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 both troposphere, UTLS and the stratosphere, can be obtained by Brewer and Dobson spectrophotometers in a special viewing mode called Umkehr. As a result, this type of observations can be used in the validation of both satellite IR instrumentation, that cover from the UTLS upwards, as well as UV instrumentation, that also cover the troposphere albeit with a coarser vertical resolution.

Within the IDEAS+ framework new efforts have been made to improve the operational Umkehr analysis algorithm and provide a more robust and unique validation dataset for ozone profile observations by space-born sensors such as S5P/TROPOMI, as well as GOME2 and IASI instruments on the Metop platforms.

Within this work, Dobson and Brewer Umkehr retrieval methods have been optimized and applied to Umkehr ozone profile measurements for a number of selected ground-based stations. Umkehr observations were then compared to satellite ozone profile measurements from the merged NOAA Solar Backscatter UV ozone profiles, as well as those by the Global Ozone Monitoring Experiment (GOME-2) instruments on board the EUMETSAT Metop platforms.

In the following sections, the Umkehr observations retrieval methodology is briefly explained, the particular settings used in each type of instrument, Brewer and Dobson so as to perform Umkehr measurements are given, and the optimization methodology of the measurements is separately described. The results section comprises of the final updated time series of Umkehr observations for 4 Brewer and 4 Dobson stations, and first comparisons of the optimized Umkehr profiles to SBUV and GOME2 satellite measurements in the form of case studies for Thessaloniki, Greece (Brewer) and Lauder, New Zealand (Dobson). Finally, some additional comparisons of the optimized Dobson data with models (Modern-Era Retrospective Analysis for Research and Applications, Version 2, Global Modeling Initiative, M2GMI and the CTM model Global Modelling Initiative MERRA2, GMI-MERRA2), complimentary satellite observations (Aura MLS, S-NPP OMPS, SBUV and SAGE III/ISS records) and co-located ozonesonde records are analyzed (Petropavlovskikh et al., 2021). The comparisons to all available satellite data are used to provide confirmation of the Umkehr data quality and to establish their suitability for future validation of ozone profiles products from various satellites, such as TROPOMI/S5P.

2 Data and methods

2.1 The Umkehr observations

The Umkehr 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 has an inflection point at about 86° SZA, which grants the observation its name since Umkehr stands for reversal or “change” in German (Petropavlovskikh et al., 2021).

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 (311/332 nm for Dobson and 310/326 nm for Brewer, the temporal range 60°-90° SZA). Following, the N-Values, 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), are interpolated at 12 nominal SZAs: 60°, 65°, 70°, 74°, 77°, 80°, 83°, 85°, 86.5°, 88°, 89° and 90°. The full formula used for the calculation of the N-Values is Eq. 2 in Section 2.1.2. The algorithm for ozone retrieval, UMK04 (Petropavlovskikh et al., 2005) provides the ozone profile in 16 layers (Table 2), but according to the AK analysis not of all them contain independent information (Petropavlovskikh, et al., 2004).

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.

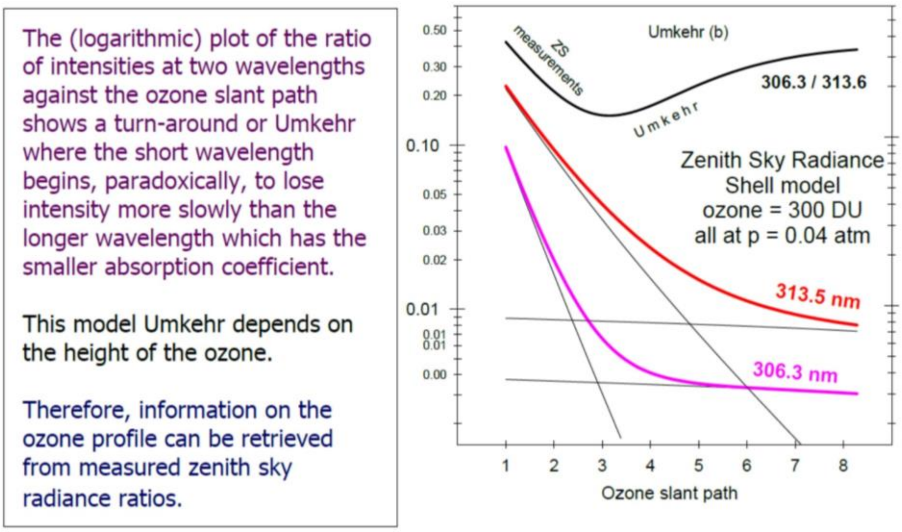


Figure 2.1: Umkehr method observations (wavelength ratio: Dobson 332/311 or Brewer 326/310 nm)

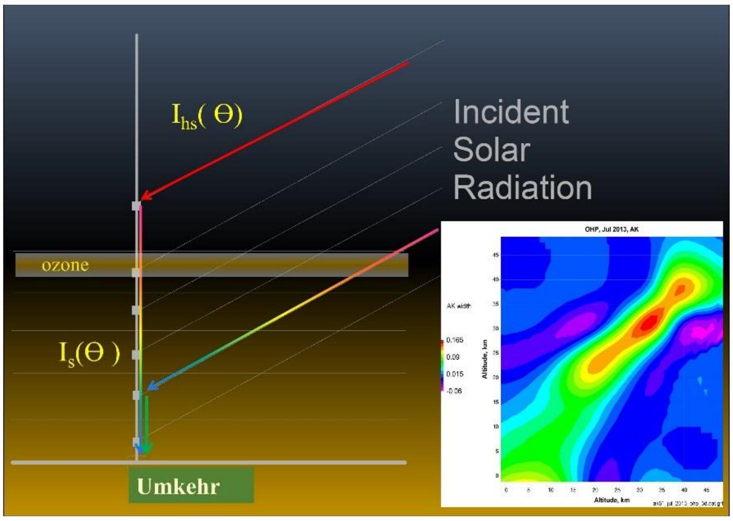


Figure 2.2: Scattering geometry information is weighted by different layers as sun sets/rises

2.1.1 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 (SZA) 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 so-called 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 (v3.2) software is used, which has been developed by M. Stanek and is based on the UKM04 algorithm (Petropavlovskikh et al., 2004; 2005). 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: Standard Umkehr layers and their typical altitude range

Layer	Layer boundaries (km)	Pressure levels (hPa)
0	0 – 5.5	1013 – 506.5
1	5.5 – 10.3	506.5 – 253.25
2	10.3 – 4.7	253.25 – 126.63
3	14.7 – 19.1	126.63 – 63.31
4	19.1 – 23.5	63.31 – 31.66
5	23.5 – 28.0	31.66 – 15.83
6	28 – 32.6	15.83 – 7.91
7	32.6 – 37.5	7.91 – 3.96
8	37.5 – 42.6	3.96 – 1.98
9	42.6 – 47.9	1.98 – 0.99
10	47.9 – 53.2	0.99 – 0.49
11	53.2 – 58.3	0.49 – 0.25
12	58.3 – 63.1	0.25 – 0.12
13	63.1 – 67.8	0.12 – 0.06
14	67.8 – 72.2	0.06 – 0.03
15	72.2 – top of atmosphere	0.03 – 0

The retrieved profile is reported in a 16-layer scheme (Table 1), with each layer being approximately 5 km thick. The overall uncertainty of the Umkehr method has been estimated to 25% for the troposphere, 15% for the lower stratosphere, within ±10% for the middle and upper stratosphere, while errors increase further in layer 8 (~37.5

km) and above (Petropavlovskikh, et al., 2005). Therefore, the profiles are analyzed either in 8 independent layers, consisting of layers 0+1, 2+3, 4, 5, 6, 7, 8 and a broad top layer 8+, combining all layers from 9 and above (Petropavlovskikh, et al., 2004), or in a 10-layer scheme (Table 2).

2.1.2 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).

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

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) (Figure 2.1 and Figure 2.2).

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

The total ozone Dobson measurement from the morning or afternoon is used for adjusting the stray light correction prior to the ozone profile retrieval. Ozone profile retrievals are reported in terms of a 10-pressure-layer system (Table 2).

Table 2: Layers used for Umkehr ozone profile retrievals

Umkehr Layer	Pressure (hPa)	Altitude (km)
1 (0 + 1)	1013 - 253	0 - 10
2	253 – 126.7	10 - 15
3	126.7 – 63.3	15 - 20
4	63.3 – 31.7	20 - 25
5	31.7 – 15.8	25 - 30
6	15.8 – 7.9	30 - 35
7	7.9 – 3.96	35 - 40
8	3.96 – 1.98	40 - 45
9 +	1.98 – 0.0	45 -top of atmosphere

2.2 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.

Total ozone column

The total ozone column which is derived from direct sun measurements is an essential parameter for the retrieved Umkehr ozone profile. The TOC measured by the Brewer spectrophotometers is stored also in the B-files and is used directly by the Umkehr retrieval algorithm. However, since the instrument's sensitivity may change with time, the TOC is often post-processed.

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+). Of course, these differences were only preliminary estimates, since even larger diurnal variability could occur in TOC (as recorded in the B-files) and lead to much larger errors in the Umkehr ozone profile. For this reason, the profiles were re-evaluated using the post-processed TOC.

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 more representative for this location Teff 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. Figure 2.3 shows results for Layer 4: the differences between the derived ozone amounts using the climatological effective temperature (i.e. built-in the Brewer Umkehr processing software) and the daily-adjusted Teff. 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 %). The impact of using the calculated ozone effective temperature, instead of the climatological one for all layers is shown in Table 3.

Although the differences introduced by using a more representative effective temperature (Teff) are generally small, it was decided to re-process the entire time-series of Thessaloniki using the Teff calculated for each day. It should also be noted that these results are based only in one year of measurements (2008), thus they are only indicative. Higher or lower differences may appear during other years, depending on the actual temperature of the atmosphere. Figure 2.4 shows the long-term climatological ozone effective temperatures for Thessaloniki as derived from the combination of the measured temperature profiles with the climatological ozone profile for the years 2000 - 2020, along with the climatological ozone effective temperature that is used in the standard Brewer Umkehr retrieval for the latitude band where Thessaloniki is. It is obvious that the latter underestimates the observed effective temperatures.

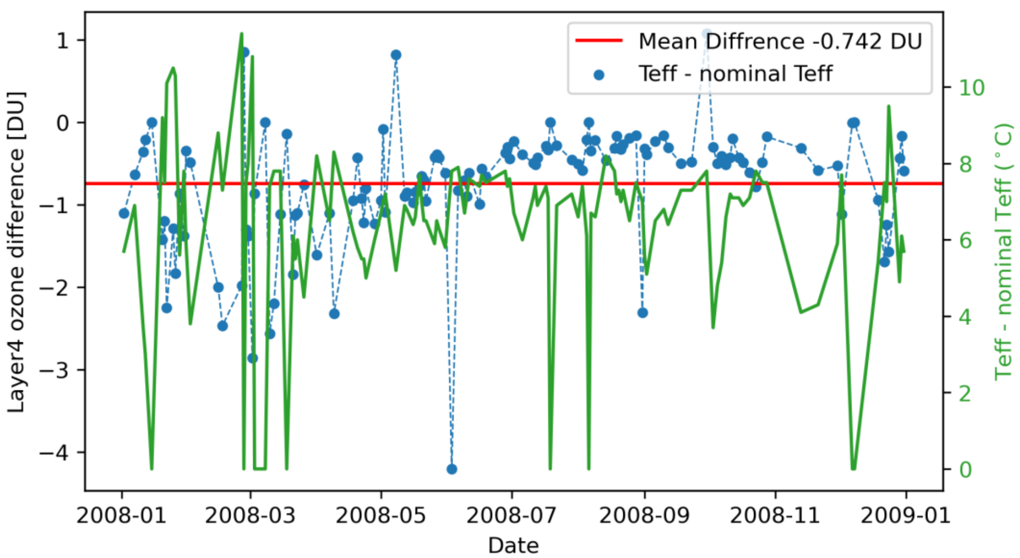


Figure 2.3: Effect of using the daily-adjusted instead of the climatological ozone effective temperature in the Umkehr retrievals of Brewer #005 in Thessaloniki for the year 2008 and for layer 4. Blue dots show the difference in the ozone amount between the two retrievals, while the green line shows the difference between two sets of Teff. The red line shows the average difference in the ozone amount.

