, 88°, 89° and 90°. The complete equation used for the calculation of the N-Values is given by Eq. 2 in Section 2.1.2. The algorithm for ozone retrieval, UMK04 (Petropavlovskikh et al., 2005) derives the ozone profile in 61 layers (Table 1) that are then combined into 10 layers for archiving at the World Ozone and Ultraviolet Radiation Data Centre (WOUDC) and National Oceanic and Atmospheric Administration (NOAA) repositories. According to the Averaging Kernel analysis, which demonstrates the information content of the profile observations, not all sub-layers contain enough independent points of information. This in practice means that the Umkehr Dobson method does not have sensitivity to ozone variability above Umkehr layer 9 (Petropavlovskikh, et al., 2004).



The (logarithmic) plot of the ratio of intensities at two wavelengths against the ozone slant path shows a turn-around or Umkehr where the short wavelength begins, paradoxically, to lose intensity more slowly than the longer wavelength which has the smaller absorption coefficient.

This model Umkehr depends on the height of the ozone.

Therefore, information on the ozone profile can be retrieved from measured zenith sky radiance ratios.

Figure 1-1: Umkehr method observations (wavelength ratio: Dobson 332/311 or Brewer 326/310 nm)

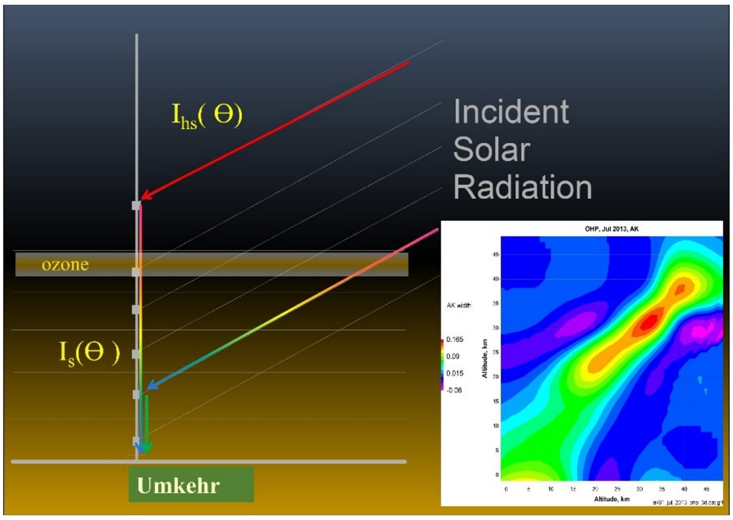


Figure 1-2: Scattering geometry information is weighted by different layers as sun sets/rises.

1.1.1 Brewer Umkehr settings

Ozone profiles using the Umkehr method can be derived by Brewer spectrophotometers through the analysis of a sequence of diffuse zenith radiance measurements at selected wavelengths recorded while the solar zenith angle is varying during a day. The intensity is measured quasi-simultaneously at eight discrete wavelengths: the five standard “short” wavelengths, used regularly for total ozone observations, as and, additionally, three “long” wavelengths. The full set of the eight Umkehr wavelengths are nominally: 306.3, 310.1, 313.5, 316.8, 320.1, 323.2, 326.4, and 329.5 nm. When the three “long” wavelengths are sampled, by moving appropriately the spectrometer’s grating, the last two “short” wavelengths are also sampled. The two sets (short and long) are about 80 sec apart, so the measurements at the two common wavelengths (316.8 and 320.1 nm) can be used to determine the stability of the radiation field during this period. Specifically, the ratio of the radiance at 320.1 nm for the two sets is used for screening the data for cloud effects. The Umkehr measurements are typically performed around sunrise and/or sunset at a number of different SZAs, ranging from ~60° to ~90°.

The Brewer Umkehr measurements are stored in the so-called B-files together with the measured total ozone column (TOC) which is derived from direct sun radiance measurements at the last four “short” wavelengths. The B-files of many Brewer spectrophotometers are available through international databases, for example the European Brewer Network, EUBREWNET, (http://rbcce.aemet.es/eubrewnet), or by direct contact with the instrument PIs.

The logarithm of the radiance measurements at two selected wavelengths centered at ~310 nm (short wavelength) and ~326 nm (long wavelength) forms the, previously discussed, single-pair N-value which is used for the retrieval of the ozone profile. The recorded N-values are then interpolated at 12 nominal SZAs (60°, 65°, 70°, 74°, 77°, 80°, 83°, 85°, 86.5°, 88°, 89° and 90°) to create the characteristic Umkehr curve. Then the N-values are normalized to the measurement at the smallest of the nominal SZAs (typically 60° or 70°), which makes the analysis insensitive to calibration and solar flux uncertainties.

For the analysis of the Brewer Umkehr measurements, the O3BUmkehr (v3.9) software is used, which has been developed by Martin Stanek at the Solar and Ozone Observatory of the Czech Hydrometeorological Institute (private communication). The main difference from the previous version (v3.2), which is based on the UKM04 algorithm (Petropavlovskikh et al., 2004; 2005), is the fact that the user can choose profile resolution of the retrieved ozone profile, in either a 61- or a 16-layer scheme. For this analysis, we used the 61-layer ozone profile, with the layers’ thickness range between 1.1 and 1.4 km (Table 1). The software has been recently modified to take into consideration the effect of the stray light contribution to the measured radiances, which introduces significant uncertainty in the retrieved ozone profiles (Petropavlovskikh et al., 2011), and is available online at http://o3soft.eu/. The analysis is performed iteratively and the retrieval of an ozone profile is deemed successful when less than 3 iterations are required to reach equilibrium and the root mean square of the residuals from an a priori profile is less than 1%.

Table 1: The 61 Umkehr layers and their typical altitude range.

Layer	Layer boundaries (km)	Pressure levels (hPa)
0	0 – 1.4	1000 – 840.896
1	1.4 – 2.8	840.896 – 707.107
2	2.8 – 4.2	707.107 – 594.604
3	4.2 – 5.5	594.604 – 500

4	5.5 – 6.7	500 – 420.448
5	6.7 – 7.9	420.448 – 353.553
6	7.9 – 9.1	353.553 – 297.302
7	9.1 – 10.3	297.302 – 250
8	10.3 – 11.4	250 – 210.224
9	11.4 – 12.5	210.224 – 176.777
10	12.5 – 13.6	176.777 – 148.651
11	13.6 – 14.7	148.651 – 125
12	14.7 – 15.8	125 – 105.112
…	…	…
59	71.1 – 72.2	0.036 – 0.031
60	72.2 – top of atmosphere	0.031 – 0

1.1.2 Dobson Umkehr settings

Umkehr measurements are performed by traditional Dobson instruments using the information from the C-wavelength pair (311.5, 332.4 nm, the temporal range 60°-90° SZA). The measured N-value is described as the ratio of the zenith sky intensities normalized with the solar flux at the top of the atmosphere, at 2 spectral channels (Eq. 2).

$$N(w,Z) = 100 * log_{10}\left\{\frac{\dfrac{I_{(w,z,Ls)}}{I_{(w,z,Ll)}}}{\dfrac{F_{(w,z,Ls)}}{F_{(w,z,Ll)}}}\right\} + k \qquad (Eq.2)$$

The Umkehr method uses N-values observed during either morning or afternoon period at 14 nominal SZAs. The algorithm for ozone retrieval, UMK04 (Petropavlovskikh et al., 2005) is provided with the ozone profile from two models (forward and inverse). Independent zenith sky cloud detector data are used for the screening of N-value measurements for interference of clouds in the zenith view. The automated Dobson instrument measures zenith sky ratios at solar zenith angles of 60°-90° for A, C and D pairs.

The Umkehr ozone profile processing is biased by the interference of out-of-band stray light into the measurement (Petropavlovskikh et al., 2011). The algorithm takes into account the stray light correction ($dN_{slc,}$ Eq. 3). dN_{slc} is estimated from look up tables that are dependent on latitude, station pressure (p), solar zenith angle (z), and total ozone (O_3).

$$N_{slc} = N(w,Z) + dN_{slc}(O_3,P,Z) \qquad (Eq.3)$$

The total ozone Dobson measurement from the morning or afternoon is used for adjusting the stray light correction prior to the ozone profile retrieval.

We modified the Umkehr Dobson retrieval to optimize tropospheric ozone information. The ozone column profile in DU is calculated in 61-layers based on the pressure level grid as described below.

$$BTM\_Press_{(j)} = 1013 * 2^{\left(-\frac{j}{4}\right)}$$

where *j* is the layer number from 0 to 60.

In addition to the 61 layers of ozone partial columns (DU) derived by Umkehr retrievals, the ozone number density is included in the output. It is used for validation with space-born, such as from S5P/TROPOMI & GOME-2/Metop satellite ozone records. The output also includes the full Averaging Kernel matrix in 61 layers. A temperature profile is required for conversion of DU to the number density. Temperature profiles are taken from the e Naval Research Laboratory, NRL, temperature climatology. Figure 1-3 shows the ozone profile and averaging kernel in 61-layers for the Dobson Umkehr retrieval at Arosa, Switzerland in 2020 as example.

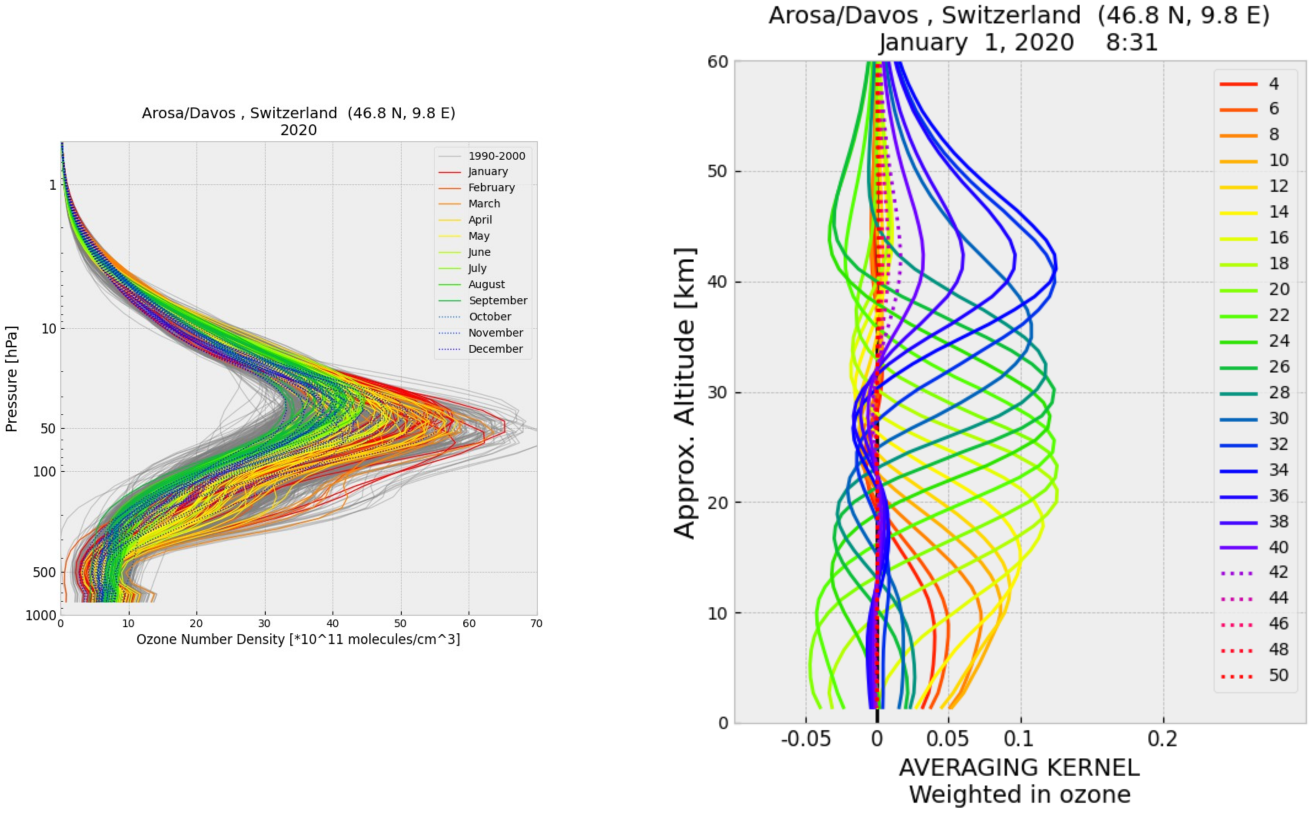


Figure 1-3. a) The ozone number density profile for the Umkehr retrieval at 61 levels, profiles are observed in 2020 at Arosa/Davos Dobson station in Switzerland. b) ozone weighted averaging kernel at 61-layers for ozone profile observed on January 1, 2020 at Arosa, Switzerland.

In Figure 1-4, we present the ozone profile error due to measurement noise uncertainty. This is obtained by comparing the ozone as retrieved using as a priori the N_M2GMI+N_residual profile versus the retrieval using as a priori the M2GMI profile. The McPeters Climatology vs M2GMI a priori obtains the residual N value (N_residual) from the retrieval of the simulated N value.

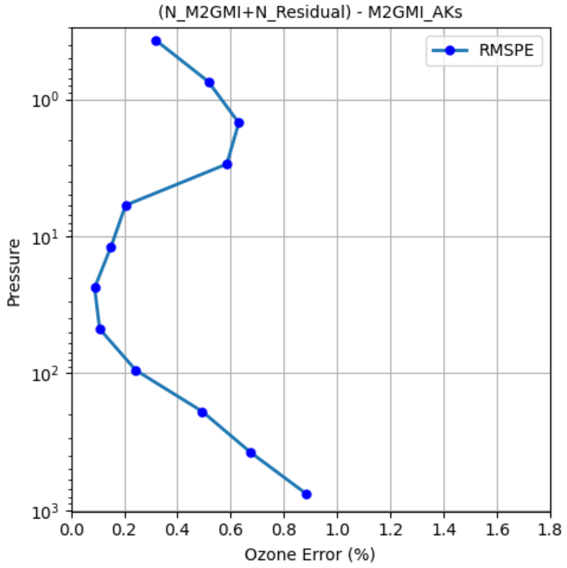


Figure 1-4: Ozone profile error due to measurement noise uncertainty.