Table 3: Effect of using the calculated vs the climatological ozone effective temperature for each Umkehr layer

Layer	climatological Teff - Teff (DU)	climatological Teff - Teff (%)
0+1	0.271	0.8
2+3	-0.005	-0.008
4	-0.742	-1.05
5	-0.485	-0.73
6	0.114	0.27
7	0.040	0.18
8	-0.043	-0.45
8+	-0.067	-0.47

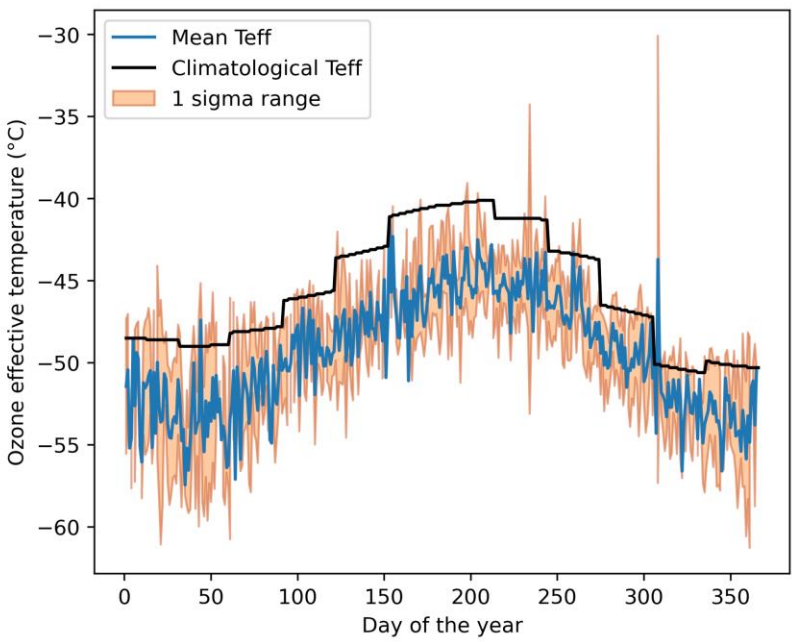


Figure 2.4: Annual cycle of the daily-adjusted(blue line) and the climatological (black line) ozone effective temperatures used in the Umkehr retrieval algorithm for Thessaloniki. The shaded orange area shows the standard deviation of the multiyear mean based on 21 years of observations (see *Figure 2.5*).

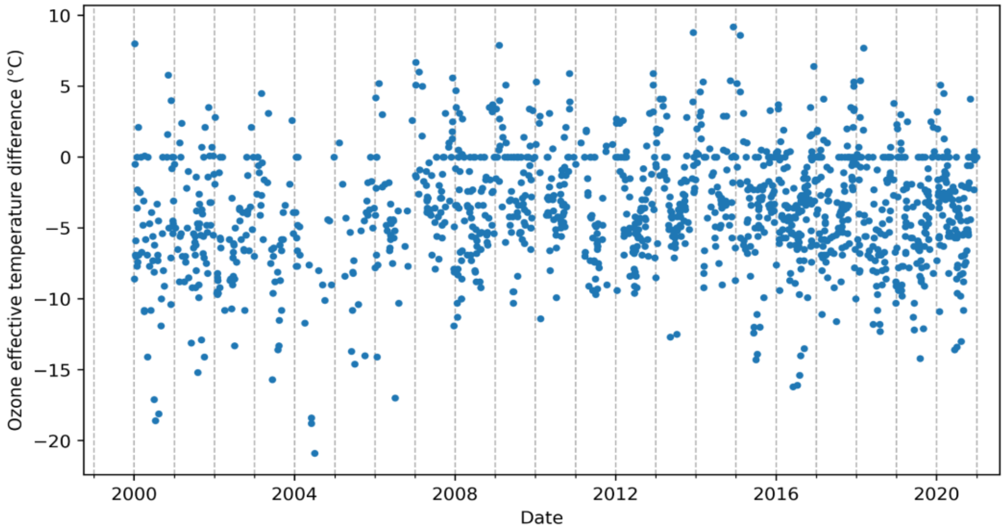


Figure 2.5: Time series of the differences in the daily-adjusted and climatological ozone effective temperature for the period 2000 – 2020 over Thessaloniki.

Figure 2.5 illustrates the difference between the daily-adjusted and climatological ozone effective temperature for each individual day. Please note that the difference is zero in days without radiosonde measurements, or when the balloon bursts at low altitudes not allowing the computation of the ozone effective temperature. For these cases, the climatological effective temperature has been used in the profile retrieval.

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. They can be different for each individual instrument and rough estimates are used in the algorithm, which were derived from the comparison of two Brewers in Arosa. The standard deviation of the residuals provides information about the instrumental noise and should be comparable with the error covariance values in the settings of the retrieval algorithm.

To assess the quality of the retrievals, the normalized (to 70° SZA) N-Values from 4 years of measurements at Thessaloniki with Brewer #005 were used. Figure 2.6 shows the time series of the normalized residuals at 74°, along with the standard observational error and the standard deviation of the residuals (shaded areas). As can be seen, the standard deviation of the residuals is close to the observation error, but slightly higher. The same pattern is observed for the other standard Umkehr SZAs with the results summarized in Table 4. These 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. The same procedure was followed also for other Brewers used in this study.

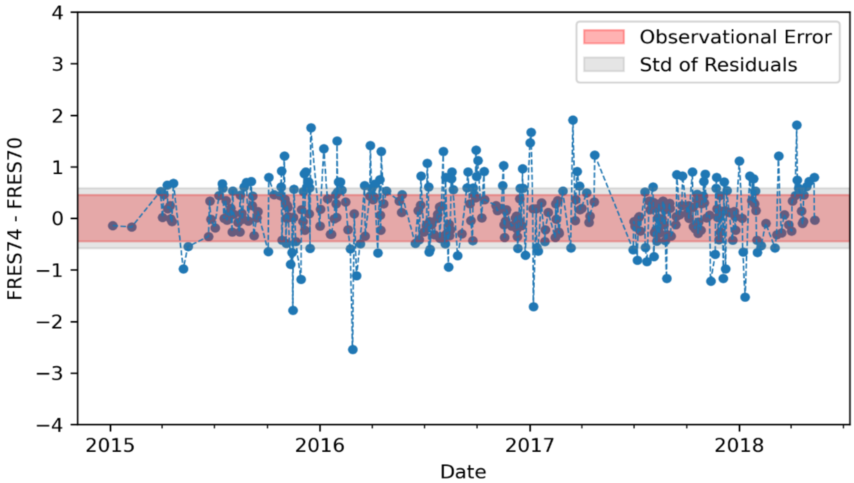


Figure 2.6: Time series of the N-values at 74° SZA normalized to 70°. The shaded areas show the observations error (red) and the standard deviation of the residuals (grey).

Table 4: Square root of observation error and standard deviation of the residuals for different SZAs

SZA (deg)	observation error (sqrt(var))	std(Res)	Var(Res)
60	-	0.44	0.19
65	0.40	0.62	0.39
70	0.42	-	-
74	0.45	0.58	0.33
77	0.47	0.69	0.48
80	0.50	0.75	0.57
83	0.52	0.79	0.63
85	0.54	0.71	0.51
86.5	0.55	0.77	0.59
88	0.63	0.79	0.63
89	0.77	0.99	0.98
90	0.89	1.19	1.42

2.3 Dobson optimization methodology

For the purposes of this work, the World Ozone and Ultraviolet Radiation Data Centre (WOUDC) database was searched for Umkehr Dobson data archived since 2007. The search was limited to identify records that have at least several years of data between 2006 and 2020, and these records have the relatively high (minimum of 4 observations per month) frequency of the Umkehr observations. The assessment of archived Umkehr level1 data resulted in the selection of several records suitable for GOME 2007-2020 satellite validation. Table 5 shows the list of stations and number of ozone profiles deposited on WOUDC since 2007.

Several versions of Umkehr record from Arosa station in Switzerland were made available in the last 4 years for NOAA Umkehr data processing through private communications with Dr. Eliane Maillard-Barras (ELB, MeteoSwiss) (Table 5). This project uses the 2021 version of the data provided by Dr. Maillard-Barras (Figure 2.7).

This project created the Stray light corrected and Optimized (OPT) Dobson Umkehr records for Boulder, MLO, Lauder, OHP and Arosa (Figure 2.8) stations.

Table 5: List of stations that deposited Umkehr data to the WOUDC archive from 2007 to 2020. The Arosa/Davos record includes Dobson Umkehr data from Arosa prior to 2017 and from Davos startting in 2017.

Platform Name	Agency	gaw_id	Platform_id	Lat	Lon	Started	Last date	Instrument	model	# instrument	number of profiles since 2007
Arosa / Davos	MeteoSwiss	ARO / DAV	35 / 501	46.8	9.7	1956	2020	dobson	BECK	51	1787
Aswan	EMA	ASW	245	24.0	32.8	1985	2011	dobson	BECK	69	233
Boulder ESRL HQ (CO)	NOAA-CMDL	BLD	67	40.0	-105.3	1982	2020	dobson	BECK	61	3122
Brisbane	ABM	BBN	27	-27.4	153.1	1962	2019	dobson	BECK	111	55
Cairo	EMA	CAI	152	30.1	31.3	1969	2006	dobson	BECK	96	1
Darwin	ABM	DWN	84	-12.4	130.9	1966	2018	dobson	BECK	78	63
Fairbanks (AK)	NOAA-CMDL	FBK	105	64.8	-147.9	1993	2020	dobson	BECK	63	1457
Haute Provence	NOAA-CMDL	OHP	40	43.9	5.7	1983	2020	dobson	BECK	85	2131
Hurghada	EMA	HUR	409	27.3	33.8	2002	2011	dobson	BECK	59	236
Lauder	NIWA-LAU	LAU	256	-45.0	169.7	1987	2020	dobson	BECK	72	1991
Mauna Loa (MLO)	NOAA-MLO	MLO	31	19.5	-155.6	1982	2020	dobson	BECK	76	5047
Naha	JMA	NAH	190	26.2	127.7	1974	2014	dobson	BECK	127	640
Perth	NOAA-CMDL	PTH	159	-31.9	116.0	1969	2012	dobson	BECK	81	1989
Sapporo	JMA	SAP	12	43.1	141.3	1958	2014	dobson	BECK	126	546
Singapore	MSS	SIN	214	1.3	103.9	1979	2012	dobson	BECK	7	65
Syowa	JMA	SYO	101	-69.0	39.6	1977	2013	dobson	BECK	122	291
Tateno (Tsukuba)	JMA	TKB	14	36.1	140.1	1957	2014	dobson	BECK	125	1381

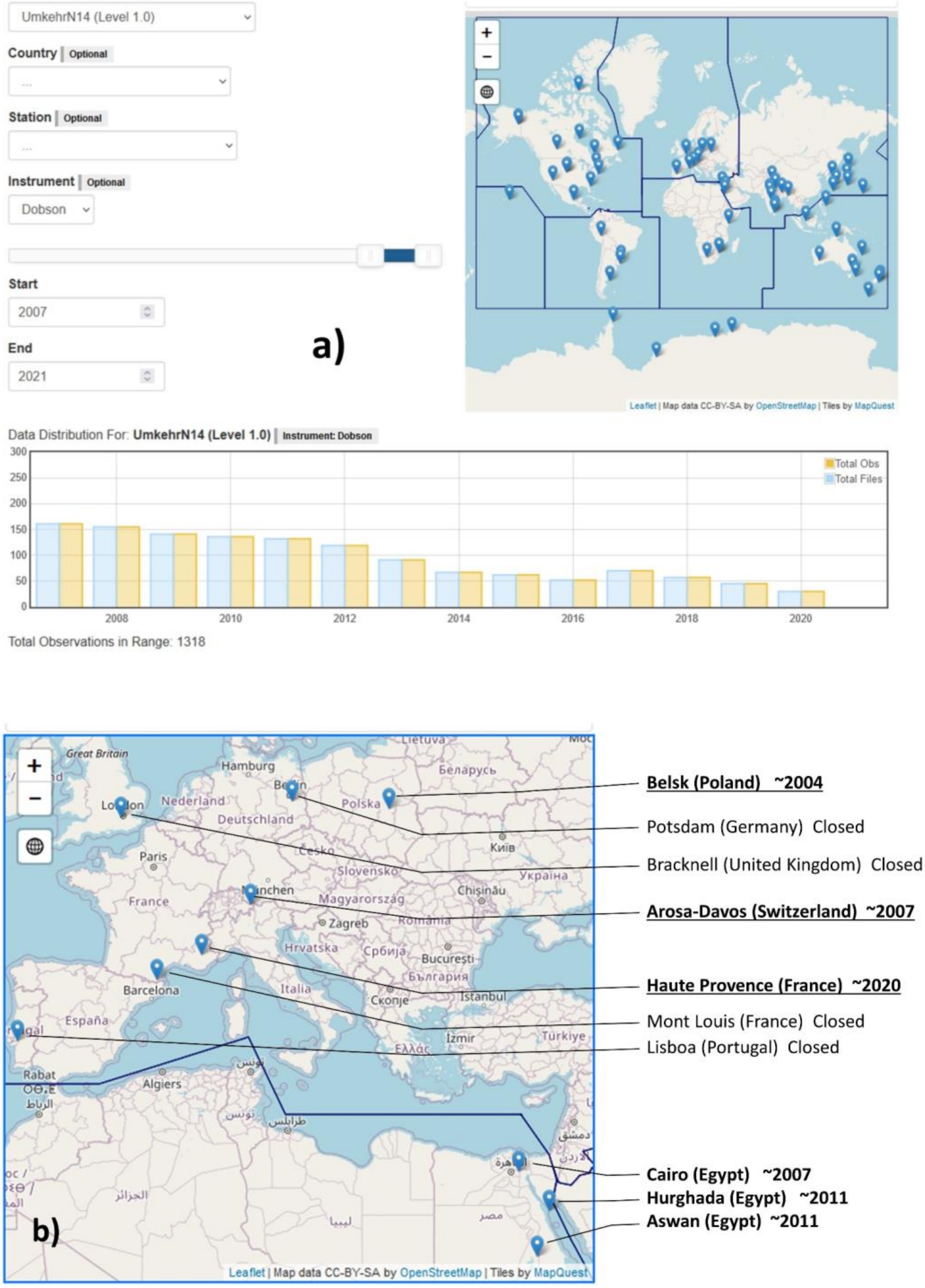


Figure 2.7: a) Statistics of the Dobson Umkehr Level-1 data archived at the WOUDC since 2007. b) Selected Umkehr stations in Europe and Africa that have long and systematic record of Umkehr observations.

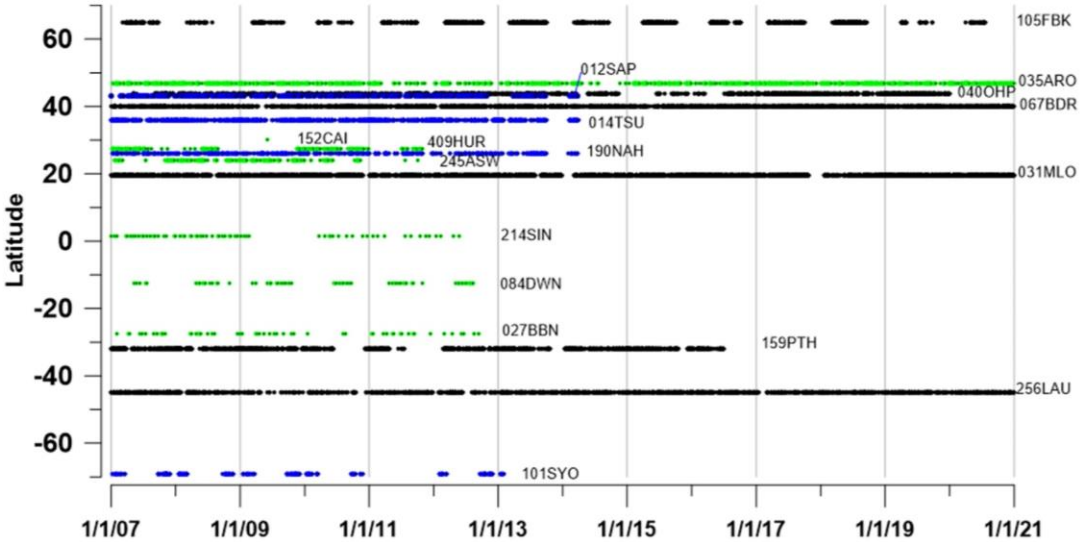


Figure 2.8: The frequency of Umkehr observation at several stations (presented as dotted line at the latitude of the station and marked with the WMO station number and3-letter station name abbreviation) as available from the WOUDC archive from 2007 to 2020.

Regular re-calibration of Dobson station instrument for total ozone, or change of instruments operated at the station, can affect the station's Umkehr measurement record. Figure 2.9 shows the frequency of Umkehr observations since 1956 as represented in four records for Arosa (Table 6). The best-quality Umkehr ozone profile retrievals are collected under the clear-sky conditions. In the NOAA data processing protocol, all Umkehr observations under cloudy conditions are removed prior to extracting N-values at 14 nominal SZAs. If the removal of cloud-impacted observations results in the portion of the Umkehr curve missing, the entire set of Umkehr data is discarded. At Arosa station, a different procedure is applied for cloud-impacted Umkehr observations. Instead of discarding an observation, it is adjusted based on the look-up tables created by semi-simultaneously taking cloudy and clear sky readings. The corrected Umkehr curves are marked with index 5 in the level1 data and therefore can be easily screened out. The ELIANE_CLEAR dataset contains only Umkehr observations under the clear sky conditions and typically has about 10 ozone profiles per month since the beginning of the record. The ELIANE_ALL dataset is similar in frequency of observations contained in the Irina2017 dataset (Arosa Umkehr data were processed through 2016 and provided in 2017 for the SPARC LOTUS trend analyses) and in the WOUDC archived record. These three records in addition to the clear-sky observations also hold Umkehr data corrected for cloudy conditions. The highest number of observations (up to 50 per month or more) is consistently found in 1989-2010 and even higher frequency is observed in 2015-2020.

Using the ELIANE_CLEAR dataset, which has only clear-sky Umkehr profiles, as a reference record, the other three Umkehr datasets were compared to it to assess the difference between cloudy and clear-sky data. The difference between ELIANE_ALL and ELIANE_CLEAR shows a drop in layer 8 ozone after 1995. We also found an increase in bias after 2000 in ozone retrieved from the WOUDC and IRINA2017 records (Figure 2.10). Therefore, we use ELIANE_CLEAR dataset to derive corrections for the Umkehr record. Arosa dataset was homogenized in the past to account for instrumental artifacts (Zannis et al, 2006). However, the new discontinuities were detected starting in 2012 and have not been yet homogenized.

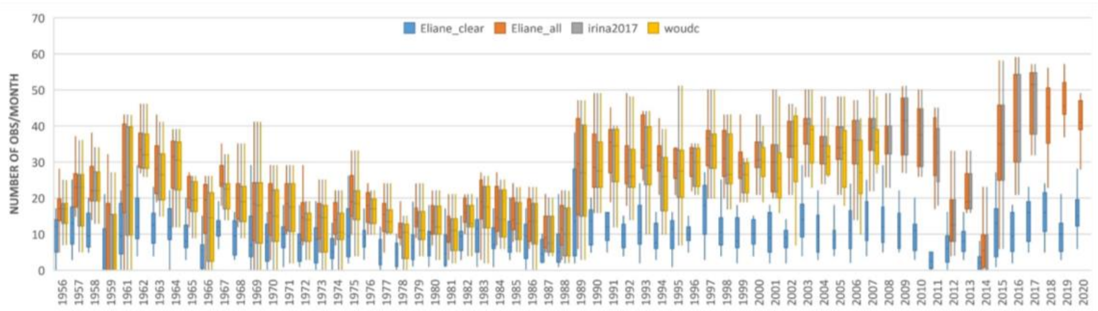


Figure 2.9: The mean and standard deviations of the yearly frequency of Umkehr observations is shown for four Arosa datasets.

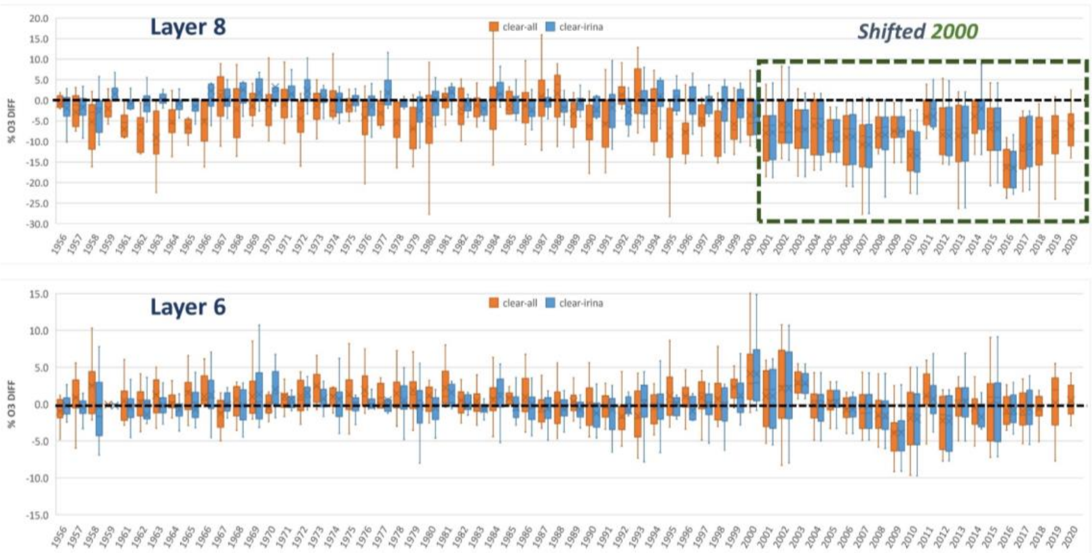


Figure 2.10: Layer 8 ozone (ELIANE_ALL and IRINA2017) percent difference with regard to the ELIANE_CLEAR dataset.

The Umkehr optimization includes updates for the a priori profiles in the retrieval code, standardized stray light corrections, and N-value empirical corrections derived using the subset of the ozone and temperature profiles from the NASA's M2GMI Chemistry Transport Model matched to the Umkehr station location. The operational Umkehr record is optimized using the subset of data from the M2GMI model matched to the station location and to the dates when Umkehr observation is taken. The optimization of Umkehr ozone profiles record at Arosa/Davos is similar to the homogenization process of the Umkehr record performed on the NOAA Umkehr network (Petropavlovskikh et al., 2021).

Here is the short summary of the homogenization process. The Umkehr ozone profile processing is biased by the interference of out-of-band (OOB) stray light into the measurement that is not considered in the retrieval algorithm (Petropavlovskikh et al., 2011). The updated algorithm takes into account the stray light correction (dNslc) that is simulated based on a set of standard ozone profiles and with the assumption of the stray light levels in a generic Dobson instrument. Figure 2.11a shows a Generic Stray light correction of N-value at Arosa (47 N, 812 hPa). Instrument calibration or replacement of an instrument occasionally creates a bias if stray light levels differ between instruments. The exact characteristics of the OOB and other stray light in each Dobson instrument is not available, therefore the optimization technique (Figure 2.11b) that is using the M2GMI model to evaluate the ozone profile bias and its uncertainty, is applied. The following equations detail the optimization method:

$$N_{opt} = N(w, Z) + dN_{slc}(O_3, P, Z) + dN_{opt}(t, Z) \qquad (Eq. 4)$$

where N_{opt} is the optimized N-value, *N* is the original Umkehr simulation based on the first guess profile (selected based on the latitude and total ozone at the station), dN_{slc} is the OOB stray light correction, and dN_{opt} is optimized correction N-value derived for a period between two consecutive calibrations.

$$dN_{opt} = N'_{fmodel} - N'_{obs} + C \qquad (Eq. 5)$$

$$N'_{fmodel} = N_{firstguessGMI}(fmodel) \qquad (Eq. 6)$$

N'_{fmodel} is the Umkehr N-value simulated using the M2GMI ozone profile as the first guess in the UMK04 algorithm. dNopt is the difference between simulated and observed N values. C is the uncertainty parameter.