We also estimated the uncertainty introduced in the retrievals due to errors in the total ozone column. Figure 2-5 provides an estimation of the impact on the ozone layer retrievals when errors are present in the TOC integrated from the Umkehr retrieval profile. The results show an impact similar to the TOC errors in the upper stratosphere. However, large errors are observed in the lower stratosphere.

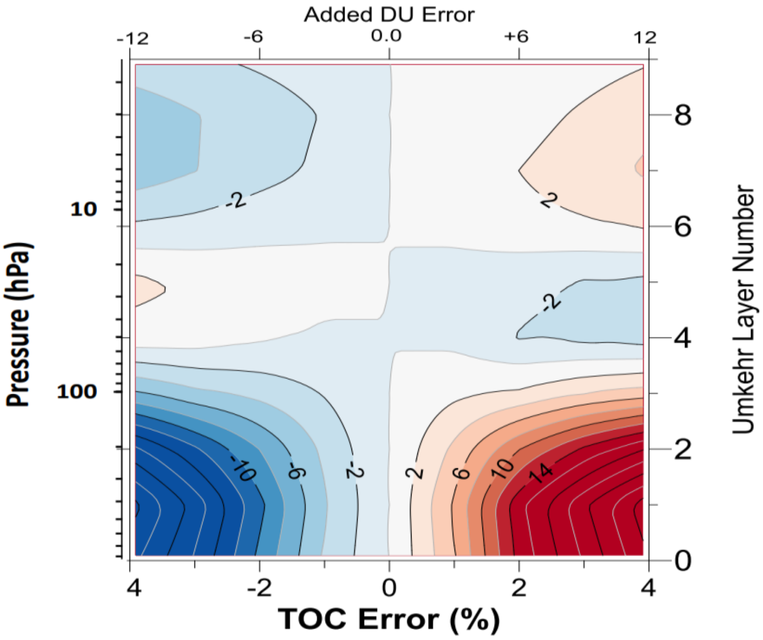


Figure 1-5: Impact on ozone profiles from Umkehr retrievals when given the total ozone error.

1.2 Brewer optimization methodology

Several factors can affect the quality of the derived Umkehr ozone profiles, such as the accuracy of the measured total ozone column, the effective temperature of the ozone absorption throughout the atmosphere, as well as various optimizations in the settings of the retrieval software. In Garane et al., 2021, these have already been investigated and explained in detail. We briefly mention here that:

Total ozone column. The effect of using post-processed TOC instead of the one stored in the B-files was assessed on 2 years of data in Thessaloniki by manually inserting the post-processed TOC in the retrieval algorithm. The effect on these 2-years of data is generally small, within ±2.5 DU (or ±5%) for layers 0+1 and 2+3 that are the most affected, and much smaller for the higher layers (4 to 8+).

Ozone effective temperature. The effect of the ozone effective temperature (Teff) on the Umkehr retrievals was assessed by analyzing the data of Brewer #005 in Thessaloniki for the year 2008. Instead of the climatological ozone effective temperature, a Teff more representative for this location was calculated from the combination of radiosonde temperature profiles and climatological ozone profiles, and the post-processed total ozone column amount derived from the direct sun measurements of the same instrument. Temperature differences were found to be up to 10°C which changed layer 4 ozone between about 0.5 and -2.5 DU with an average difference of ~-0.75 DU (~-1.05 %).

Optimization of the Observation Error. In the O3BUmkehr algorithm the user can specify the observation errors which are used in the error covariance matrix and are provided at the 12 nominal SZAs used in the retrieval. To assess the quality of the retrievals, the normalized (to 70^{o} SZA) N-Values from 4 years of measurements at Thessaloniki with Brewer #005 were used. Results suggest that the observation error used in the algorithm is comparable to the standard deviation of the residuals and can be applied in the retrieval algorithm.

1.3 Dobson optimization methodology

The Dobson optimization methodology has already been extensively described in Garane et al., 2021.

Parallel to the optimization efforts of this project, MeteoSwiss group applied the optimization to the Dobson Umkehr record at Arosa based on comparisons with other Dobson and Brewer observations at the same station. The NOAA and MeteoSwiss homogenized records were compared and differences in two versions were assessed and published by Maillard-Barras et al. (2022, further referred as MB22). The nonlinear trend model (DLM, Ball et al, 2017) was used to study trend evolution over time and vertically (Figure 7 from MB22). Based on the difference found in BM22 comparisons, the optimization of the Arosa Umkehr record was continued with a special focus on the 2012-2020 time period. It is important to reconcile these differences in the Arosa Dobson record due to its impact on the 2000-2020 trends.

According to Table 4 of the MB22 paper the 2012-2013 and 2018 periods experienced instrumental changes and therefore required close attention to the development of optimization corrections. The continuity of the M2GMI modelled ozone record was assessed with respect to the Arosa ozone record in the 2012 -2014 period. It was also found that some data were missing in 2014 that have originally created a correction bias. The decision was made to extend the shift correction through the end of 2013. In the previous version of Arosa optimized record, the correction was applied in 2017, but the actual instrumental change occurred in 2018. Hence, corrections were added for year 2018. The MLS overpass ozone profile is used to verify detection of instrumental shifts and developed corrections (Figure 1-6). The one-year smoothed fit is applied for Umkehr (MLS) records and the trends indicate 4.54 (0.84) %/decade that indicate the erroneous impact of Umkehr step changes on the ozone recovery trend detection. The difference between two records is shown in the bottom panel and the drift trend is evaluated at -3.5±1.47 %/decade. The correction was developed and applied to correct Umkehr records.

The optimized Umkehr records were compared with the MLS record (panel c in the Figure 1-6) and the biases are reduced to less than ± 5% which is the MM uncertainty of Umkehr ozone retrieval in layer 8 (pink envelope around zero). The drift between optimized Umkehr and MLS is reduced to 0.14 ± 0.73 %/decade.

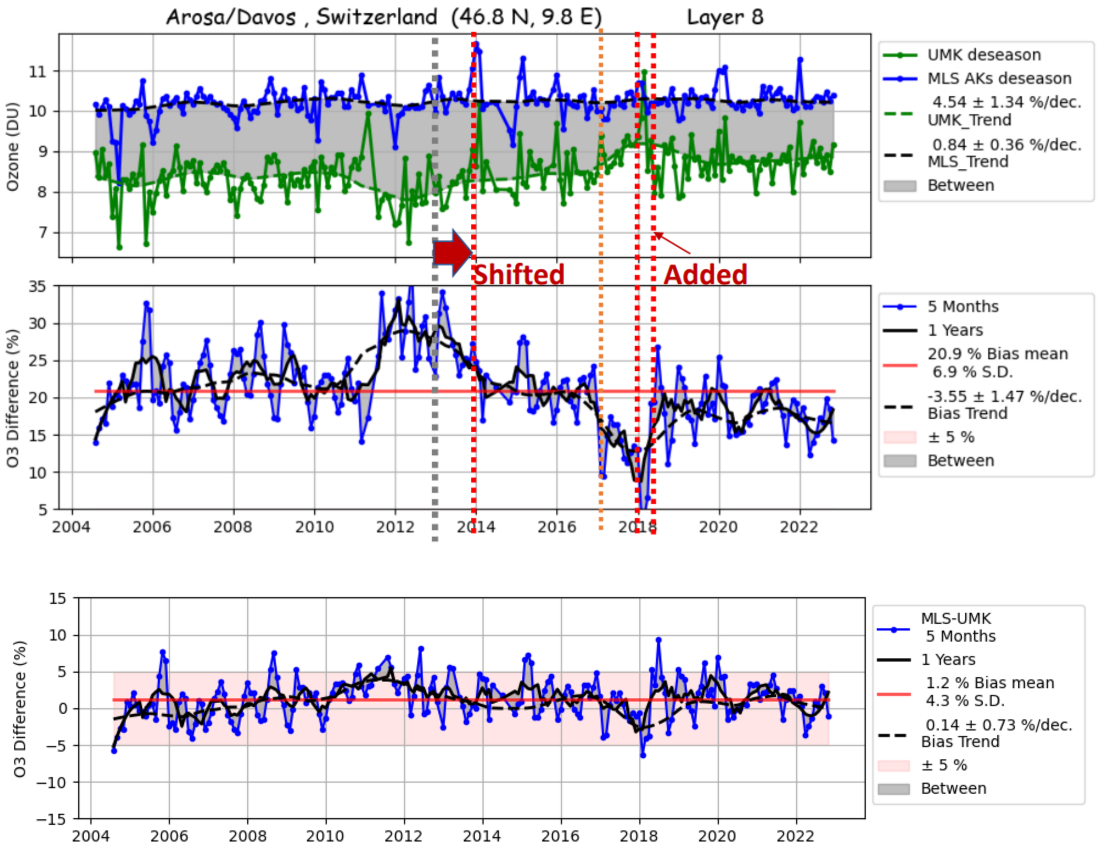


Figure 1-6. a) Operational Umkehr (green) and MLS (blue) deseasonalized ozone data are shown as time series between 2005 and 2022 in the top panel, the grey area between two lines indicates time dependent bias. MLS ozone profiles are smoothed with Umkehr AK. The one-year smoothed fit is done for Umkehr and MLS records, the trends are assessed as %/decade (shown in the legend). Three vertical red dashed lines indicate the time for the instrumental changes in Umkehr record. b) The difference between two records is shown in the middle panel and the drift trend is evaluated at -3.5+/- 1.47 %/decade. c) the same as b) but for the difference between the optimized Umkehr and MLS monthly mean records

Full comparisons between optimized Umkehr (reference), MLS (green), S-NPP OMPS Limb profiler (NASA, V2.6, orange) and ozonesonde (Payerne, blue) are shown in Figure 1-7. The drifts between satellite records and Umkehr record in 2012-2022 in the middle and upper stratosphere are reduced in the new optimized version of Arosa record but become consistently negative in the lower stratosphere (left/right panel shows the Umkehr old/new version). The Umkehr drift from ozonesonde record in the upper troposphere is reversed from negative to positive for the new version. The drift between ozonesonde and Umkehr at 50 hPa is somewhat increased in the new version, a fact that requires further investigation.

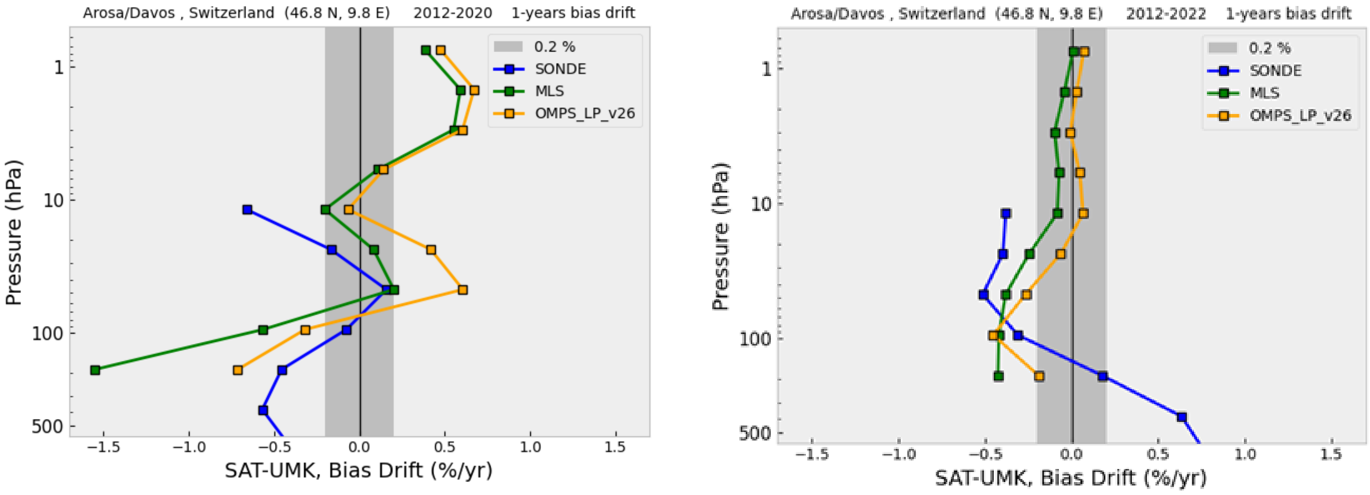


Figure 1-7. Drifts of satellite (MLS and S-NPP OMPS LP) and ozonesonde records relative to the Umkehr record at Arosa in 2012-2020. Left panel: old Umkehr version. Right Panel: new Umkehr version. The vertical grey envelope is +-0.2 %/decade.

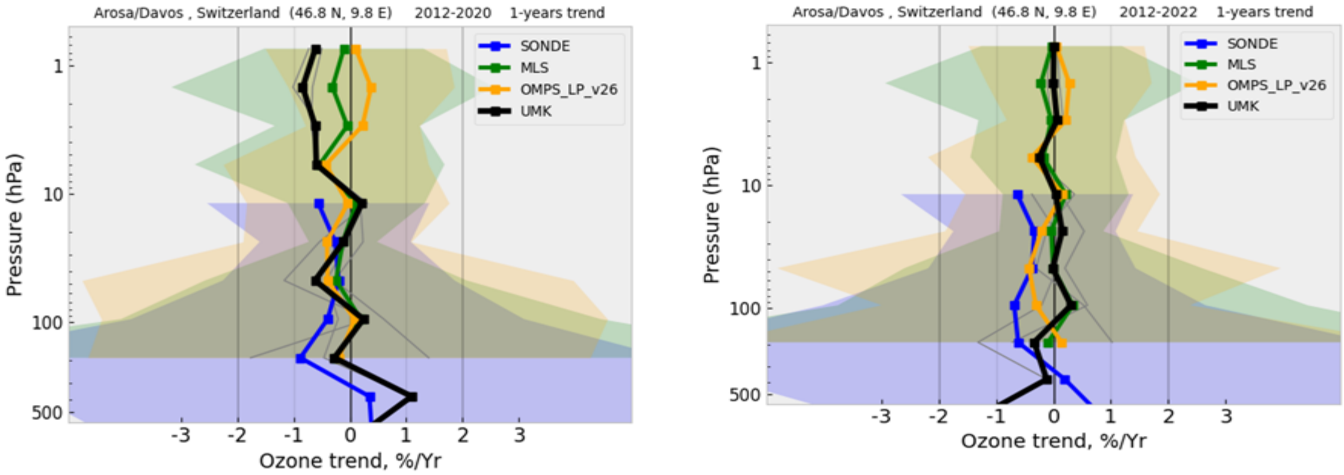


Figure 1-8. Trends derived from 2012-2022 period for Umkehr (black), ozonesonde (blue), MLS (green) and S-NPP OMPS LP (orange). The left panel shows the older version of optimized Umkehr and the right panel shows trends with the updated Umkehr data (results for other record have slightly changed due to sampling differences).