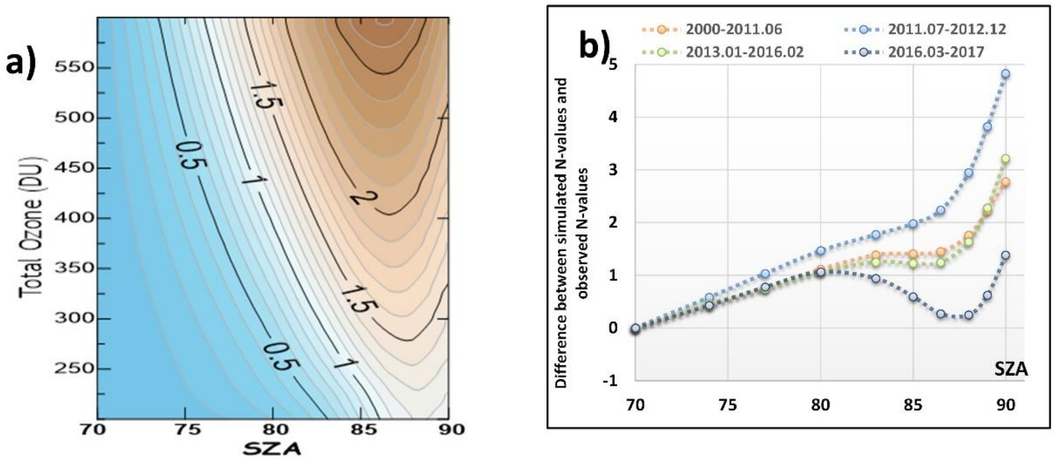


Figure 2.11: Stray light correction and Optimized correction. ***a)*** *Generic stray light correction N-value at Arosa (47 N, 812 hPa).* ***b)*** *The simulated N-values are based on the M2GMI model ozone profile data matched with station observations in time and space. Difference between simulated N-values and observed N-values is illustrated for four observational periods.*

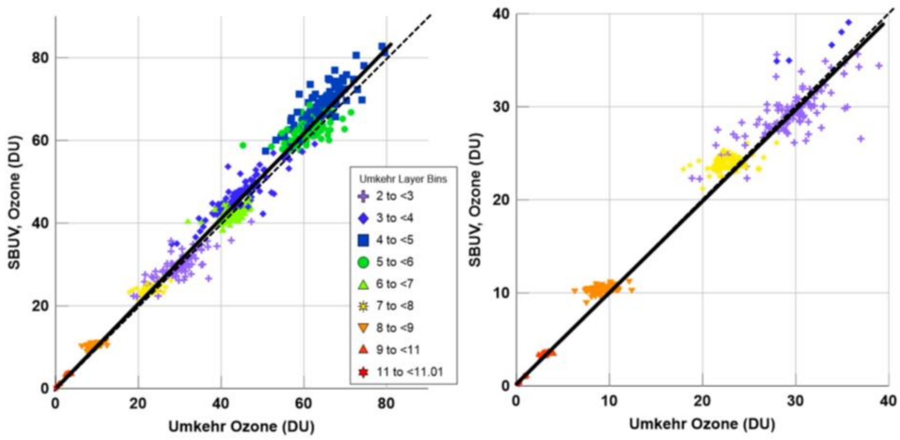


Figure 2.12: Scattering plot shows comparisons between the optimized Umkehr ozone (legend provides information about Umkehr layers) and ozone from the NASA SBUV AGGREGATED (AGG) record selected as the overpass over Arosa station. Optimized Umkehr includes the Stray light correction (SLC), and AKs smoothing is applied for. Comparisons are shown for monthly mean (MM) data.

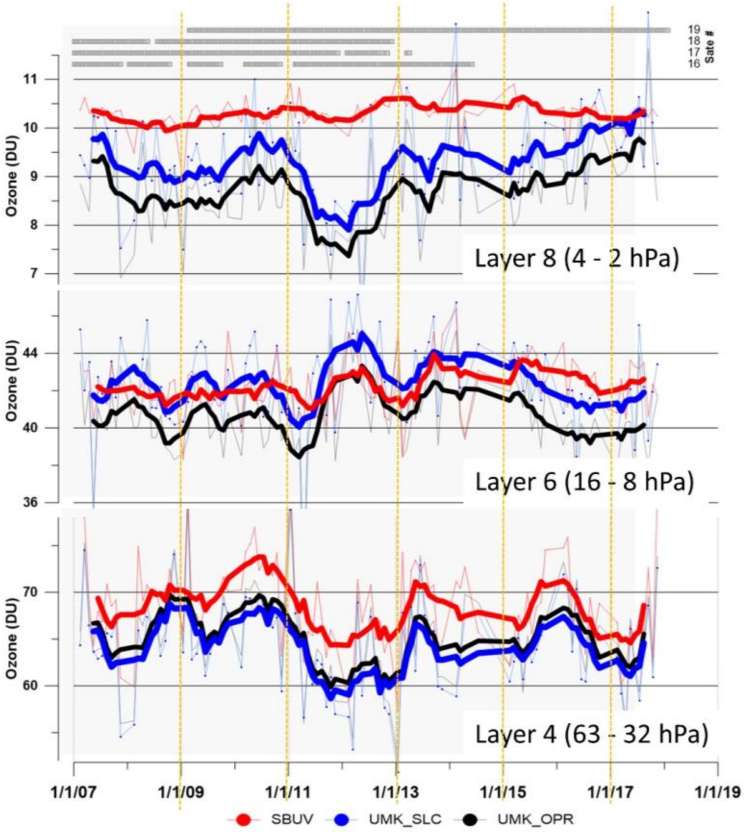


Figure 2.13: Time series of comparisons between ozone derived from the satellite AGG (Red line) and two Umkehr records at Arosa, first processed with the operational algorithm (Red line) and after applying the Standard Stray light correction (Blue line). This plot shows de-seasonalized anomalies in three Umkehr layers – layer 8, 6, and 4. The time for satellite overpass is selected within +/- 24 hours of Umkehr observations. A thin line is for monthly mean data. A solid line shows a running average for 13 months.

Figure 2.12 shows comparisons between the optimized Umkehr ozone retrieval and ozone from the NASA SBUV AGGREGATED (AGG) record selected as the overpass over Arosa station. Optimized Umkehr includes the Stray light correction (SLC), while the averaging kernel smoothing is applied to the satellite ozone profile prior to comparisons. Figure 2.13 shows the deseasonalized time series of ozone in layers 8, 6 and 4. The ozone time series are from the satellite AGG record (Red line), operational Umkehr algorithm (Red line) and the Umkehr processing that has the Standard Stray light correction (Blue line). The time for satellite overpass is selected within ± 24 hours of Umkehr observations. A thin line represents monthly mean data. A solid line represents data smoothed with a 13-month running average. Large bias and step change can be found in comparison to an SBUV satellite record. Figure 2.14 illustrated the standardized stray light correction (a) for 12 Umkehr values as function of time correction, optimized correction (b) based on M2GMI model data, and a combination of SLC and Optimized correction (c).

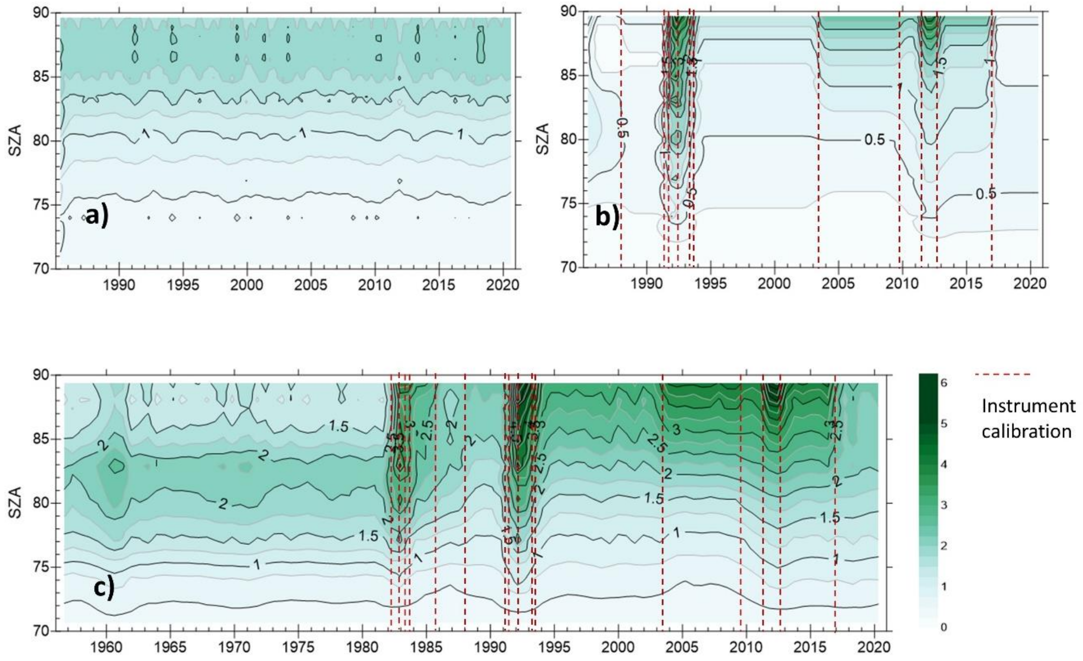


Figure 2.14: The optimized stray light correction for Umkehr record at Arosa. A) Standrad stray light correction, b) optimized correction, c) both corrections combined. Red dotted lines indicate the dates of Dobson calibrations, which are selected as the beginning/end of the optimized correction. The period of 1991-1993 in Umkehr record is impacted by the Pinatubo volcanic aerosol load in stratosphere that creates errors in operational Umkehr retrieval. Correction for the volcanic period is applied in the optimized version of data.

Table 6: The Table lists information about Umkehr records available from the WOUDC archive at Arosa/Davos, including information about station, period of available data.

Name	**Period**	**Note**	**qc**
WOUDC	1956-2007	Downloaded from WOUDC	
Irina2017	1956-2017	Provided by EMB in 2017 for LOTUS Report trend analyses	
Eliane_Clear	1956-2020	Provided by EMB, w flag 3= clear sky measurement	High
Eliane_ALL	1956-2020	Provided by EMB, w flag 5= data with QC cloud correction	

3 Results

3.1 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 – 2020. Additionally, Umkehr measurements from four Dobson stations (Boulder, USA; MLO, USA; Lauder, New Zealand and Haute Provence, France) have been optimized and are presented for the same time period. Table 7 shows the list of the stations for both types of instruments and their exact locations.

Table 7: 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 (#256)	45.05 S	169.68 E

3.1.1 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 2020. 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, leaving 406 acceptable profiles in this period. 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 (Figure 3.1), 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.

For the construction of the monthly mean averages all available daily profiles have been used, without applying any filter. The time series of the monthly mean ozone for each layer is shown in Figure 3.2. All layers show the expected distinct annual cycle in ozone, which is more pronounced (~80% of the mean) at the first two combined layers (0+1 and 2+3). The mean layer ozone amount ranges between 9.40 and 69.31 DU for layers 8 and 4, respectively. Table 8 summarizes the mean ozone amount per layer and its standard deviation.

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 2017-2020. 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^o) 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.

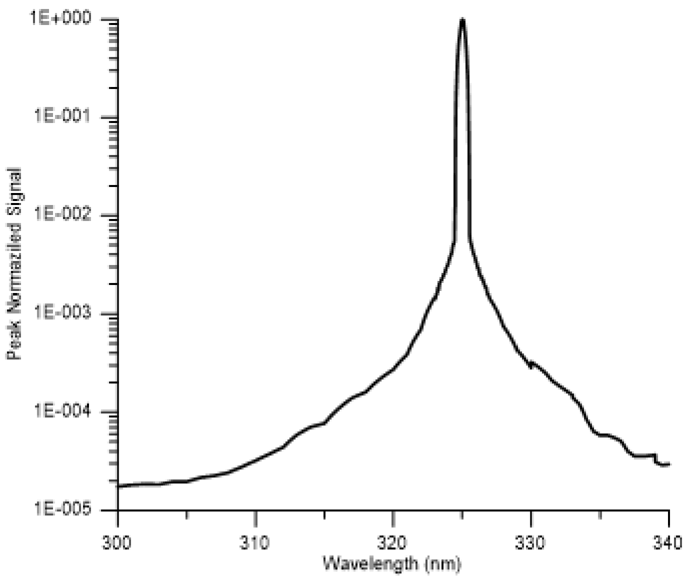


Figure 3.1: Slit function of Brewer #005, measured with a HeCd laser for slit #1 during the X Intercomparison Campaign of the Regional Brewer Calibration Center Europe (http://rbcce.aemet.es).

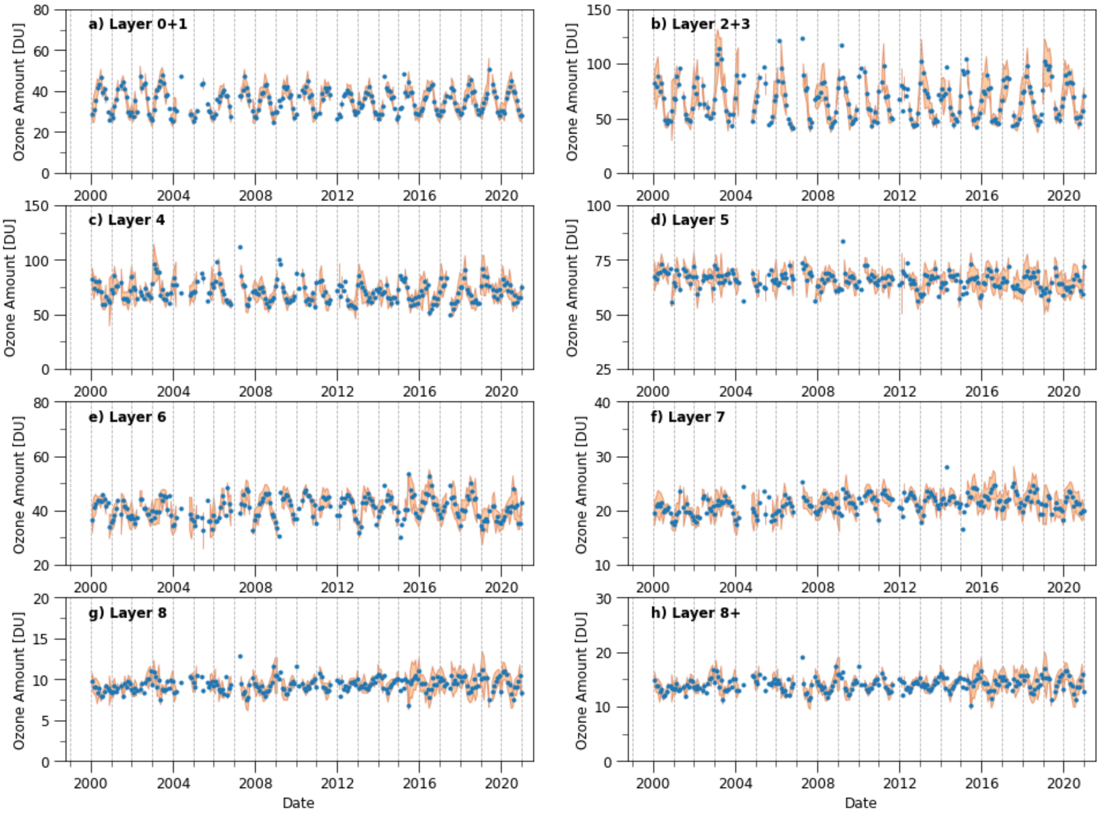


Figure 3.2: Time series of monthly mean ozone column amounts (in DU) at the 8 Umkehr layers over Thessaloniki, Greece, for the period 2000–2020. The orange shaded area shows the standard deviation of the monthly values.

Table 8: Average partial ozone column (DU) and its standard deviation in individual Umkehr layers

Layer	Mean O_3 [DU]	Standard deviation [DU]
0+1	35.47	6.24
2+3	64.63	19.30
4	69.31	11.39
5	65.55	5.41
6	41.37	5.01
7	21.54	2.30
8	9.40	1.25
8+	14.11	1.80

Seven stations that have good observations of at least a few months have been initially selected. Out of these, B-files of Brewers MKIII operating at Hradec Kralove (#184), Warsaw (#207) and Madrid (#186) were downloaded from EUBREWNET for the period 2017–2020. These data were analyzed with the O3BUmkehr algorithm and the retrieval settings were optimized for each particular station. The time series of partial ozone columns at the 8 standard Umkehr layers were derived separately for the morning and evening twilight hours.

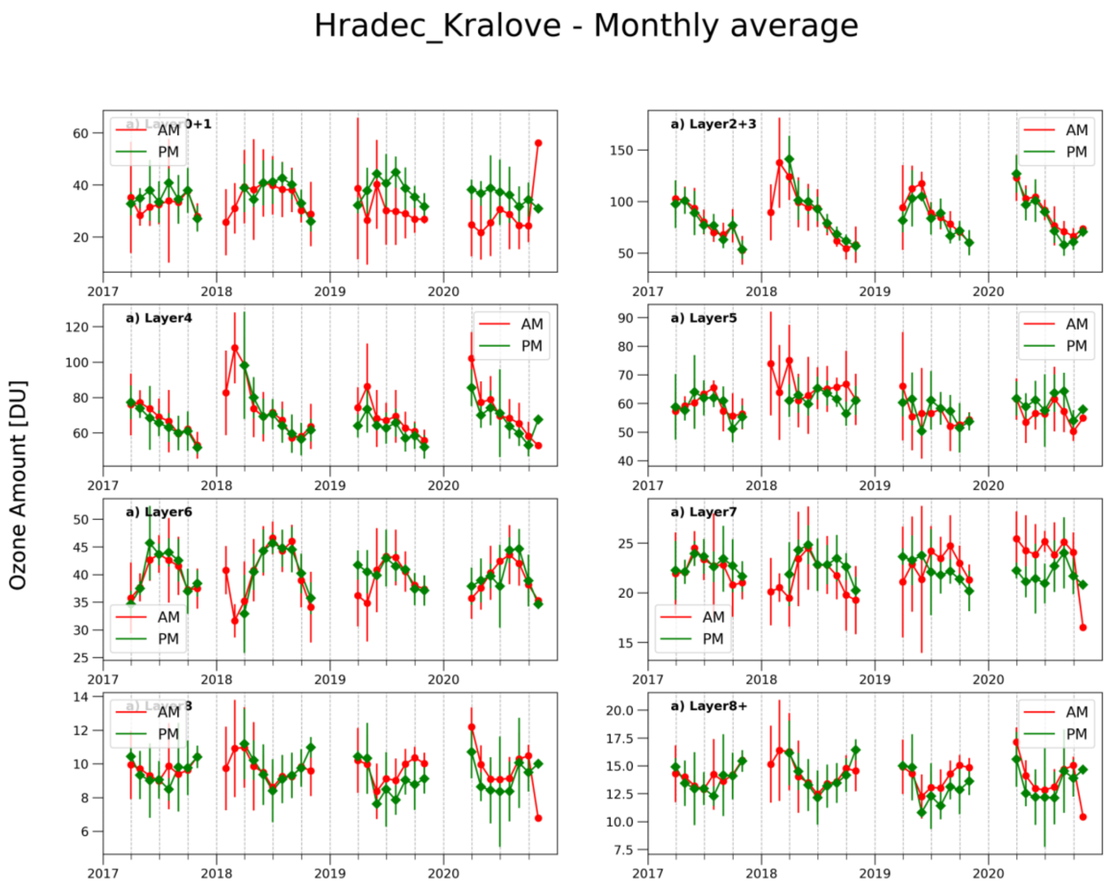


Figure 3.3: Time series of monthly mean ozone column amount (in DU) and the associated standard deviation in the 8 layers derived from Umkehr observations over Hradec Kralove, Czech Republic, for the period 2017 – 2020. AM and PM data are plotted in different colors and vertical bars correspond to one standard deviation.

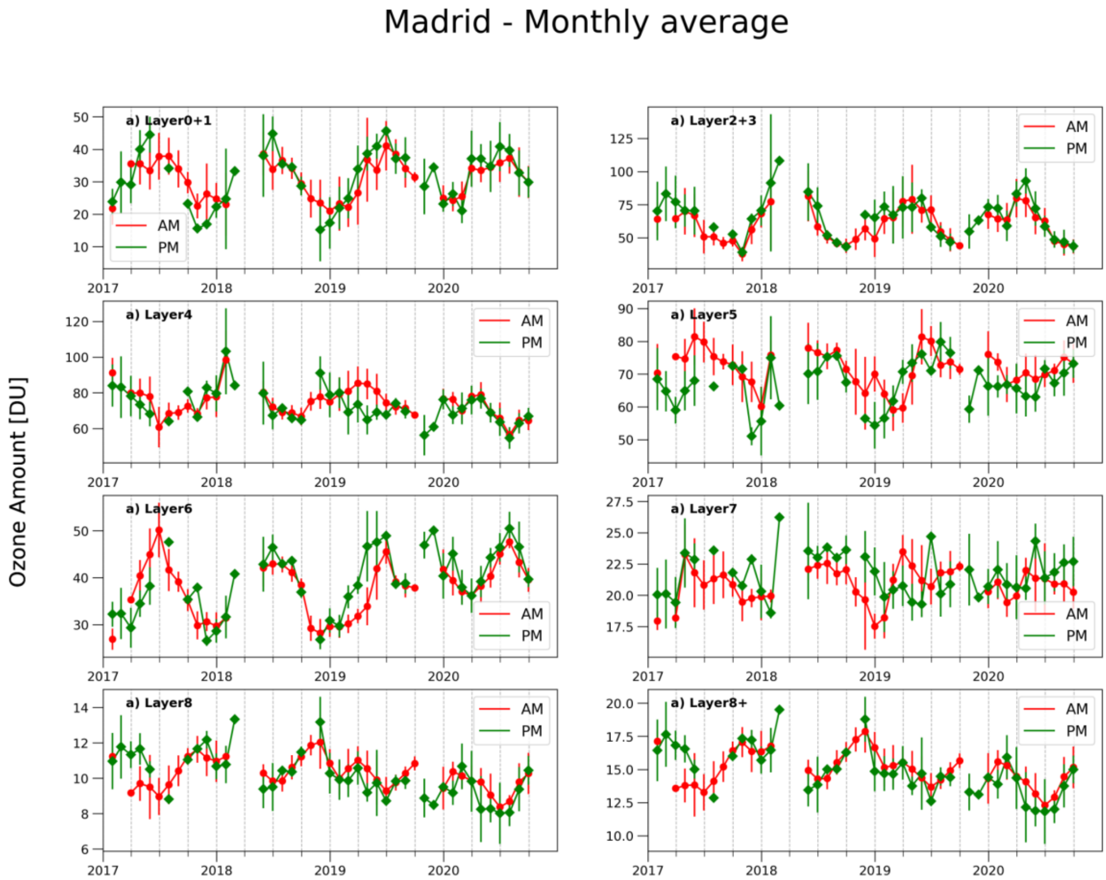


Figure 3.4: Same as Figure 3.3 but for Madrid, Spain.

Figure 3.3 to Figure 3.5 show the time series of monthly mean ozone column amount (in DU) for each of the 8 layers along with the standard deviation of each monthly value, for the three 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 good, at least qualitatively, with the monthly values always lying within the standard deviation.

Figure 3.6 summarizes the time series of monthly mean ozone column amount (in DU) in the 8 layers for the period 2017 – 2020, derived from Umkehr observations performed at the four selected Brewer stations. All stations have annual ozone cycles that depend on their location and on the atmospheric layer. For example, for the lower combined layer (0+1), the seasonal cycle has a peak-to-peak amplitude of ~ 10 DU for Thessaloniki and ~ 20 DU for Madrid and Warsaw.

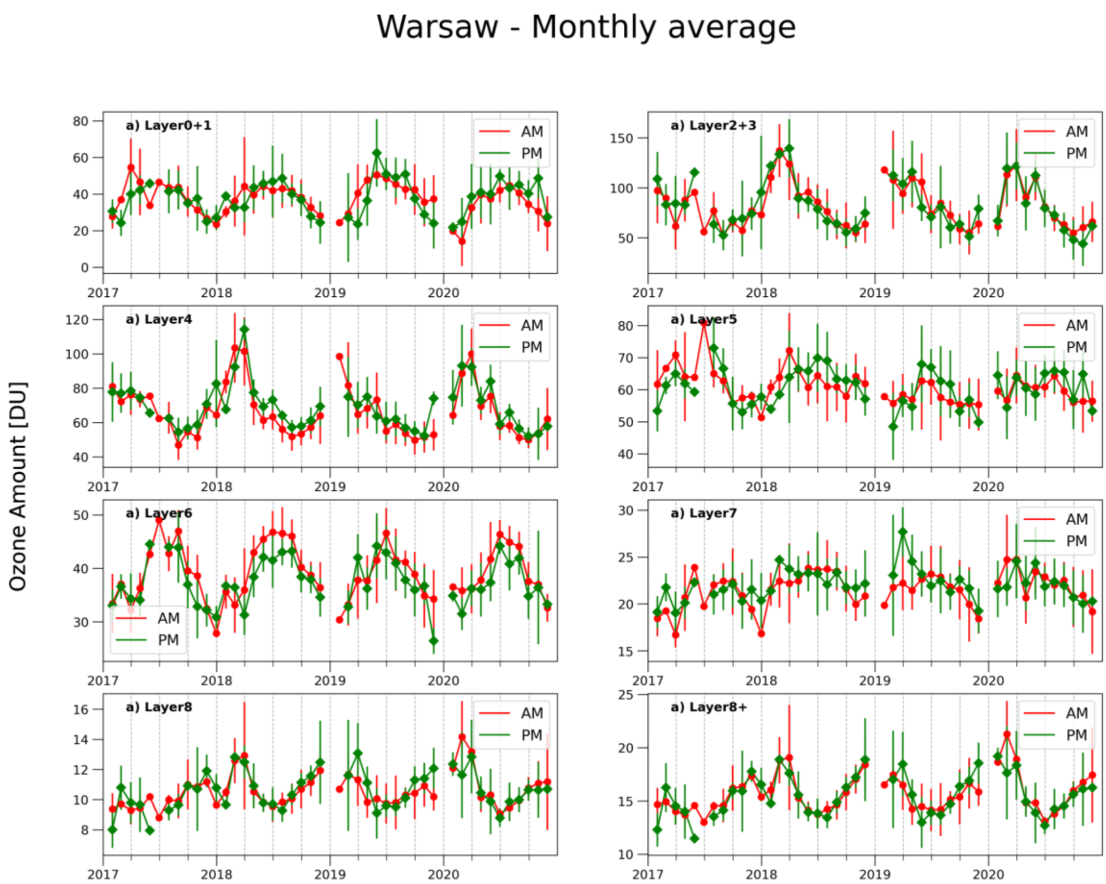


Figure 3.5: Same as Figure 3.3 but for Warsaw, Poland.