2 Results

2.1 The updated Umkehr timeseries

Umkehr measurements from four Brewer instruments (3 type MKIII and 1 type MKII) operating at Madrid, Spain; Hradec Kralove, Czech Republic; Warsaw, Poland and Thessaloniki, Greece were studied for the period 2017 – 2022. Additionally, Umkehr measurements from five Dobson stations (Boulder, USA; Mauna Loa, USA; Lauder, New Zealand; Haute Provence, France and Arosa, Switzerland) have been optimized and are presented for the same time period. Table 2 shows the list of the stations for both types of instruments and their exact locations.

Table 2: The list of stations and instruments that were used in this study.

Station	Instrument Type/ Number	Latitude	Longitude
Thessaloniki	Brewer MKII (#005)	40.63 N	22.96 E
Hradec Kralove	Brewer MKIII (#184)	50.18 N	15.84 E
Madrid	Brewer MKIII (#186)	40.45 N	3.72 W
Warsaw	Brewer MKIII (#207)	52.25 N	20.94 E
Boulder	Dobson (#061)	40.02 N	105.25 W
Mauna Loa	Dobson (#076)	19.53 N	155.58 W
Haute Provence	Dobson (#085)	49.93 N	5.71 E
Lauder	Dobson (#072)	45.05 S	169.68 E
Arosa	Dobson (#051)	46.78 N	9.68 E

2.1.1 Brewer timeseries

The Umkehr measurements of Brewer #005 (MKII) operating at Thessaloniki, Greece, have been already analyzed up to 2017 and results have been reported in several publications (Fragkos et al., 2016; Fragkos et al., 2018; Kosmidis et al., 1997; Kosmidis et al., 2004). In the frame of this project the data have been re-evaluated to include the optimizations described above (e.g. post-corrected total ozone column, ozone effective temperature calculated from local temperature profile measurements and climatological ozone profiles) and the time series of the ozone profiles has been extended to the end of 2022. The data were analyzed with the “O3BUmkehr” algorithm. To ensure the highest possible quality in the retrieved profiles the N-values have been visually checked for detection of outliers and all data contaminated (e.g., by clouds that have skipped the automated cloud flagging, or affected by other instrumental issues) were manually removed. All profiles were stray-light corrected based on the effect of the near-field stray-light on the ozone absorption coefficients, which has been determined from the shape of the slit function of Brewer #005 (see discussion in Garane et al., 2021), following the methodology developed by Petropavlovskikh et al. (2011). It should be noted that Umkehr measurements at Thessaloniki are performed only in the evening, therefore only PM profiles are shown.

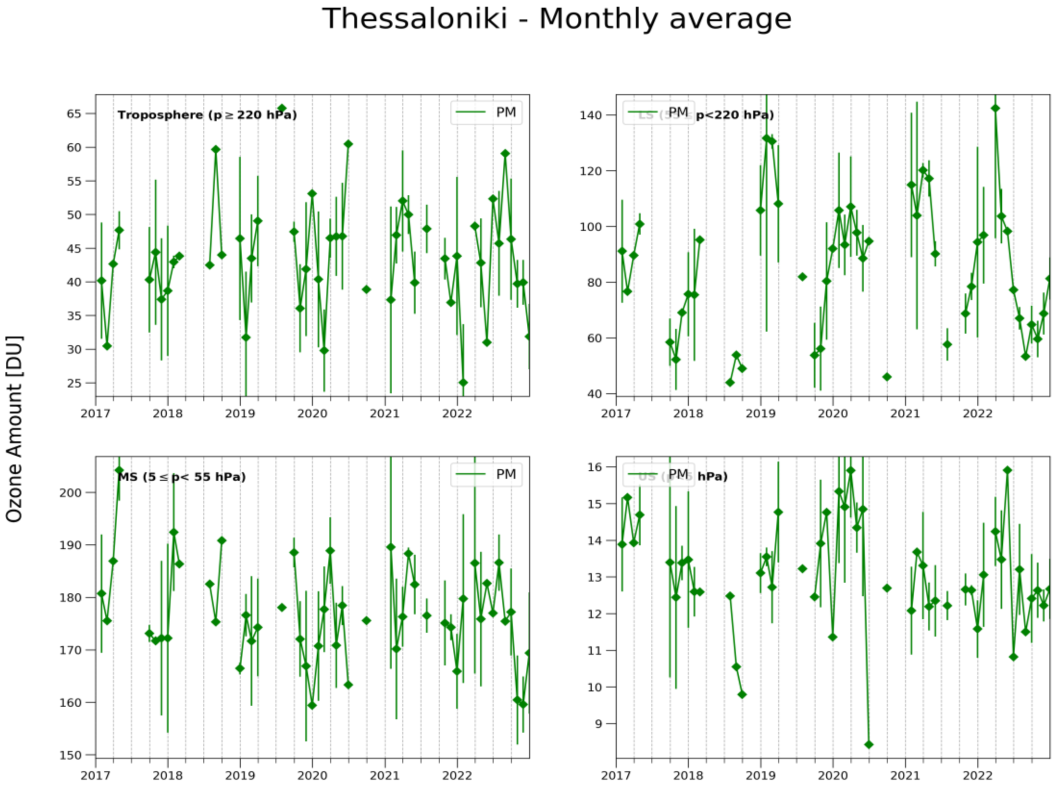
Additional stations that submit data to the EUBREWNET database were investigated for possible Umkehr measurements that could be further analyzed. The available data cover the period 2017 – 2022. While many (around 20) stations were identified to perform Umkehr observations, only about half of them have observations covering the range of solar zenith angles (at least 70-90°) required to successfully retrieve the ozone profile. One additional criterion for the final selection of stations was the type of Brewer: double monochromator spectrophotometers, type MKIII, were chosen in order to eliminate the effect of stray light.

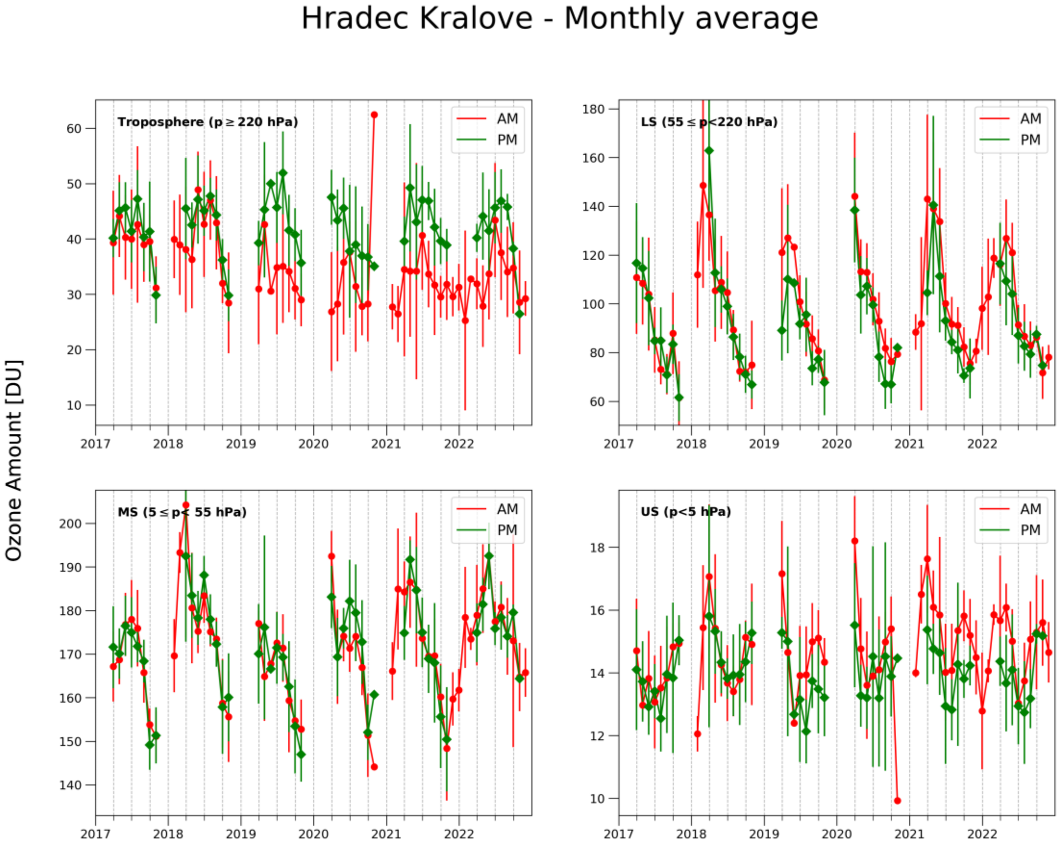
Three other Brewer stations, apart from Thessaloniki, have hence been selected, which have sufficient observations of at least a few months. The B-files of Brewers MKIII operating at Hradec Kralove (#184), Warsaw (#207) and Madrid (#186) were downloaded from EUBREWNET for the period 2017–2022. The Umkehr measurements from these three stations were performed both morning and evening. Thus, both AM and PM profiles are presented. These data were analyzed with the O3BUmkehr algorithm, and the retrieval settings were optimized for each particular station. The partial ozone columns were divided into 4 certain layers: Troposphere, containing the tropospheric ozone, Lower Stratosphere (LS), containing the ozone between the tropopause and the ozone peak, Main Stratosphere (MS), containing the ozone peak and Upper Stratosphere (US), containing the ozone content above the ozone peak. The time series of partial ozone columns at those certain layers were derived separately for the morning and evening twilight hours. The boundaries of each one of these 4 layers are presented in Table 3.

Table 3: Boundaries of the four standard layers

Layer	Boundaries in km	Boundaries in hPa
Troposphere	0 – 11	1013.25 – 220
Lower Stratosphere	11 – 20	220 – 55
Main Stratosphere	20 – 40	55 – 5
Upper Stratosphere	40 – 50	5 – 2

For the construction of the monthly mean averages, all available daily profiles have been used up to the pressure level where P ≥ 2 hPa, since there is no significant ozone information for P < 2 hPa. The time series of the monthly mean ozone for each layer, for all four stations, are shown in Figure 2-1.


Thessaloniki - Monthly average
Ozone Amount [DU]
Troposphere (p ≥ 220 hPa)
PM
p<220 hPa)
PM
MS (5 ≤ p< 55 hPa)
PM
hPa)
PM
2017
2018
2019
2020
2021
2022


Hradec Kralove - Monthly average
Ozone Amount [DU]
Troposphere (p ≥ 220 hPa)
AM
PM
LS (55 ≤ p<220 hPa)
AM
PM
MS (5 ≤ p< 55 hPa)
AM
PM
US (p<5 hPa)
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2018
2019
2020
2021
2022