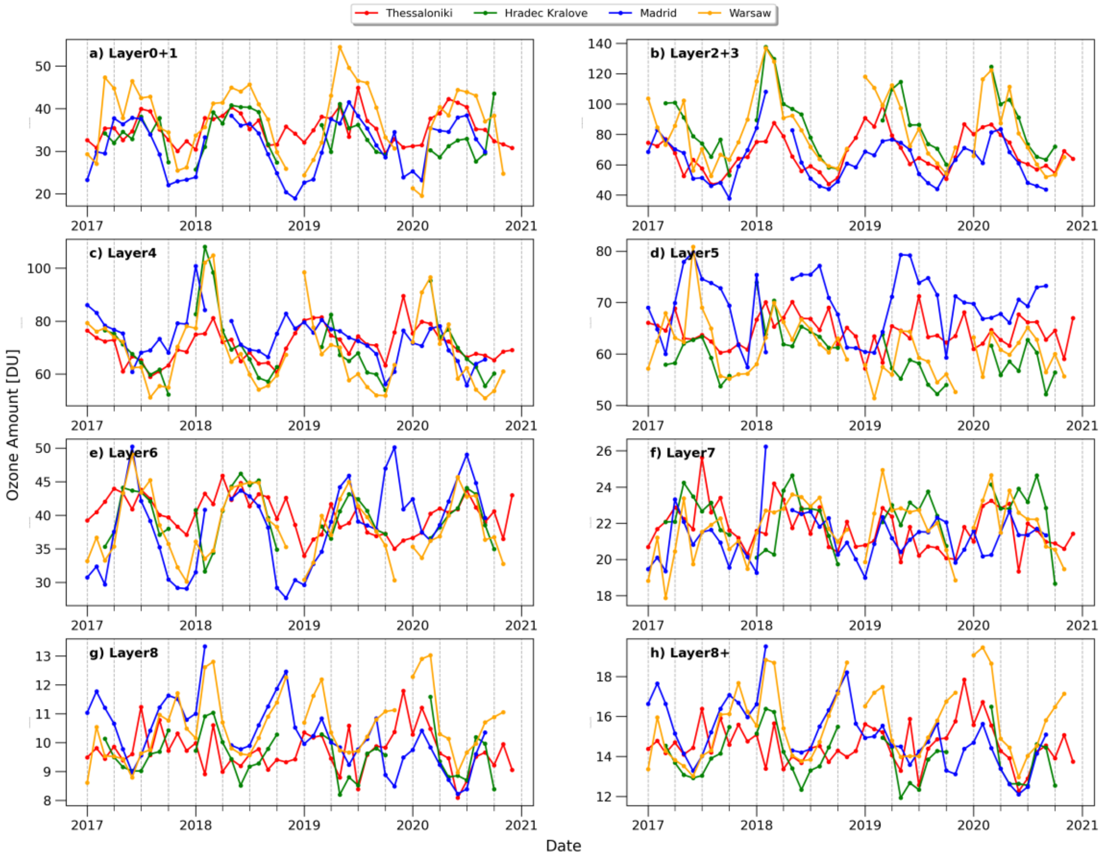


Figure 3.6: Time series of monthly mean ozone column amount (in DU) in the 8 layers for the period 2017 – 2020, derived from Umkehr observations performed at the four selected Brewer stations.

3.1.2 Dobson timeseries

This project optimized the SZA bias in Umkehr curves which were impacted by instrument-specific out-of-band and internal stray light. All records were reprocessed.

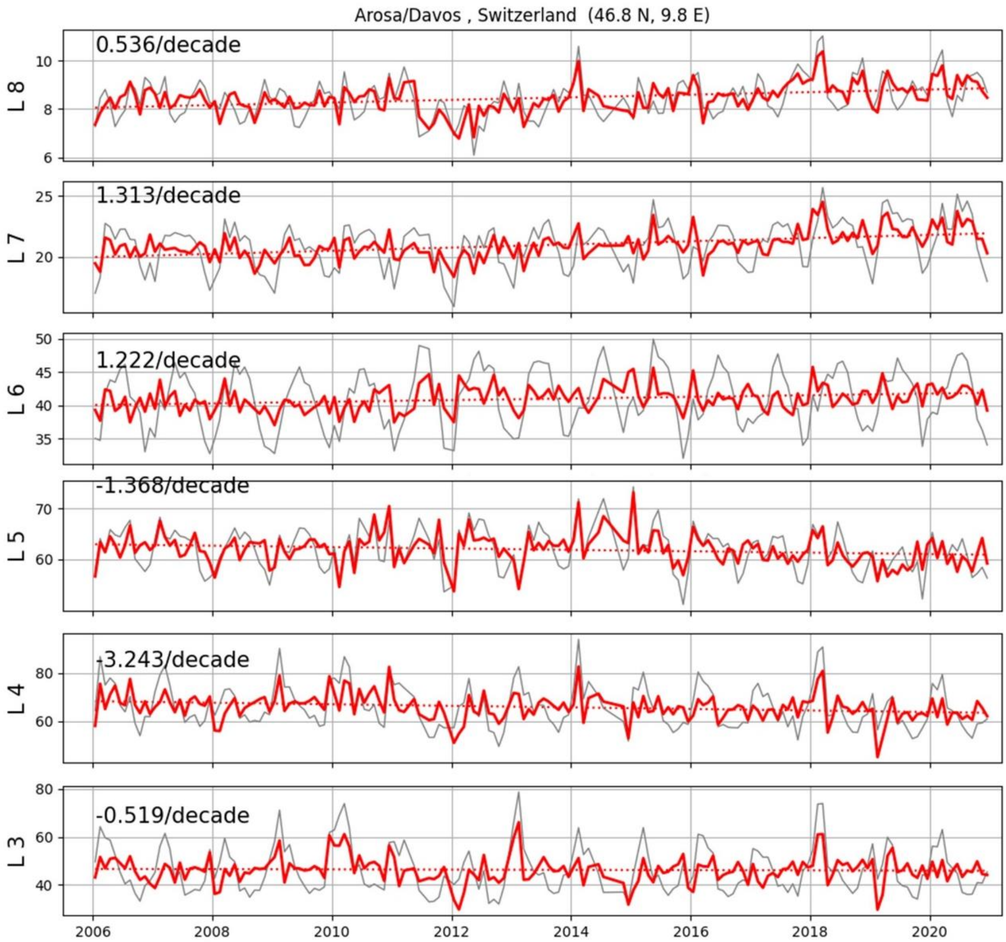
Panel a in Figure 3.7 shows the ozone timeseries from Arosa/Davos station in six Umkehr layers, based on operational retrievals (not homogenized) for 2006-2020 period. Panel b shows results for optimized retrievals. Figure 3.7c shows ozone time series from four optimized NOAA Umkehr stations. Only three selected layers are shown for NOAA Umkehr stations: Umkehr layers 8, 6 and 4. The linear trends (dashed lines) are derived from de-seasonalized records (red solid lines) and trend estimates (DU per decade) are included in the upper left corner of each panel.

Figure 3.8 shows the 2017-2020 ozone monthly mean time series in 8 layers for the four Dobson stations: Boulder, USA (red); Haute Provence, France (pink); Mauna Loa, Hawaii (green) and Lauder, New Zealand (blue).

Figure 3.9 shows the ozone seasonal cycle based on the optimized retrievals for Umkehr profiles in 10 layers at Arosa/Davos and Boulder stations, from 2007 to 2020. The color contour represents percent difference between the 2007-2020 averaged (OZN) ozone in reference to the 1995-2005 average (ANO3), calculated as follows:

% diff = (OZN-ANO3)/ANO3 * 100.

a)



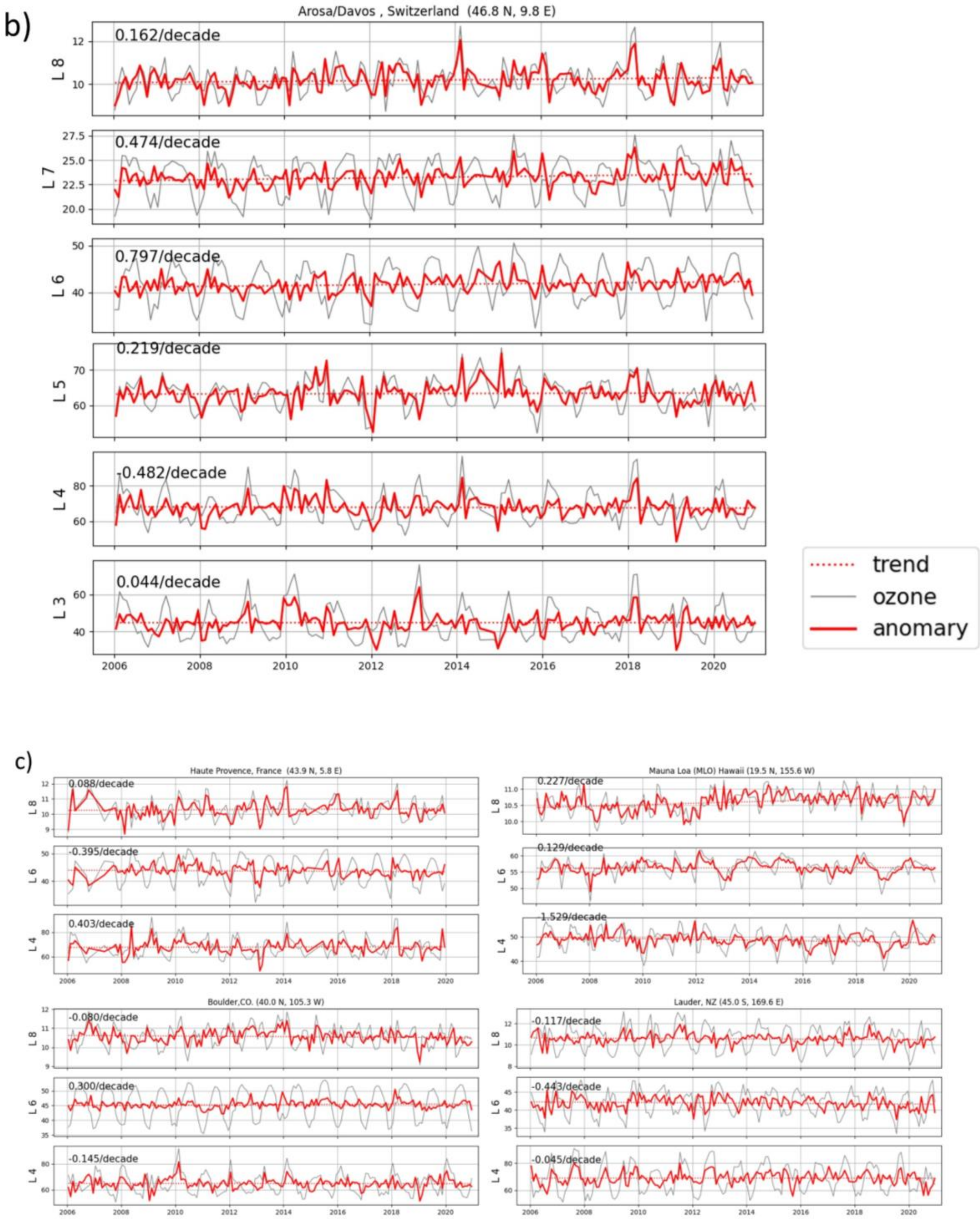


Figure 3.7: The ozone time series of Dobson Umkehr vertical ozone profile at Arosa/Davos. a) based on operational observational retrievals (not homogenized). The red dashed line represents ozone trend derived after time series were de- seasonalized (red solid line). b) Same as panel (a) but the results are from the optimized Umkehr retrievals. c) Similar to panel (b), but results are shown for three selected layers (Umkehr layers 8, 6 and 4) and in 4 blocks representing four NOAA optimized Umkehr records.