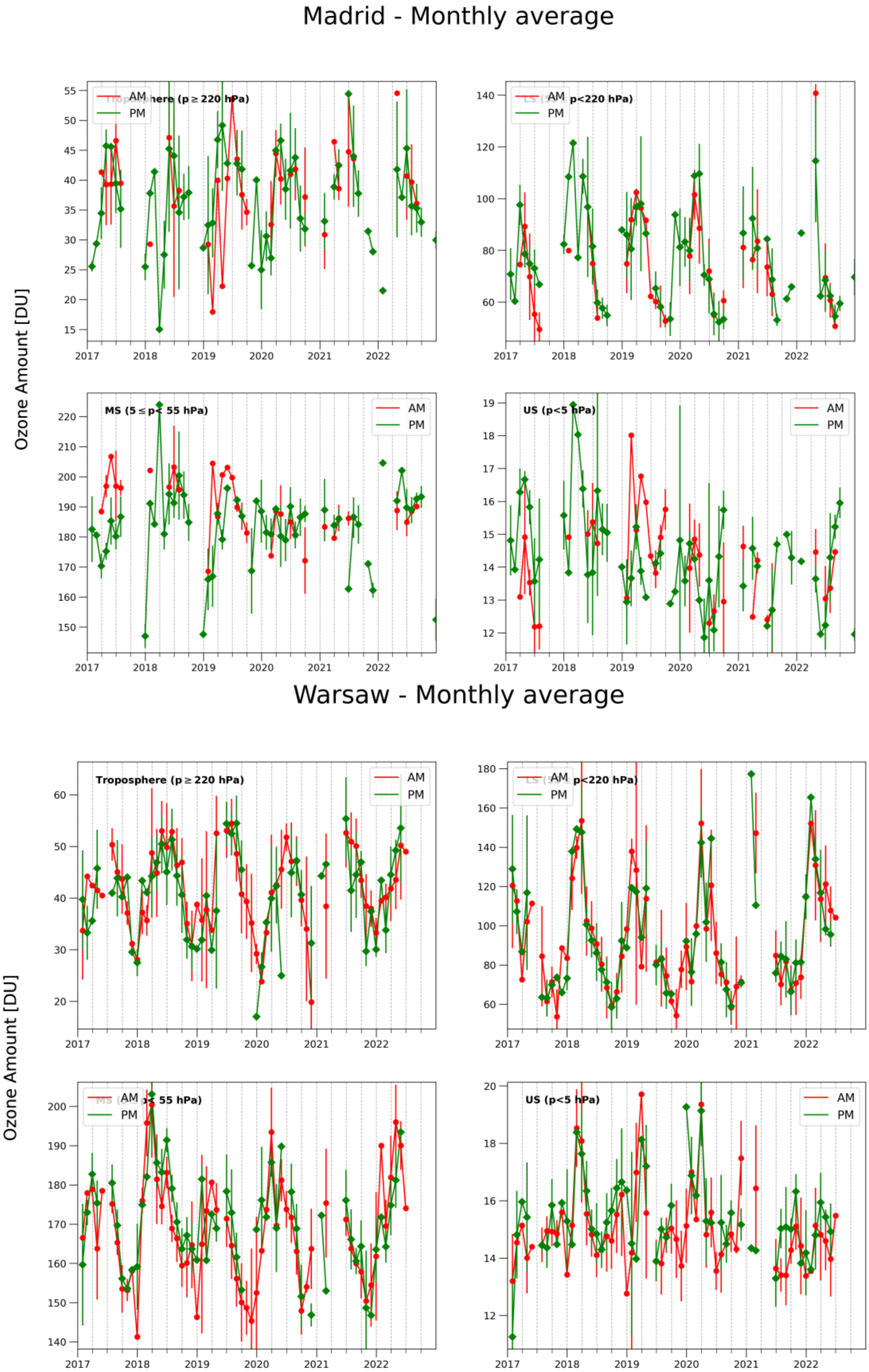


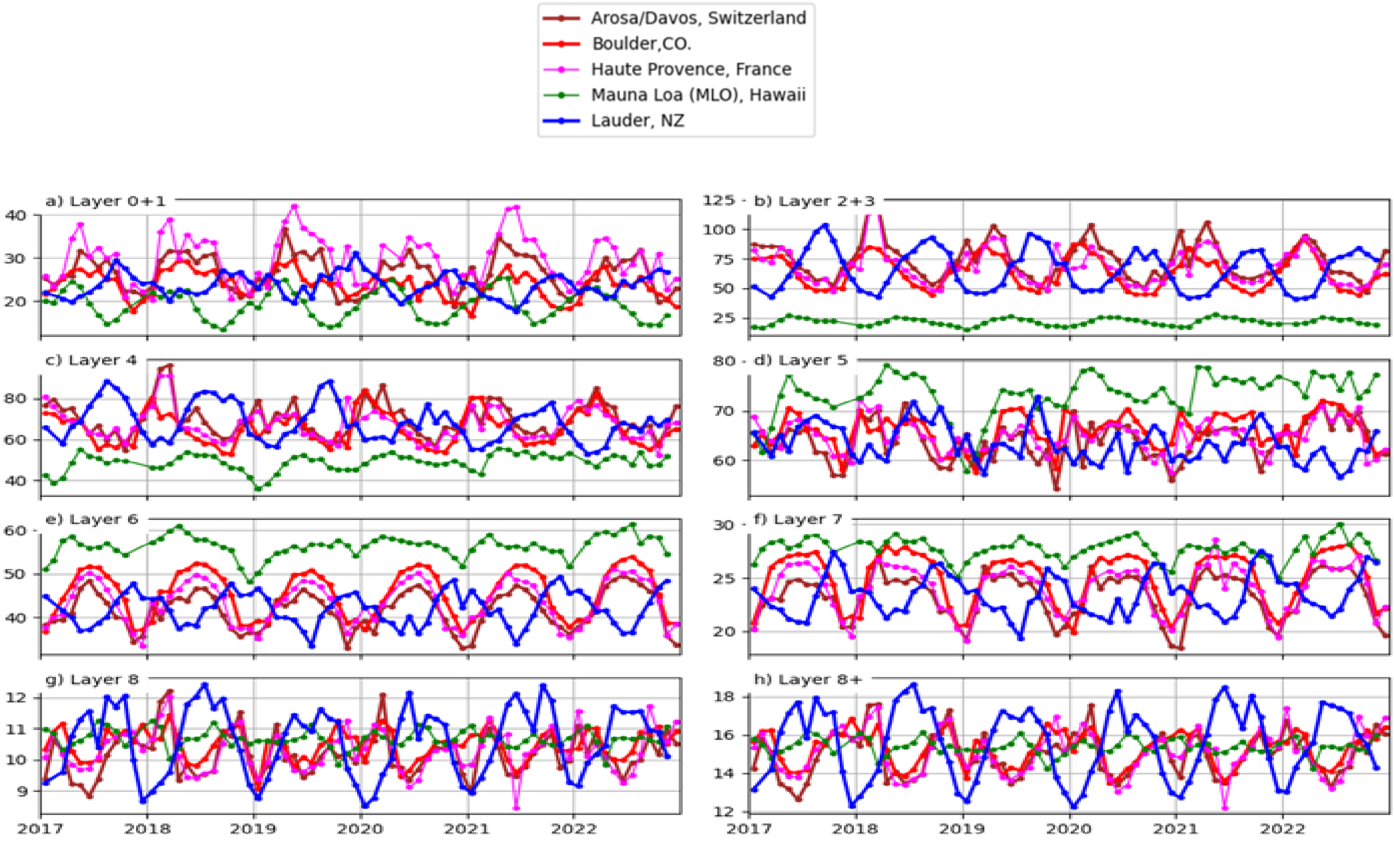
Figure 2-1: Time series of monthly mean ozone column amount (in DU) in 4 layers: Troposphere (upper left panel), Lower Stratosphere (LS, upper right panel), Main Stratosphere (MS, lower left panel) and Upper Stratosphere (US,

lower right panel) over Thessaloniki, Hradec Kralove, Madrid and Warsaw, respectively, for the period 2017 – 2022. AM and PM data are plotted in different colors and vertical bars correspond to the standard deviation.

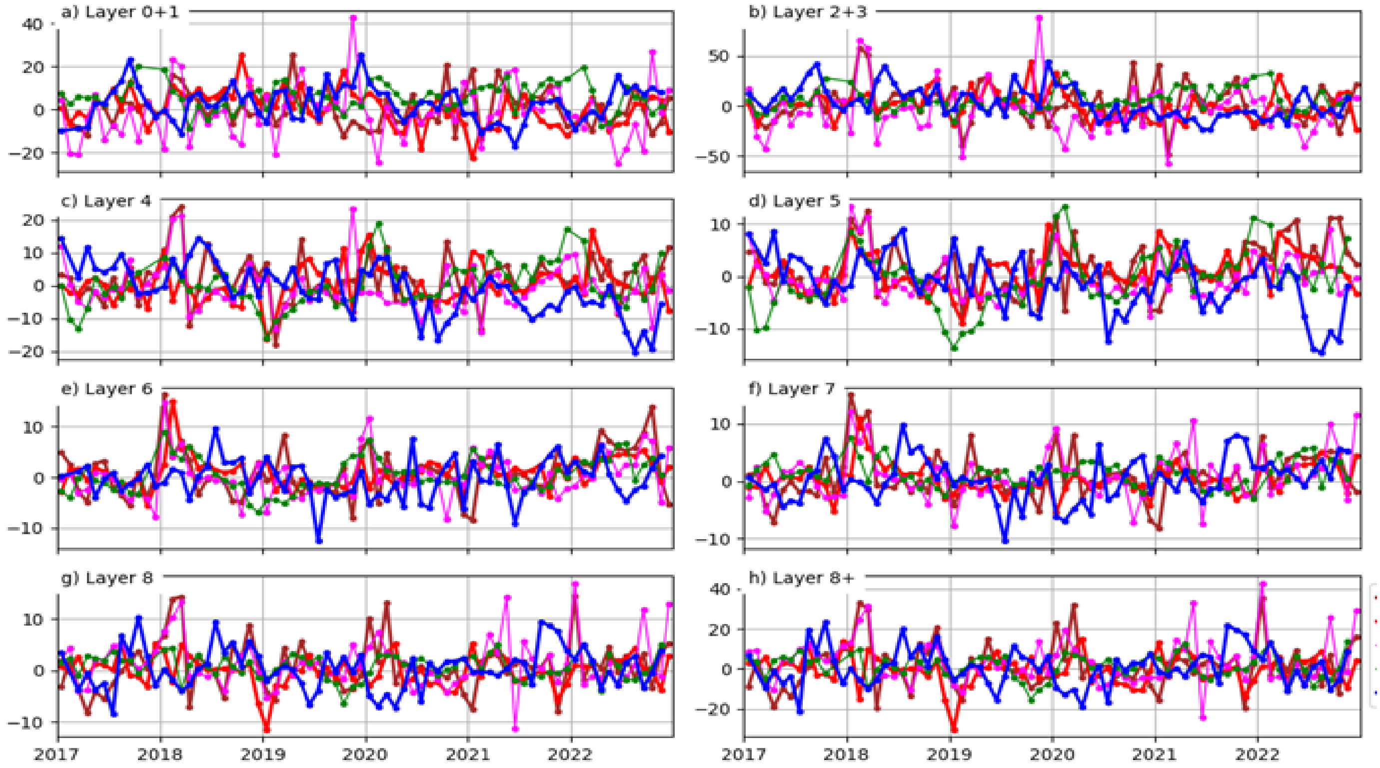
Figure 2-1 shows the time series of monthly mean ozone column amount (in DU) for each of the 4 layers along with the standard deviation of each monthly value, for the four selected Brewer stations. A direct comparison between AM and PM profiles is difficult since on many occasions the monthly means are derived from different days. However, the comparison of AM and PM data is promising in most of the stations, at least qualitatively. In addition, in some cases, such as in Hradec Kralove, in the Troposphere layer (upper left panel), a certain bias between the AM and PM data appear. The reason for this is still under investigation.

2.1.2 Dobson timeseries

Figure 2-2, panel a, shows the 2017- 2022 ozone monthly mean time series in 8 layers for the five Dobson stations: Arosa, Switzerland (purple); Boulder, USA (red); Haute Provence, France (pink); Mauna Loa, Hawaii (green) and Lauder, New Zealand (blue). Data from Arosa, OHP and Boulder share similar seasonal cycle in most of the layers, but the largest differences are found in layer below 250 hPa. The Lauder seasonal cycle is shifted by 6 months as is expected from ozone variability in the Southern Hemisphere. The seasonal cycle at MLO is reduced in phase. Panel (b) shows the same data but as deseasonalized time series. The 1995-2020 data were used to create the climatology that was subtracted from the 2020-2022 record.



(a)



(b)

Figure 2-2 a) Time series of monthly mean ozone column amount (in DU) in 8 layers for the period 2017 – 2022, derived from Umkehr observations performed at the five selected Dobson stations. b) the same as a), but for deseasonalized records (in %) relevant to the 1995-2020 climatology

Scatter plot between the Upper/Mid stratosphere and the Umkehr ozone are shown in Figure 2-33 over Arosa/Davos, and the Mid/Low stratosphere is compared with the ozonesonde stations at Payerne and Hohenpeissenberg (DWD).

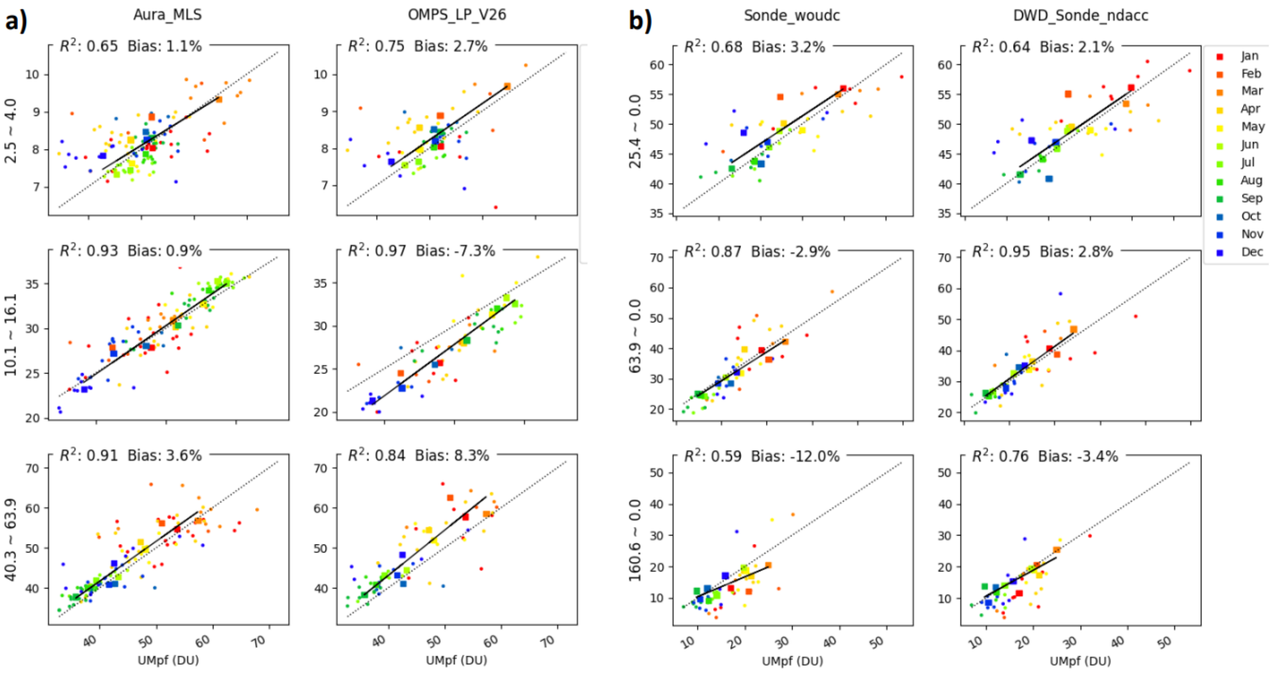


Figure 2-3. a) Scatter plot between NASA satellites (Aura MLS, OMPS_LP_v2.6) overpass and Umkehr ozone over Arosa/Davos station in 2020. b) Scatter plot with Ozonesonde between Payerne and Hohenpeissenberg (DWD) and Davos Umkehr.

2.2 Umkehr Ozone profile comparison to satellite datasets

2.2.1 The satellite observational datasets

S5P/TROPOMI

TROPOMI (TROPOspheric Monitoring Instrument) is a nadir-viewing spectrometer and the only instrument on the Sentinel-5 Precursor (S5P) satellite launched in October 2017. S5P is part of the Copernicus Earth observation programme and is designed to prevent a potential gap in global atmospheric monitoring that could arise between existing missions such as OMI and GOME-2 and the upcoming Sentinel-4 and Sentinel-5. S5P is in a sun-synchronous orbit with an Equator crossing time of 13:30 local time (LT). TROPOMI consists of four spectrometers in the UV, UVIS, NIR and SWIR spectral range. For the ozone profile retrieval, UV1 and UV2 bands are used. One measurement pixel in the middle of the swath covers 28.8×5.6 km^2 (across track × along track) in UV1 and 3.6×5.6 km^2 in UV2 channels. Further information on the instrument and updates on its status and data products can be found in Veefkind et al., 2012 and Lambert et al., 2023 respectively.

The aim of the TROPOMI ozone profile product is to continue the record of stratospheric ozone, monitor changes, and improve the accuracy of the retrieved stratospheric profiles. The TROPOMI ozone profile product provides vertical information of ozone in two ways: as a number density profile at 33 pressure levels and as 6 sub-columns with a vertical sampling of 6 km up to an altitude of 24 km and lower sampling above (24-32 km, and 32 km to TOA). The full profile information is used in this work, so that the averaging kernels are also considered in the comparisons with the Umkehr observations. It should be noted that the UV spectrum allows retrieving approximately 6 independent pieces of information on the ozone profile (Veefkind et al., 2021).