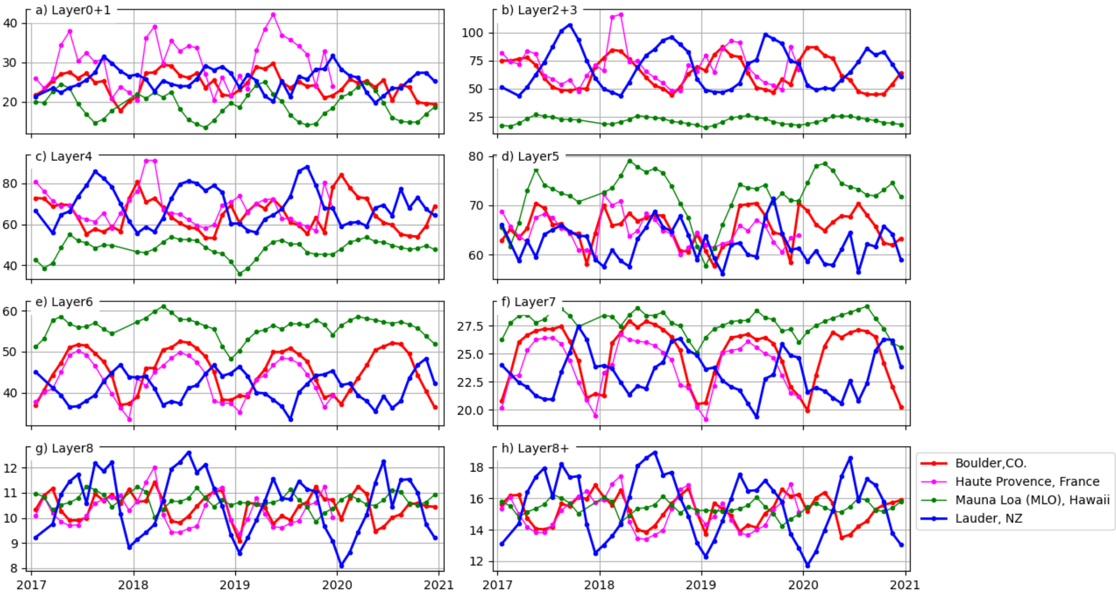


Figure 3.8: Time series of monthly mean ozone column amount (in DU) in 8 layers for the period 2017 – 2020, derived from Umkehr observations performed at the four selected Dobson stations.

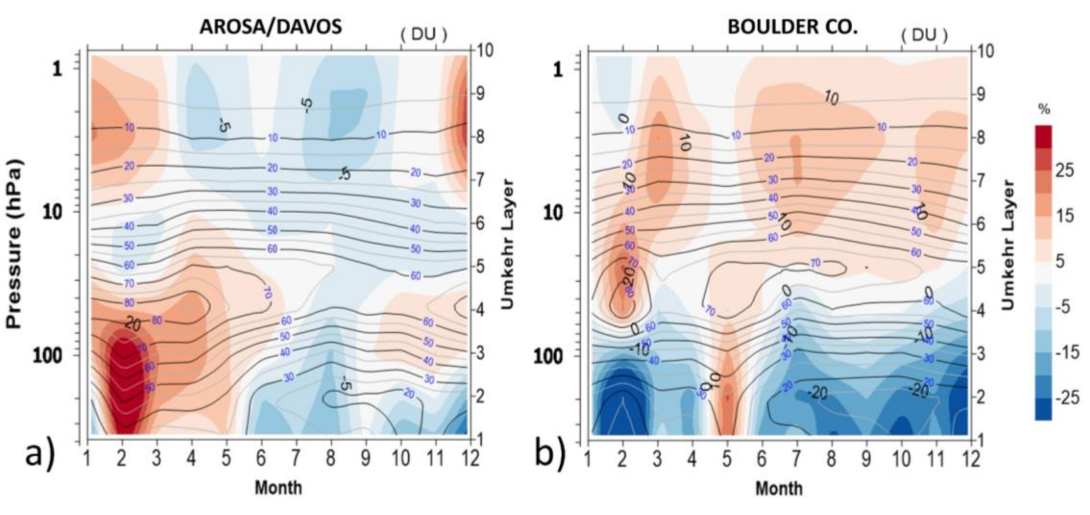


*Figure 3.9: The ozone seasonal cycle based on the optimized retrievals for Umkehr in 10 layers. Results are shown for Arosa/Davos and Boulder records. Ozone is averaged from 2007 to 2020 (black solid contour lines). The colors represent the difference between the 2007-2020 averaged ozone and the averaged ozone from the 1995-2005 period. The difference is calculated as a percent of ozone change; % = (OZN-ANO3)/ANO3 * 100.*

3.2 Umkehr Ozone profile comparison to satellite datasets

3.2.1 The satellite observational datasets

3.2.1.1 SBUV/NOAA

The second-generation Solar Backscatter Ultraviolet (SBUV) merge ozone datasets provide daily mean ozone products constructed by merging individual SBUV (total and profile ozone) satellite data sets (McPeters et al., 2013) with no external calibration adjustments. Intercalibration of the SBUV instruments in Version 8.7 used in this work is accomplished within the algorithm at the radiance level. Version 8.7 uses the same core algorithm as Version 8.6 (Firth et al., 2020a), but includes new inter-instrument calibration adjustments for instrument records since 2000 (NOAA-16 SBUV/2 though OMPS NP) based on a new approach to radiance intercomparisons across overlapping instruments. Version 8.7 also incorporates an updated a priori with improved tropospheric representation and diurnal adjustments to ensure the a priori profile correctly reflects the local solar time of each measurement. A post-retrieval diurnal correction is applied to adjust each instrument record to an equivalent measurement time of 1:30pm. Remaining offsets between instruments exist, but their cause is not understood (Firth et al., 2020b). Validation of different parts of this dataset have already been performed against ground-based instrumentation (for e.g. Sterling et al., 2018; Zerefos et al., 2018).

The SBUV overpass daily files were extracted from the official NASA pages, SBUV Merged Ozone Data Set (nasa.gov) and provide ozone profiles as partial ozone columns in Dobson Units (DU) in 21 layers from the surface up to 0.1 hPa.

3.2.1.2 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, for MetopB and –C this means 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 and dusk observations.

3.2.1.3 COH

The station overpass data are selected from each SBUV/2 NOAA and S-NPP OMPS satellite records and adjusted using the SBUV COH technique developed for zonal average data to create a coherent long-term time series (J. Wild, private communications).

The SBUV/2 and OMPS COH station overpass data (referred to as COH) are available at NOAA ftp://ftp.cpc.ncep.noaa.gov/SBUV_CDR.

3.2.1.4 SAGE II, III

SAGE is an ongoing series of solar occultation instruments spanning several decades providing high-precision vertical profiles of ozone from the troposphere to the mesosphere with ~1 km vertical resolution. Providing the longest single-instrument record of stratospheric ozone, SAGE II (Mauldin et al., 1985) was operational onboard the Earth Radiation Budget Satellite between October 1984 and August 2005.

SAGE III/ISS instrument is similar to SAGE II, but includes extra near-IR channel to improve aerosol observations. The instrument started routine operation from the international space station in 2017 (McCormick et al, 2020). The ozone profile retrieval algorithm is similar to the SAGE II ozone profile product (Damadeo et al, 2013)

3.2.1.5 S-NPP OMPS

The Suomi National Polar-orbiting Partnership (S-NPP) satellite of the Joint Polar Satellite System (JPSS) was launched in October 2011 (Flynn et al, 2006). The ozone profile retrieval is very similar to Rodger's optimal statistical method deployed in the SBUV and Umkehr retrieval techniques.

3.2.1.6 Aura MLS

The Microwave Limb Sounder (MLS) measured ozone profiles from the UARS and Aura satellite platforms (Waters et al, 1999). We use Aura MLS Version 4.2 data for comparisons with Umkehr observations during the 2005 – 2020 period. Ozone profiles are provided on a 1 km vertical resolution grid, although the vertical resolution of MLS AK is about 2.6 km in the stratosphere.

3.2.2 Comparison for Thessaloniki, Greece | a Brewer case study

In this section, the optimized Brewer Umkehr data record for Thessaloniki is compared to NASA SBUV Version 8.7 MOD v2 Release 1 dataset aggregated overpass records, as well as to the GOME2-MetopA and -MetopB ozone profiles, for verification of instrumental bias corrections.

The SBUV and GOME2 ozone profiles over Thessaloniki are interpolated in Umkehr layers analysis and then smoothed using the Umkehr average kernels and a priori profiles (Miyagawa et al., 2009):

$$X\_sm(j) = \sum_k \left\{ AK(j,k) x \left[X_t(k) - AP(k) \right] \right\} + AP(j) \quad \text{(Eq. 7)}$$

where j is the layer number, $X_t(k)$ the SBUV ozone profile in layer k, AP(k) is the Umkehr a priori in layer k and Σ_k the integral of the smoothed differences in all layers.

In Figure 3.10 and Figure 3.11, the vertical distribution of the mean percentage differences between ground and satellite observations for the period of 2017-2020, is shown. The blue line and symbols with the respective blue shadow (i.e. the ±1σ standard deviation) represent the mean difference per layer, while the orange line and symbols show the mean differences per layer when the satellite profiles are additionally smoothed with the Umkehr Averaging Kernel and a priori profiles.

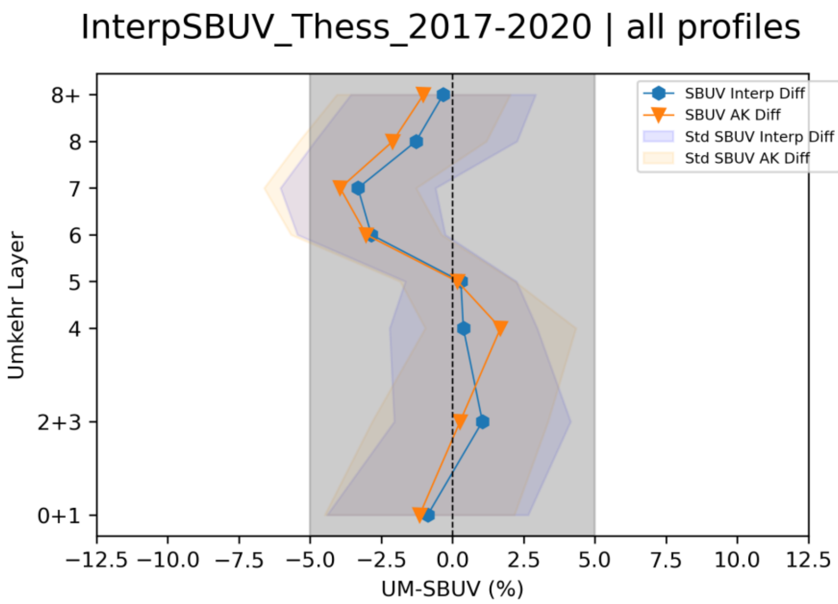


Figure 3.10: Vertical distribution of the mean profile difference between the Thessaloniki Brewer Umkehr observations and a) SBUV interpolated in the Umkehr analysis (blue square and line) and b) SBUV interpolated in the Umkehr analysis and smoothed with the Umkehr AK and AP (orange triangle and line) for the period 2017 – 2020. The shaded areas show the ±1 standard deviation of the mean.