The TROPOMI ozone profile datasets shown in this report are publicly available from the Copernicus Data Space Ecosystem webpages, Copernicus Data Space Ecosystem | Europe's eyes on Earth.

Overpass files over each of the locations of the Brewer and Dobson stations studied in this project were extracted using the recommended filters (Keppens et al., 2021; di Pede et al., 2023). All satellite profiles within 0.5° from the ground-based station were averaged and compared to the Umkehr profile for that day, both for the dawn and dusk observations.

GOME2/Metop

The Global Ozone Monitoring Experiment-2 (GOME-2) instrument, on board the MetopA, -B and –C platforms, measures the radiance spectrum of sunlight scattered from the atmosphere in the (UV) wavelength region 260-330 nm (Hassinen et al., 2016). Since the absorption of ozone decreases with increasing wavelength, this differential absorption makes it possible to derive the vertical distribution of ozone in the atmosphere from the measured UV spectrum (Tuinder et al., 2019).

Within the EUMETSAT Atmospheric Composition Monitoring Project, ACSAF, the Ozone ProfilE Retrieval Algorithm (OPERA) iteratively finds the vertical ozone profile best matching the GOME-2 reflectance using optimal estimation (van Peet et al., 2014). The forward model is based on LidortA and uses an externally prescribed instrument response slit function. The *a priori* ozone climatology is (currently) based on McPeters/Labow/Logan (McPeters et al., 2007). The surface pressure and the vertical temperature profile come from operational European Centre for Medium-Range Weather Forecasts, ECMWF, forecasts. Special adaptations have been made to handle spikes in the measured radiance spectrum in the South Atlantic Anomaly. The vertical ozone profiles are given as partial ozone columns in Dobson Units (DU) in 40 layers from the surface up to 0.001 hPa. The ground pixel size corresponds to the footprint of the Band-1b integration time, i.e for MetopB and –C 40 x 80 km^2 and for MetopA 40 x 40 km^2 (along-track x cross-track). The local equator crossing time is approximately 09:30 L.T. The high-resolution GOME-2 ozone profiles have been validated against ozonesonde, lidar and microwave profiles (Delcloo et al., 2020), against other satellite ozone profile products (Kauppi et al., 2016) and assimilated for forecasting purposes in modelling studies (van Peet et al., 2018.)

The GOME-2 high-resolution ozone profile datasets shown in this report are publicly available from the ACSAF product webpages, Offline high-resolution ozone profile (acsaf.org).

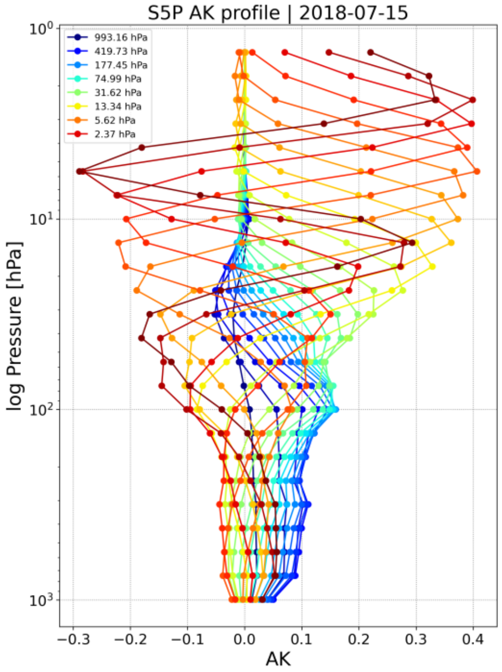
Overpass files over each of the locations of the Brewer and Dobson stations studied in this project were extracted using the recommended filters (Tuinder, 2020). All satellite profiles within 0.5° from the ground-based station were averaged and compared to the Umkehr profile for that day, both for the dawn (AM) and dusk (PM) observations.

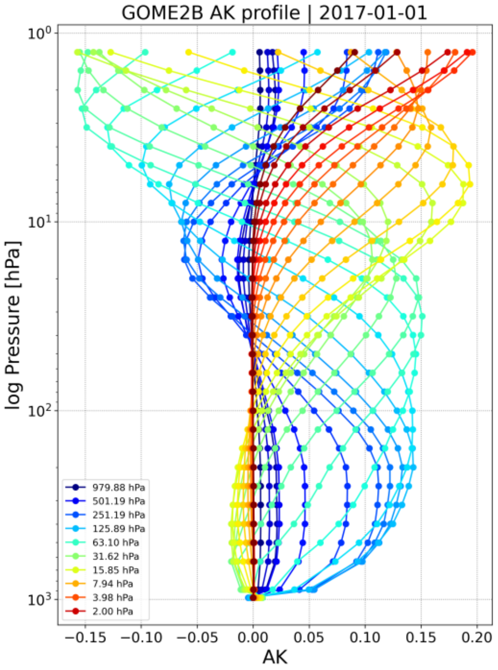
2.2.2 Comparison methodology

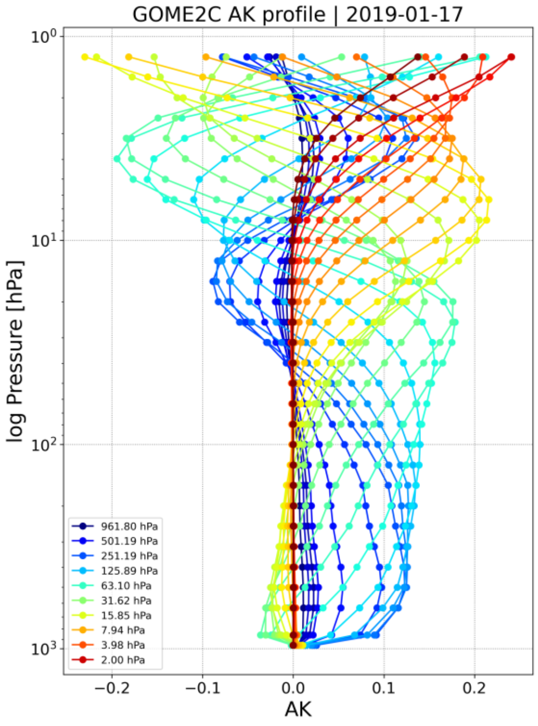
In this study the S5P-TROPOMI and GOME-2 B&C ozone profiles were compared with the 61-layer scheme Umkehr ozone profiles for the selected Brewer and Dobson stations. Both the Umkehr and the GOME-2 B&C ozone profiles were retrieved in DU. The S5P profile it is provided in number density units (molec/m^3). Thus, before the comparison procedure, the S5P ozone and apriori profiles were converted to DU. To do so, first it was converted to column number density units (molec/m^2), using the AtmosphericToolbox© Harp module, and then by dividing with the Loschmidt number ($2.687 \cdot 10^{20}$ particles/cm^3) it was converted to DU.

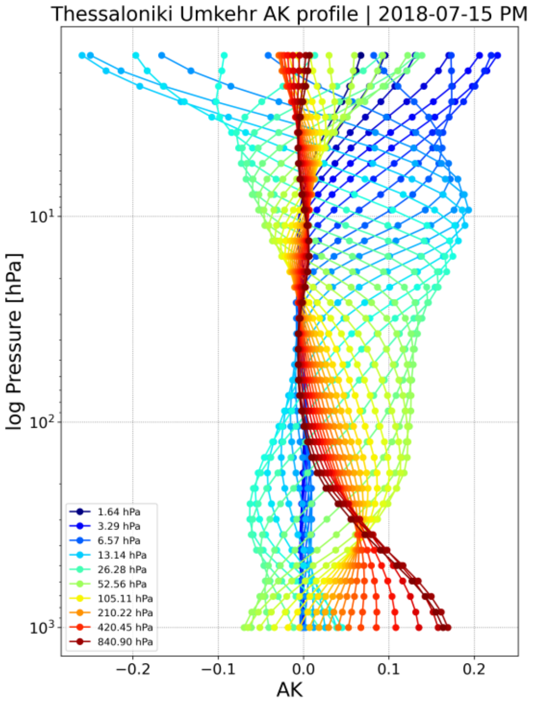
For the comparisons between the satellite (S5P-TROPOMI and GOME-2 B&C) and the ground-based datasets, we three approaches were investigated in full:

1. Interpolation of the satellite ozone profile to the Umkehr vertical resolution – Averaging Kernel (AK) smoothing by applying the square Umkehr AK to the interpolated satellite profile
2. Interpolation of the Umkehr ozone profile to the satellite vertical resolution – AK smoothing by applying the square satellite AK matrix to the interpolated Umkehr profile
3. Interpolation of the Umkehr ozone profile to the satellite vertical resolution – AK smoothing by applying the rectangular satellite AK matrix (interpolated to rows) to the interpolated Umkehr profile (Ceccherini et al., 2011)


S5P AK profile | 2018-07-15
log Pressure [hPa]
AK
10^0
10^1
10^2
10^3
−0.3
−0.2
−0.1
0.0
0.1
0.2
0.3
0.4
993.16 hPa
419.73 hPa
177.45 hPa
74.99 hPa
31.62 hPa
13.34 hPa
5.62 hPa
2.37 hPa


GOME2B AK profile | 2017-01-01
log Pressure [hPa]
AK
10^0
10^1
10^2
10^3
−0.15
−0.10
−0.05
0.00
0.05
0.10
0.15
0.20
979.88 hPa
501.19 hPa
251.19 hPa
125.89 hPa
63.10 hPa
31.62 hPa
15.85 hPa
7.94 hPa
3.98 hPa
2.00 hPa


GOME2C AK profile | 2019-01-17
log Pressure [hPa]
AK
10^0
10^1
10^2
10^3
−0.2
−0.1
0.0
0.1
0.2
961.80 hPa
501.19 hPa
251.19 hPa
125.89 hPa
63.10 hPa
31.62 hPa
15.85 hPa
7.94 hPa
3.98 hPa
2.00 hPa


Thessaloniki Umkehr AK profile | 2018-07-15 PM
log Pressure [hPa]
AK
10^1
10^2
10^3
−0.2
−0.1
0.0
0.1
0.2
1.64 hPa
3.29 hPa
6.57 hPa
13.14 hPa
26.28 hPa
52.56 hPa
105.11 hPa
210.22 hPa
420.45 hPa
840.90 hPa

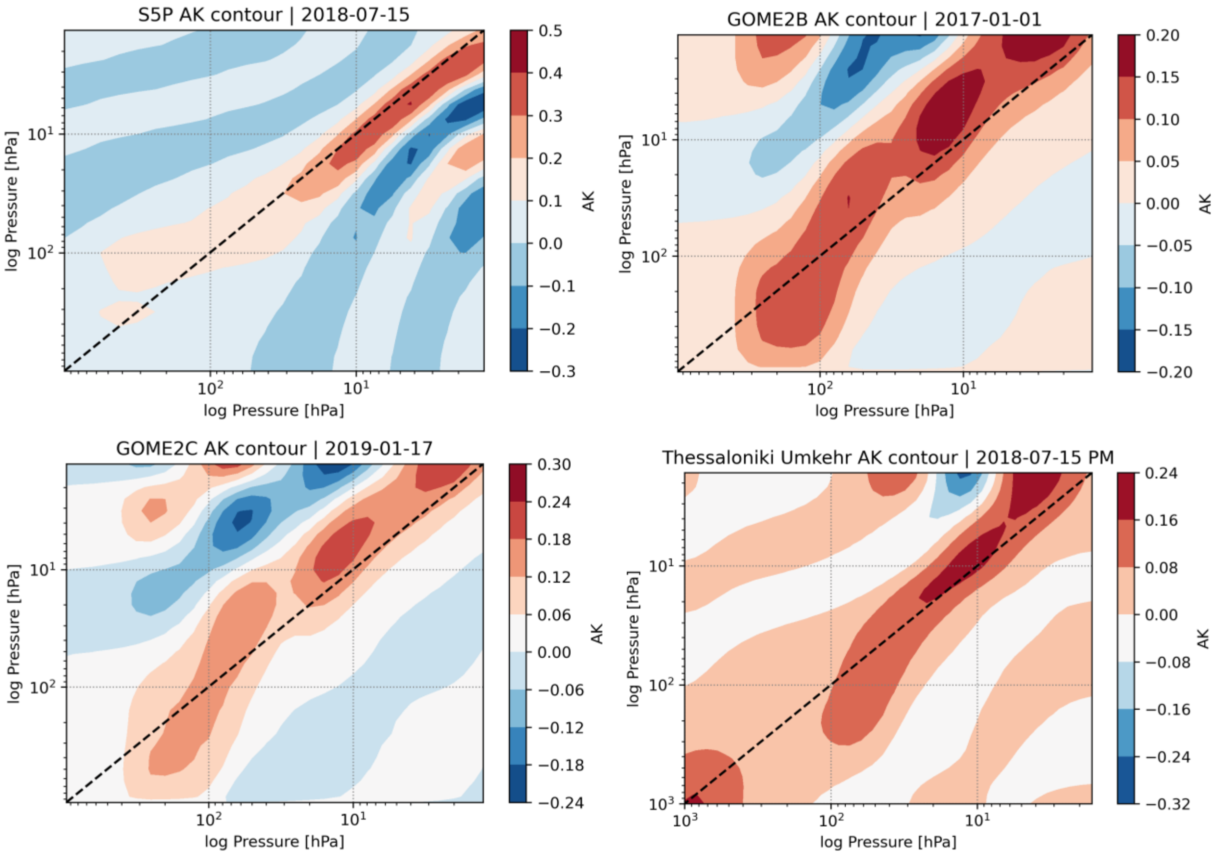


Figure 2.2: Specific cases of the AK matrix of the satellite and the ground-based datasets, as profile (upper panel) and contour (lower panel) representation. Upper left: S5P, upper right: GOME2B, lower left: GOME2C and lower right: Umkehr.

Figure 2.2 shows some cases as examples of the AK for the satellite (S5P and GOME-2 B/C) and the ground-based datasets, as profile and contour representations. These specific cases are presented here as indicators to the whole datasets. Note that for the analysis, we used the profiles where the pressure is equal or larger than 2 hPa ($p \geq 2$ hPa), since there is no significant ozone information above 2 hPa.

The AK smoothing was performed according to the equation:

$$x_{sm} = x + AK \cdot (x_{interp} - x) \qquad [1]$$

where x_{sm} is the final interpolated-smoothed ozone profile, x is the original profile, AK is the averaging kernel matrix and x_{interp} is the interpolated ozone profile. Note that those parameters are referred to either satellite or Umkehr data, according to the comparison approach that it was mentioned before. For example, in the first case (satellite to Umkehr conversion) equation$x_{sm} = x + AK \cdot (x_{interp} - x)$ *[1]* will take the form:

$$satellite_{sm} = Umkehr + AK_{Umkehr} \cdot (satellite_{interp} - Umkehr) \qquad [2]$$

where, the *satellite* factor can be either S5P, or GOME-2 B&C.

Typically, the AK smoothing procedure is performed using the apriori profile. According to literature, the smoothing procedure can also be conducted, using the ozone profile, instead of the apriori (replace x in equation xsm = x + AK · (xinterp – x) *[1]* with apriori or ozone). Thus, the above three approaches were divided in two cases, one where the smoothing were conducted using the apriori profile and one using the ozone profile. In total, this investigation resulted in six different comparison processes.

2.2.3 Results and discussion

For the comparisons between the satellite and the ground-based datasets, the mean percentage difference was calculated. The calculations were performed for all six comparison approaches. The results showed that there are no significant differences between those approaches. In this report, the conversion from satellite to Umkehr, smoothed using the apriori profile, will be presented.

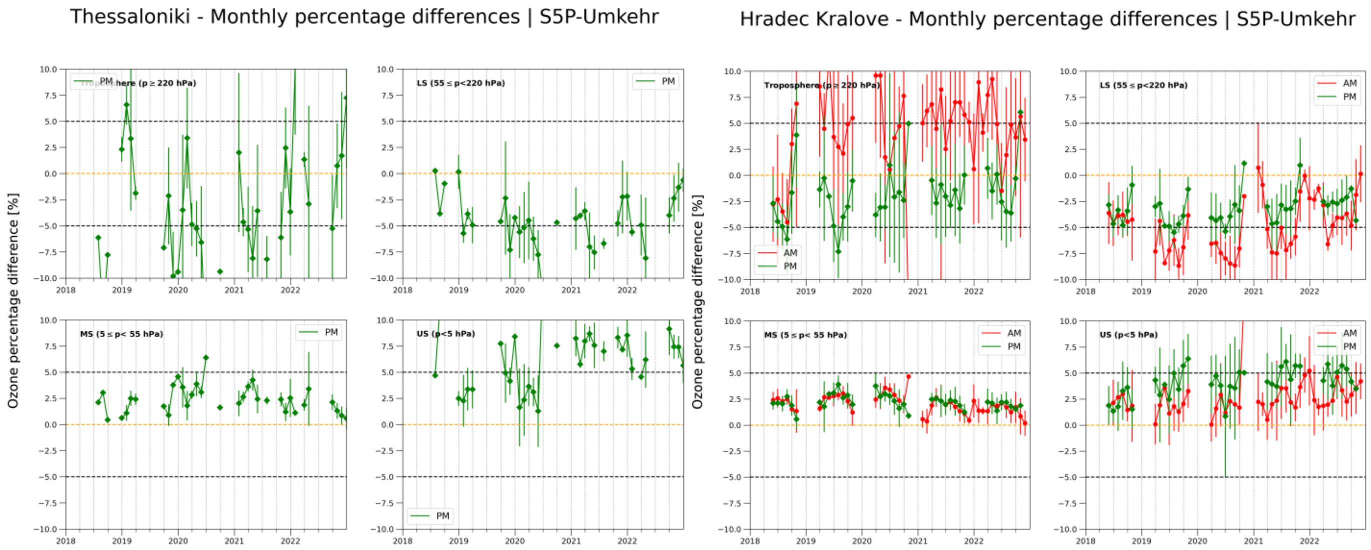
As it mentioned before, for the comparison of the profiles, the mean percentage difference was calculated, according to the equation:

$$\left(\frac{satellite_{sm}-Umkehr}{\frac{satellite_{sm}+Umkehr}{2}}\right)\cdot 100 \qquad [3]$$

where, *satellite*$_{sm}$ is the integrated satellite (S5P or GOME-2 B/C) smoothed ozone profile calculated according to equation $satellite_{sm} = Umkehr + AK_{Umkehr} \cdot (satellite_{interp} - Umkehr)$ [2] and *Umkehr* is the integrated original Umkehr ozone profile.

2.2.3.1 Monthly timeseries of mean percentage differences

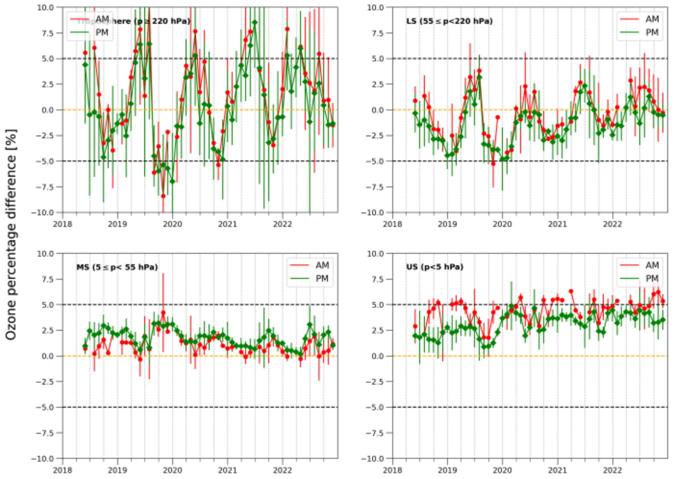
Figure 2.3 presents the monthly timeseries of the mean percentage differences for two Brewer and two Dobson stations, for the four standard layers (Troposphere, LS, MS and US), for all satellite datasets, respectively.



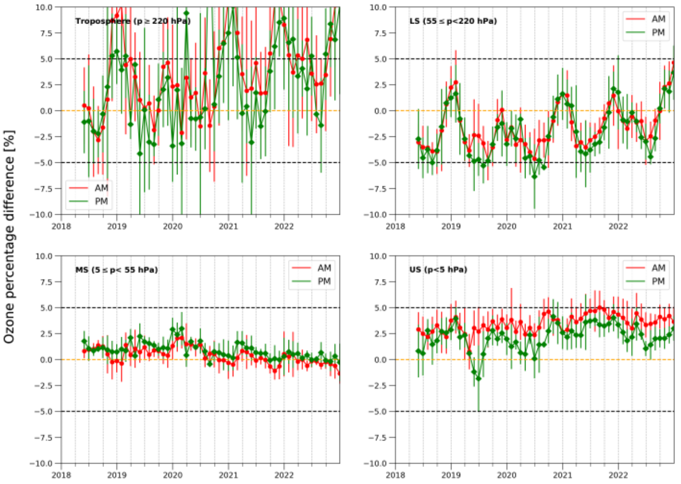
Thessaloniki - Monthly percentage differences | S5P-Umkehr

Hradec Kralove - Monthly percentage differences | S5P-Umkehr

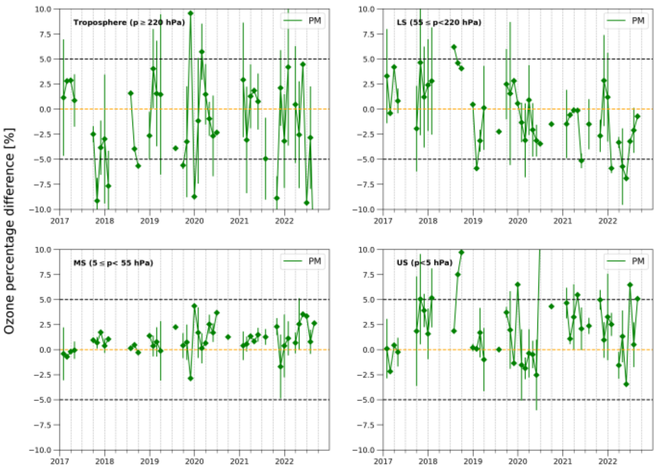
Lauder - Monthly percentage differences | S5P-Umkehr



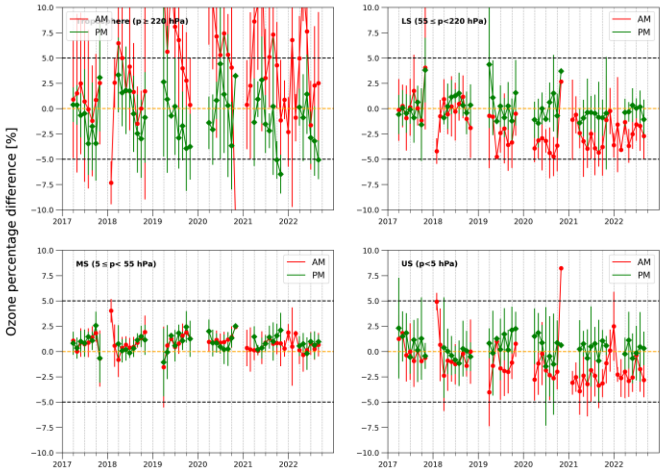
Boulder - Monthly percentage differences | S5P-Umkehr



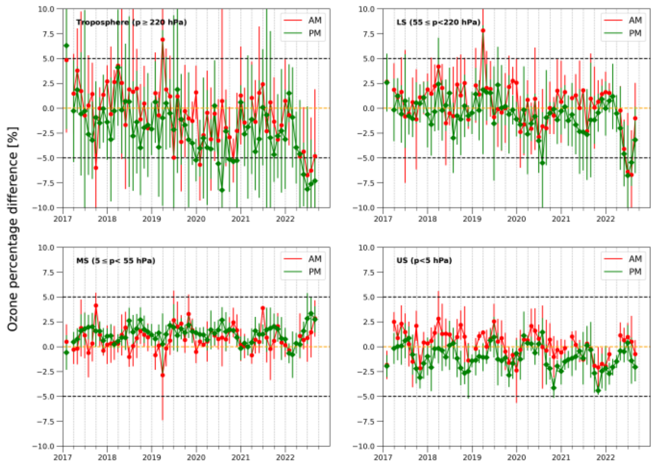
Thessaloniki - Monthly percentage differences | GOME2B-Umkehr



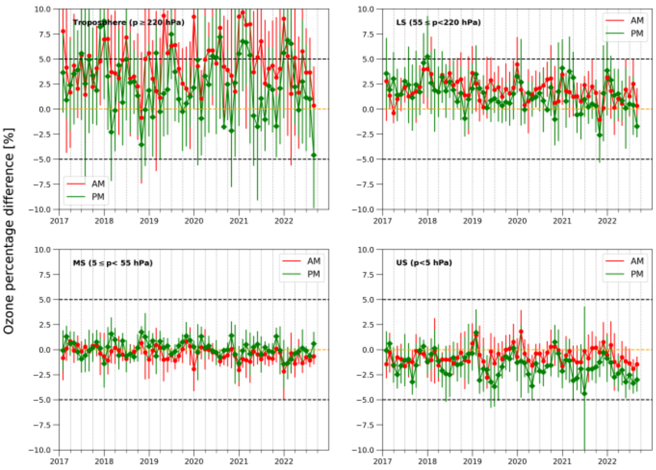
Hradec Kralove - Monthly percentage differences | GOME2B-Umkehr



Lauder - Monthly percentage differences | GOME2B-Umkehr



Boulder - Monthly percentage differences | GOME2B-Umkehr



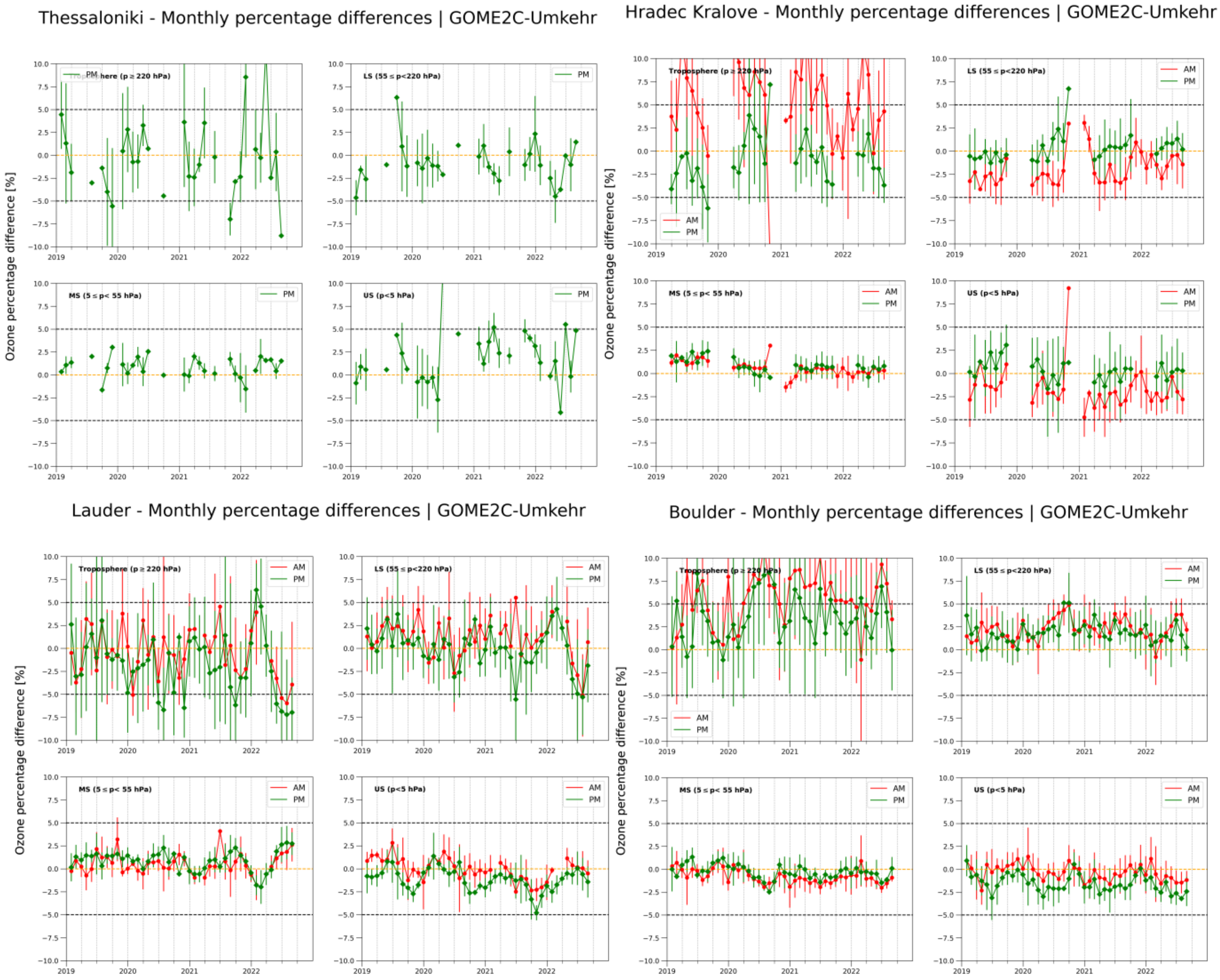
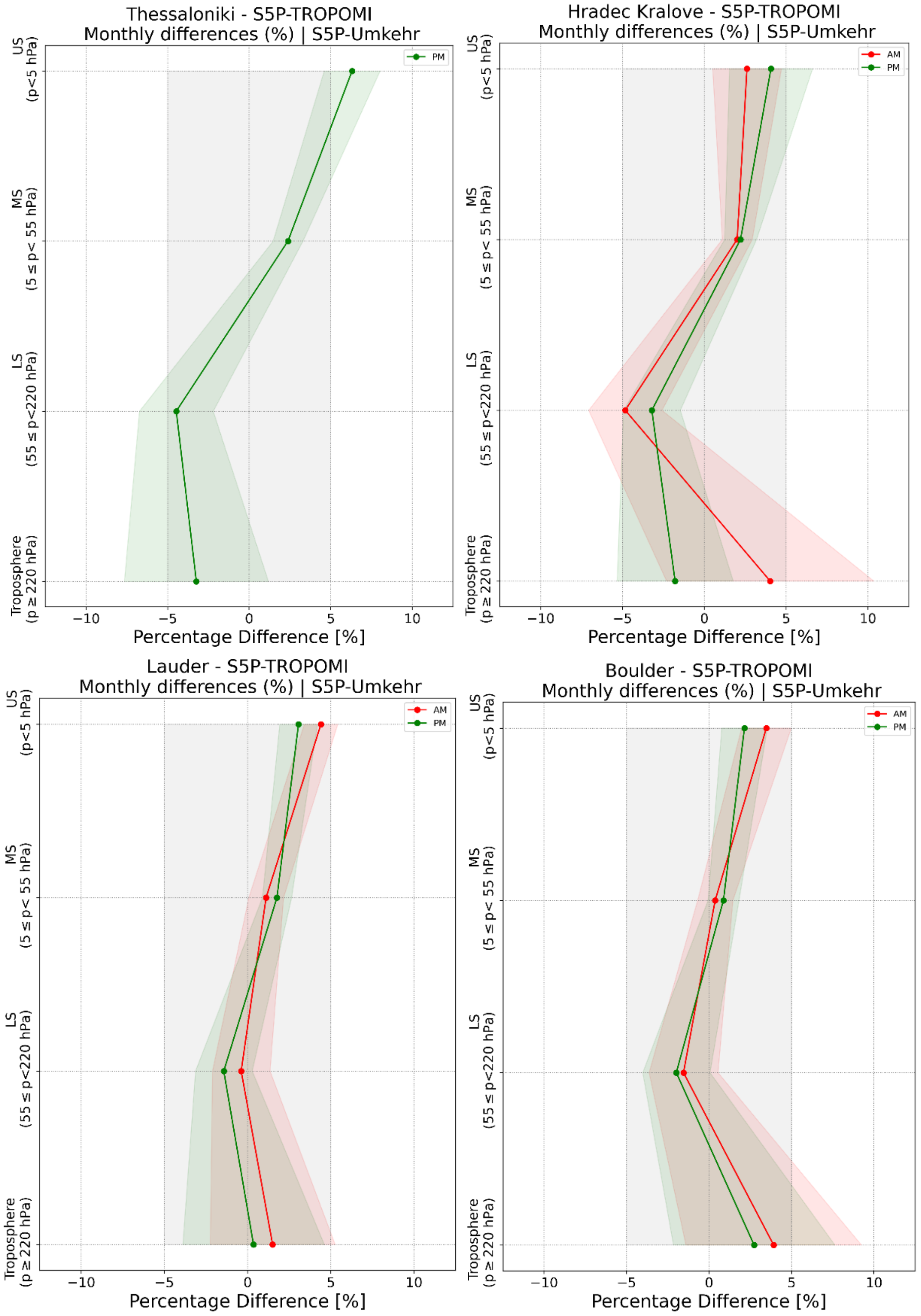


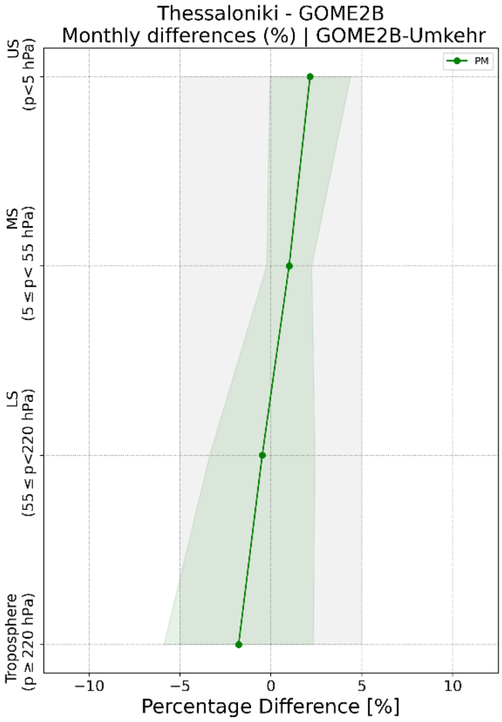
Figure 2.3: Time series of monthly mean percentage differences in 4 layers: Troposphere (upper left plot), Lower Stratosphere (LS, upper right plot), Main Stratosphere (MS, lower left plot) and Upper Stratosphere (US, lower right plot), in each panel, over Thessaloniki, Hradec Kralove, Lauder and Boulder, for S5P-TROPOMI (upper panel), GOME-2B (middle panel) and GOME-2C (lower panel), for the periods 2018 – 2022, 2017 – 2022 and 2019 – 2022, respectively. AM and PM data are plotted in different colors and vertical bars correspond to the standard deviation.

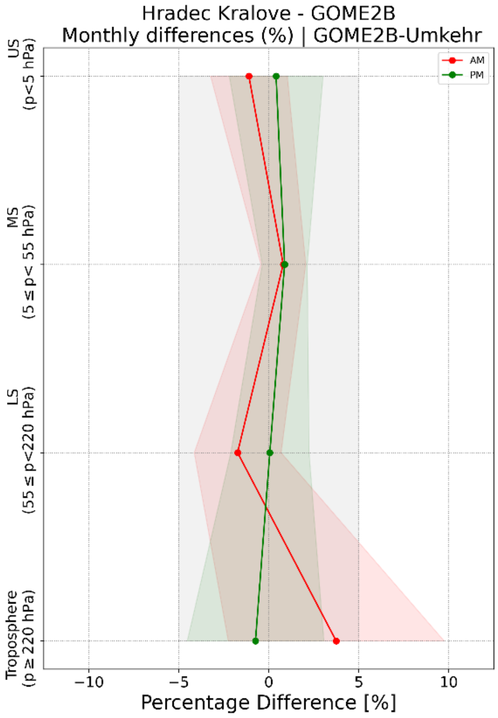
Figure 2.3 shows clearly that the highest deviations between ground and satellite appear, for most cases, in the Troposphere layer, shown in the upper left sub-panel of all figures. A good agreement appears in the Main Stratosphere layer, lower left sub-panel, in which the ozone peak can be detected, with the mean percentage differences being reported between ±5% (black dotted lines). In addition, similar to Figure 2-1, the bias between the AM and PM data that appears in Hradec Kralove, is visible here (for all three satellite datasets), as well. The comparisons for the Lower and Upper Stratosphere are similar as for the Main Stratosphere layer.

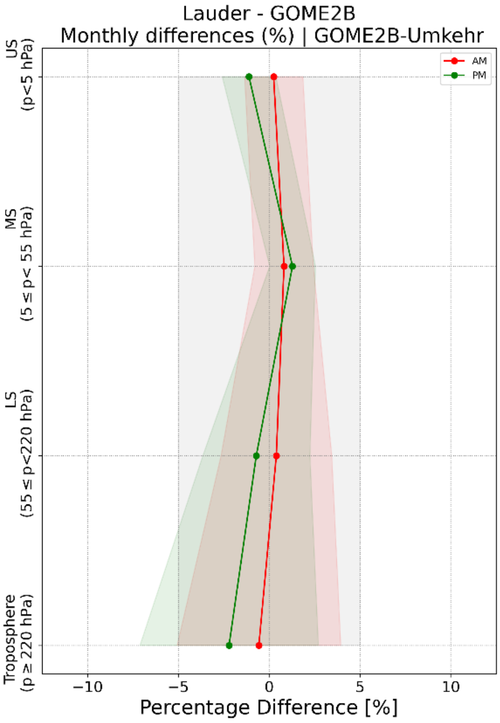
2.2.3.2 Profiles of the monthly mean percentage differences

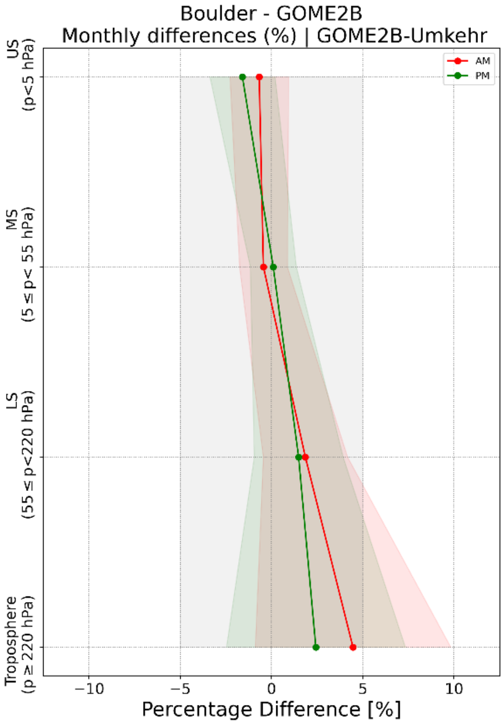
To get a better perspective of the monthly mean percentage differences, the average value of those differences was calculated, for each layer. Figure 2.4 presents the average monthly mean percentage differences for each of the four layers for selected Brewer and Dobsons stations, for both S5P-TROPOMI and GOME-2 B&C.




Thessaloniki - GOME2B
Monthly differences (%) | GOME2B-Umkehr
PM
US (p<5 hPa)
MS (5 ≤ p< 55 hPa)
LS (55 ≤ p<220 hPa)
Troposphere (p ≥ 220 hPa)
−10
−5
0
5
10
Percentage Difference [%]


Hradec Kralove - GOME2B
Monthly differences (%) | GOME2B-Umkehr
AM
PM
US (p<5 hPa)
MS (5 ≤ p< 55 hPa)
LS (55 ≤ p<220 hPa)
Troposphere (p ≥ 220 hPa)
−10
−5
0
5
10
Percentage Difference [%]


Lauder - GOME2B
Monthly differences (%) | GOME2B-Umkehr
AM
PM
US (p<5 hPa)
MS (5 ≤ p< 55 hPa)
LS (55 ≤ p<220 hPa)
Troposphere (p ≥ 220 hPa)
−10
−5
0
5
10
Percentage Difference [%]


Boulder - GOME2B
Monthly differences (%) | GOME2B-Umkehr
AM
PM
US (p<5 hPa)
MS (5 ≤ p< 55 hPa)
LS (55 ≤ p<220 hPa)
Troposphere (p ≥ 220 hPa)
−10
−5
0
5
10
Percentage Difference [%]

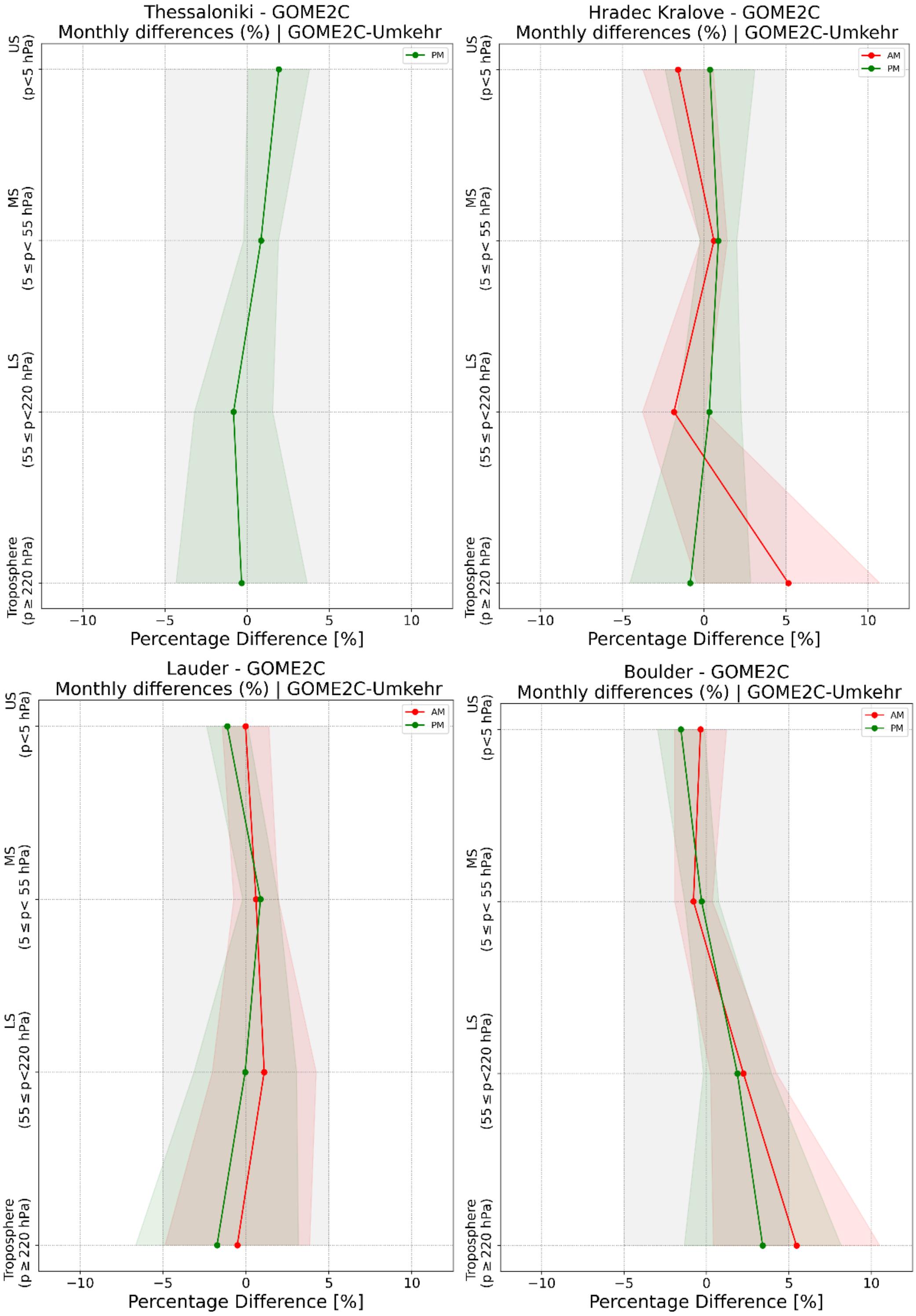


Figure 2.4: Average of the monthly mean percentage differences for each one of the 4 layers: Troposphere, Lower Stratosphere (LS), Main Stratosphere (MS) and Upper Stratosphere (US), over Thessaloniki, Hradec Kralove, Lauder and Boulder, for S5P-TROPOMI (upper panel), GOME-2B (middle panel) and GOME-2C (lower panel), for the periods 2018 – 2022, 2017 – 2022 and 2019 – 2022, respectively. AM and PM data are plotted in different colors and the shaded areas correspond to the standard deviation.

Figure 2.4 shows the mean profile comparisons for two Brewer and two Brewer stations, for all three satellite instruments. A good agreement is reported in these comparisons, since, in most cases, the percentage difference lies between ±5% (gray area). Table 4, Table 5 and

Table 6 summarize the results for all the selected stations, for all three satellites, respectively. The last row of the tables is the average value and standard deviation for all stations, for AM, PM and each layer, respectively.

Table 4: Average of the monthly mean percentage difference for all the selected stations (AM/PM) – S5P-TROPOMI

Station	**Troposphere**		**Lower Stratosphere**		**Main Stratosphere**		**Upper Stratosphere**	
	AM	**PM**	**AM**	**PM**	**AM**	**PM**	**AM**	**PM**
Arosa	1.0 ± 4.4	1.2 ± 4.9	-3.0 ± 1.6	-2.5 ± 1.5	1.3 ± 0.9	1.1 ± 1.0	2.8 ± 1.6	3.4 ± 1.6
Boulder	3.9 ± 5.3	2.7 ± 4.9	-1.5 ± 2.1	-2.0 ± 2.0	0.4 ± 1.1	0.9 ± 0.9	3.5 ± 1.5	2.2 ± 1.4
HauteProvence	4.5 ± 6.1	3.8 ± 4.6	0.0 ± 1.9	-0.2 ± 1.7	0.8 ± 1.0	1.1 ± 0.9	3.9 ± 1.6	2.9 ± 1.4
HradecKralove	4.0 ± 6.3	-1.8 ± 3.6	-4.8 ± 2.2	-3.2 ± 1.7	2.0 ± 0.9	2.2 ± 1.0	2.6 ± 2.1	4.1 ± 2.5
Lauder	1.5 ± 3.8	0.4 ± 4.3	-0.4 ± 1.7	-1.4 ± 1.7	1.1 ± 1.0	1.8 ± 0.9	4.4 ± 1.0	3.1 ± 1.1
Madrid	-0.1 ± 3.3	0.3 ± 3.7	-2.8 ± 1.8	-3.0 ± 1.9	1.4 ± 0.8	1.4 ± 0.8	3.7 ± 1.4	4.6 ± 1.6
Mauna Loa	2.0 ± 3.1	1.7 ± 3.1	-0.1 ± 1.6	-0.7 ± 1.6	0.5 ± 0.5	0.5 ± 0.5	4.1 ± 0.9	3.4 ± 0.8
Thessaloniki	n.a	-3.2 ± 4.4	n.a	-4.5 ± 2.3	n.a	2.4 ± 0.9	n.a	6.3 ± 1.7
Warsaw	-0.8 ± 4.7	-1.0 ± 4.2	-1.3 ± 3.0	-2.1 ± 2.9	1.8 ± 0.8	2.0 ± 0.8	1.4 ± 1.6	1.0 ± 1.5
Average	**2.0 ± 4.6**	**0.5 ± 4.2**	**-1.7 ± 2**	**-2.2 ± 1.9**	**1.2 ± 0.9**	**1.5 ± 0.9**	**3.3 ± 1.5**	**3.4 ± 1.5**

Table 5: Average of the monthly mean percentage difference for all the selected stations (AM/PM) – GOME2B

Station	**Troposphere**		**Lower Stratosphere**		**Main Stratosphere**		**Upper Stratosphere**	
	AM	**PM**	**AM**	**PM**	**AM**	**PM**	**AM**	**PM**
Arosa	2.2 ± 4.7	1.2 ± 4.7	0.7 ± 1.7	0.7 ± 1.9	-0.2 ± 1.2	0.1 ± 1.3	-0.6 ± 1.9	-0.2 ± 1.8
Boulder	4.5 ± 5.3	2.4 ± 4.9	1.8 ± 2.3	1.5 ± 2.4	-0.4 ± 1.3	0.1 ± 1.3	-0.7 ± 1.6	-1.6 ± 1.8
HauteProvence	3.9 ± 4.7	2.6 ± 4.9	2.2 ± 1.9	1.9 ± 2.2	-0.1 ± 1.1	0.3 ± 1.2	-0.2 ± 1.6	-1.1 ± 1.6
HradecKralove	3.6 ± 6.0	-0.7 ± 3.8	-1.7 ± 2.4	0.1 ± 2.2	0.8 ± 1.2	0.9 ± 1.3	-1.1 ± 2.1	0.4 ± 2.6
Lauder	-0.6 ± 4.5	-2.2 ± 4.9	0.4 ± 3.1	-0.7 ± 2.9	0.8 ± 1.6	1.3 ± 1.2	0.2 ± 1.6	-1.1 ± 1.5
Madrid	1.6 ± 3.2	2.2 ± 4.2	1.7 ± 2.1	0.7 ± 2.7	0.1 ± 1.0	0.2 ± 1.1	0.1 ± 1.6	0.1 ± 1.7
Mauna Loa	2.6 ± 3.7	1.8 ± 3.7	2.6 ± 1.8	1.9 ± 1.9	0.5 ± 0.6	0.5 ± 0.6	-0.5 ± 1.1	-1.2 ± 1.1
Thessaloniki	n.a	-1.8 ± 4.1	n.a	-0.5 ± 2.9	n.a	1.0 ± 1.2	n.a	2.1 ± 2.2
Warsaw	-1.7 ± 4.4	-1.2 ± 3.9	1.1 ± 3.3	0.6 ± 2.6	0.6 ± 1.2	0.6 ± 1.0	-2.0 ± 1.7	-2.7 ± 1.7
Average	**2.0 ± 4.6**	**0.5 ± 4.3**	**1.1 ± 2.3**	**0.7 ± 2.4**	**0.3 ± 1.2**	**0.6 ± 1.1**	**-0.6 ± 1.7**	**-0.6 ± 1.8**

Table 6: Average of the monthly mean percentage difference for all the selected stations (AM/PM) – GOME2C

Station	Troposphere		Lower Stratosphere		Main Stratosphere		Upper Stratosphere	
	AM	PM	AM	PM	AM	PM	AM	PM
Arosa	2.2 ± 4.4	1.3 ± 4.0	0.8 ± 1.3	1.2 ± 1.4	-0.2 ± 0.9	-0.2 ± 1.0	-0.6 ± 1.4	-0.1 ± 1.6
Boulder	5.5 ± 5.1	3.4 ± 4.8	2.2 ± 2.0	1.9 ± 2.1	-0.8 ± 1.1	-0.3 ± 1.0	-0.4 ± 1.6	-1.5 ± 1.4
HauteProvence	3.6 ± 4.5	2.4 ± 4.3	2.4 ± 1.4	2.1 ± 1.8	-0.1 ± 0.9	0.1 ± 1.0	0.0 ± 1.5	-1.1 ± 1.5
HradecKralove	5.1 ± 5.6	-0.8 ± 3.7	-1.8 ± 1.9	0.3 ± 1.9	0.6 ± 0.8	0.9 ± 1.1	-1.6 ± 2.1	0.4 ± 2.7
Lauder	-0.5 ± 4.4	-1.7 ± 4.9	1.1 ± 3.1	0.0 ± 3.1	0.6 ± 1.3	0.9 ± 1.1	0.0 ± 1.4	-1.1 ± 1.2
Madrid	2.8 ± 2.4	1.7 ± 3.5	1.6 ± 1.5	0.8 ± 2.5	0.1 ± 0.6	0.2 ± 1.0	0.2 ± 1.5	1.0 ± 1.6
Mauna Loa	5.7 ± 3.3	4.6 ± 3.3	4.2 ± 1.6	3.3 ± 1.7	-0.1 ± 0.5	0.0 ± 0.6	-0.1 ± 1.0	-0.8 ± 1.0
Thessaloniki	n.a	-0.3 ± 4.0	n.a	-0.8 ± 2.4	n.a	0.8 ± 1.1	n.a	1.9 ± 1.9
Warsaw	-1.8 ± 4.2	-1.9 ± 3.8	-1.4 ± 2.9	0.3 ± 2.7	0.4 ± 0.7	0.8 ± 0.8	-2.1 ± 1.9	-2.6 ± 1.7
Average	**2.8 ± 4.2**	**1.0 ± 4.0**	**1.1 ± 2.0**	**1.0 ± 2.2**	**0.1 ± 0.9**	**0.4 ± 1.0**	**-0.6 ± 1.6**	**-0.4 ± 1.6**

Summarizing these findings, we note similarities as well as differences in the comparisons of the temporally different Umkehr profiles to the three different satellite observations:

- The Troposphere Layer, ≥200hPa, comparisons show a marked dependency on the time of the Umkehr observations, AM or PM and the highest variability on the comparisons shown by the increased 1-sigma standard deviations reported. The monthly mean difference for all stations in the case of AM Umkehr observations ranges from 2.0 ± 4.6 to 2.8 ± 4.2% for the three satellite sensors, whereas the PM Umkehr observations provide comparisons ranging from 0.5 ± 4.2 to 1.0 ± 4.0%. The improved comparison for the Troposphere Layer PM comparisons is mainly due to the higher variability of the individual stations results and not so much on an overall improved picture in these comparisons.
  In the case of the Troposphere Layer, it is worth noting that specific stations, namely Boulder, Haute Provence, Hradec Kralove and Mauna Loa, typically report high over-estimations for all three satellite sensors. As these stations are at a higher elevation than the rest of the examined locations, the issue of the representability of the total troposphere cannot be discarded as possible reason for these high differences.
- The Lower Stratosphere Layer, between 200hPa and 55hPa, comparisons show a different result depending on the satellite sensor. The two GOME2 instruments report monthly mean differences

of 0.7 ± 2.4 to 1.1 ± 2.3% for both AM and PM Umkehr observations. The S5P instrument, on the contrary, reports a clear under-estimation to all ground-based sensors with the AM comparisons at -1.7 ± 2.0% and the PM comparisons at -2.2 ± 1.9%.

- The Main Stratosphere Layer, between 55hPa and 5hPa, comparisons also show a distinction between the two GOME2 instruments and S5P. The former report an excellent agreement, with low 1-sigma deviations, between 0.1 ± 0.9 & 0.6 ± 1.1% for both AM and PM Umkehr observations, common to all ground-based stations. The latter reports slightly higher differences, of ~1.5 ± 0.9% for both AM and PM, again common to all Umkehrs.
- The Upper Stratosphere Layer, between 5hPa and 2hPa, comparisons report the higher disagreement between GOME2BC and S5P. The two GOME2 instruments under-estimated slightly with reported monthly mean differences of -0.4 ± 1.6 to -0.6 ± 1.8% for both AM and PM Umkehr observations. The S5P instrument, on the contrary, reports a clear over-estimation to all ground-based sensors with reported monthly mean differences of 3.3± 1.5 for both AM and PM Umkehr observations.

3 Summary and Outlook

During the second phase of the ESA IDEAS + QA4EO Umkehr WP the following activities were performed:

- Modifications in the operational Umkehr algorithm were applied in order optimize the Umkehr retrievals for the validation of the S5P/TROPOMI nadir ozone profiles. This included the inclusion of 61 layers and the full AK matrix.
- Further activities were performed for optimization of the Arosa timeseries and the timeseries have been compared against MLS, OMPS and ozonesonde measurements. The new version of the Arosa timeseries shows improved performance with a reduced drift per decade in most layers.
- The Umkehr timeseries of partial ozone columns have been updated till the end of 2022 for 4 Brewer and 5 Dobson stations and netcdf files for each station have been prepared. The dataset is freely available upon request.
- Comparisons with operational S5P/TROPOMI and GOME-2/Metop ozone profiles have been performed in four atmospheric layers: troposphere, lower stratosphere, middle stratosphere and upper stratosphere. The average SAT-UMK differences are within 2% for TROPOMI for the LS and MS layers and within 1% for GOME-2B and GOME-2C for LS, MS and US layers

The suggested outlook for future steps in this research include:

- Homogenization between Dobson and Brewer Umkehr records at stations that are going through the transition of the instruments (or have undergone).
- Test and apply the newly developed option in the Brewer software for the homogenization of the Brewer timeseries using the same protocol with the Dobson ones.
- Compile a tropospheric ozone dataset from the Umkehr retrievals, verify and further investigate its potential for the validation of satellite tropospheric ozone products.

Data Availability

The optimized Dobson Umkehr records presented in this report are available upon request from NOAA in NetCDF format (please contact Irina Petropavlovskikh: irina.petro@noaa.gov).

The Brewer Umkehr retrievals presented in this report are available upon request in NetCDF format (please contact Dimitris Balis: balis@auth.gr and the PI of the instrument)

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