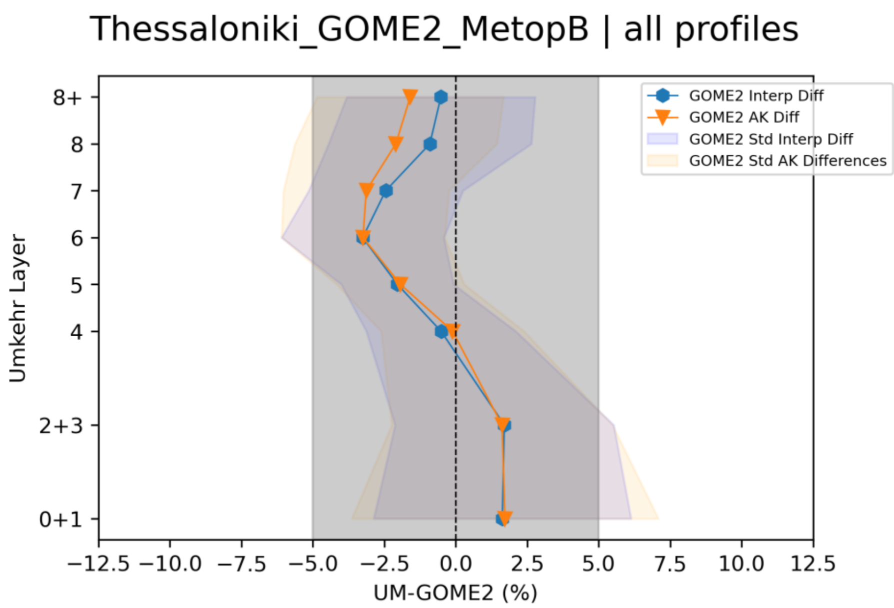


Figure 3.11: The same as Figure 3.10 for the comparison of Umkehr to GOME2-MetopB ozone profiles over Thessaloniki.

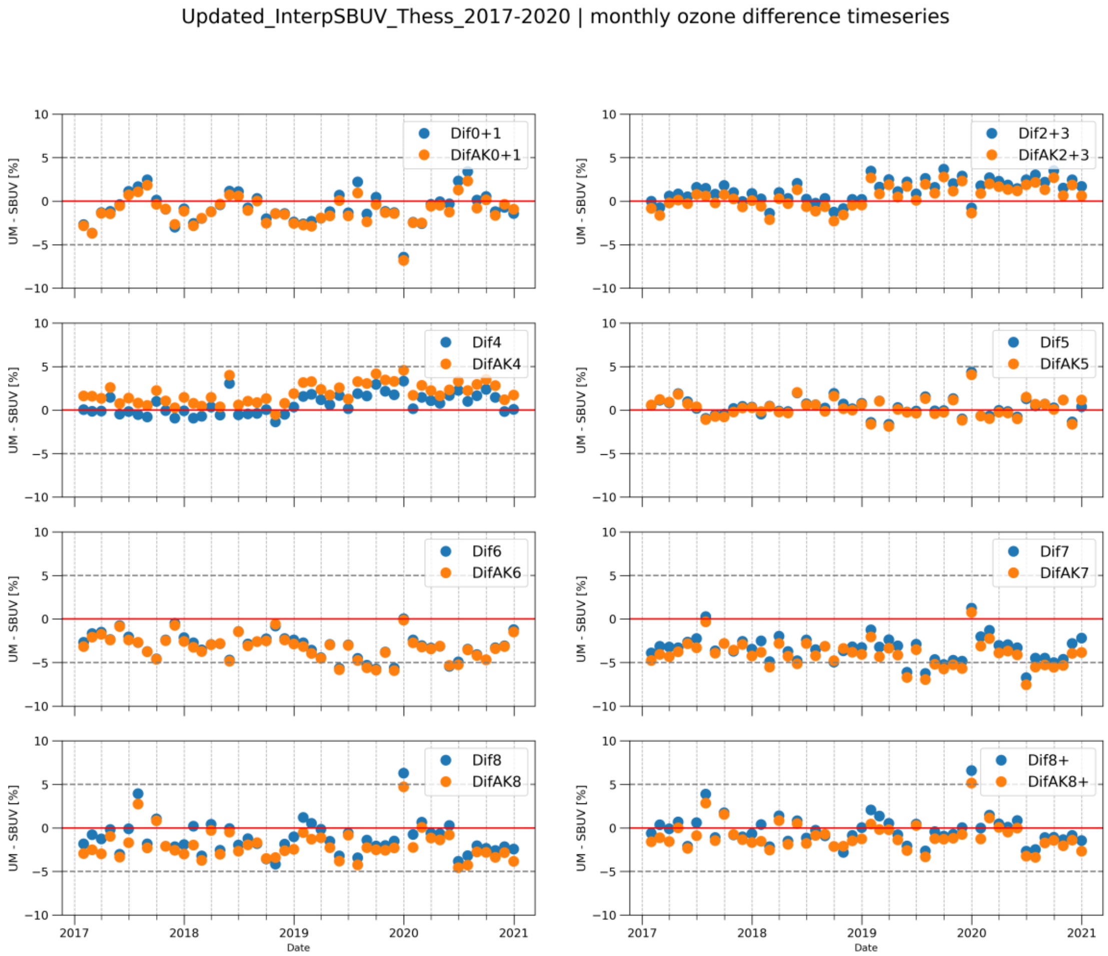


Figure 3.12: The timeseries (per layer) of the monthly mean percentage differences of the comparisons of ground-based Umkehr observations to the SBUV ozone profile overpass data, for Thessaloniki during 2017-2020 (blue symbols). The orange symbols show the differences when the AK smoothing is applied.

The overall agreement between Brewer Umkehr profiles and SBUV records (Figure 3.10) is quite satisfactory, within ±5%, for all layers. The best agreement is found for layers 2+3, 4 and 5, where the bulk of the ozone absorption occurs. The highest discrepancies between ground and satellite observations are at layers 6 and 7, but the mean differences remain within ±5%. Application of the AK smoothing does not improve the comparison, possibly because the vertical resolutions of Umkehr and SBUV are comparable.

The comparison between Brewer Umkehr and GOME2-MetopB ozone profiles (Figure 3.11) also shows a very good agreement, within ±5%, for all layers. The best agreement is found for layer 4, while the highest discrepancies between ground and satellite observations are at layers 6, 7 and below layer 3. Still, the mean differences remain within the ±5% range. Application of the AK smoothing does not change the comparison below layer 6 and is increasing the difference by about 1% above that height. The variability of the means, i.e., the ±1σ deviation, becomes higher for layers 2+3 and 1+0, thus below 20km (troposphere and lower stratosphere).

The increased biases observed in the upper layers were also seen in the original Dobson Umkehr (not optimized) profiles compared to satellite records, but they were eliminated in the optimized Dobson versions comparisons. Thus, it is expected that the application of the same optimization process in Brewer profiles will also significantly reduce the observed biases in layers 6 and above.

Figure 3.12 and Figure 3.13 show the timeseries (per layer) of the monthly mean percentage differences of the comparisons between ground-based Umkehr observations and SBUV (Figure 3.12) and GOME2-MetopB (Figure 3.13) ozone profile overpass data , for Thessaloniki during 2017-2020 (blue symbols). The orange symbols show the differences when the AK smoothing is applied.

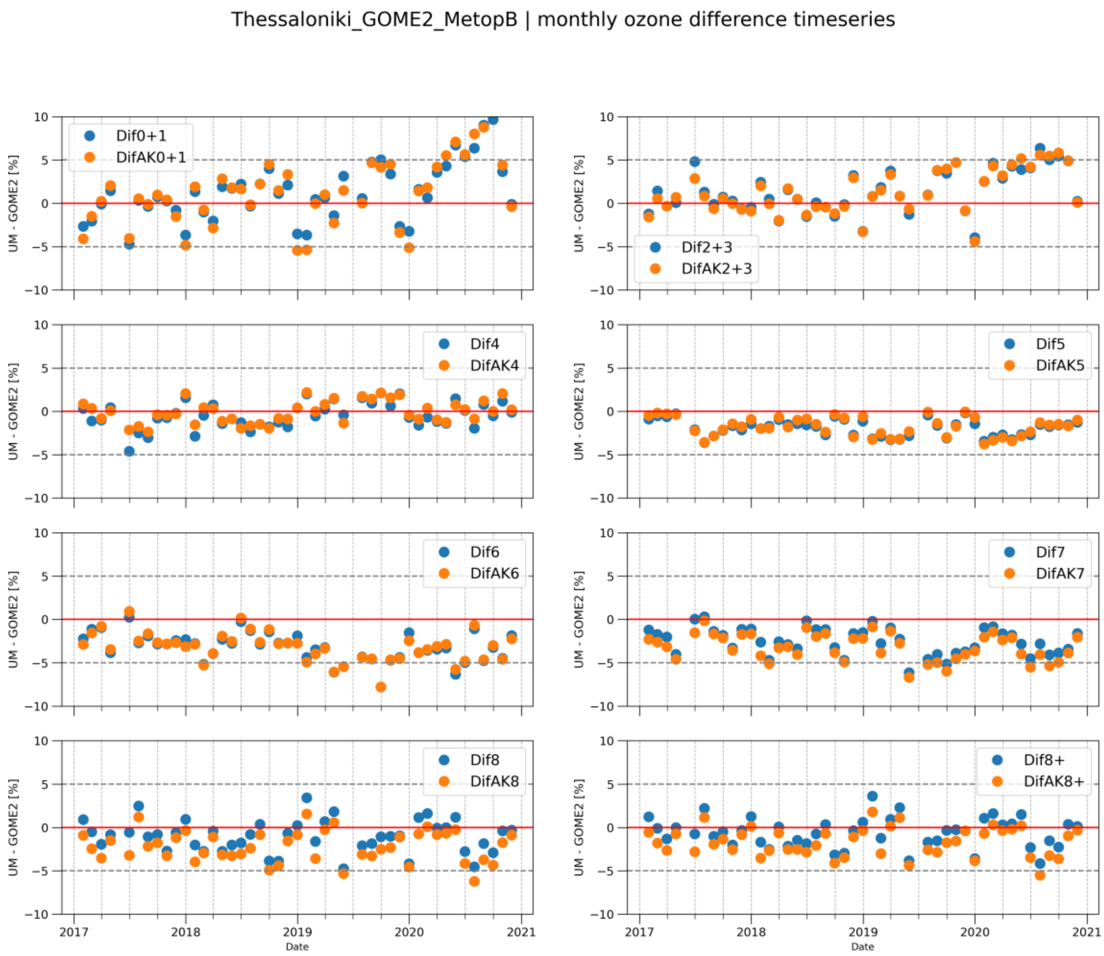


Figure 3.13: The same as Figure 3.12, for the GOME2-MetopB comparisons.

The comparisons of the Umkehr observations to SBUV overpasses are temporally stable for all layers and they are always within ±5%, with no abrupt changes for the time span of 2017 to 2020. The seasonal variation is more pronounced in the lower troposphere (layer 0+1) comparisons, with a ~5% peak-to-peak difference, showing positive discrepancies during summer months and negative during winter. The seasonal variation is reduced for the upper layers (mostly 4 and 5) and appears inversed for layers 6 and above.

When GOME2-MetopB ozone profiles are compared to Brewer Umkehr observations (Figure 3.13), the timeseries for layers 0+1 and 2+3 are noisier, with very high monthly means during the second half of 2020, up to +10% for layer 0+1. This effect can be attributed to the satellite data, since it does not agree with the respective comparisons to SBUV or GOME2-MetopC (not shown here) for the same time period. Finally, layers 4 and 5 has a limited variability, which is increasing gradually for layers 6 and above. In other respects, the time series of the Thessaloniki Brewer Umkehr comparisons to GOME2-MetopB stays within ±5% and shows no particular discontinuities or seasonal dependency for any of the layers.

3.2.3 Comparison for Lauder, New Zealand | a Dobson case study

Following the same methodology that was briefly described in the previous section, the results of the comparison between the Dobson Umkehr measurements performed at Lauder, New Zealand, and satellite ozone profile overpasses by SBUV and GOME2-MetopB, will be presented.

The vertical distribution of the mean percentage differences between ground and satellite observations for the period of 2017-2020, is shown in Figure 3.14 and Figure 3.15. As before, the blue line and symbols with the respective blue shadow (i.e. the ±1σ standard deviation) represent the mean difference per layer, while the orange line and symbols show the mean differences per layer when the satellite profiles are additionally smoothed with the Umkehr Averaging Kernel and a priori profiles.

The comparison of the Umkehr data to SBUV (Figure 3.14) is excellent, with a bias up to ± 2%. The variability of the differences is ~ 6% for the lower part of the profile (layer 0+1) and it is decreasing at higher layers to 2.5%. When GOME2-MetopB is considered (Figure 3.15) a positive bias of +2.5% is observed for tropospheric ozone amount (layer 0+1), and a negative bias of -2.5% is present for layers 4 and 5. All other layers show a very good agreement (within ±1 %) with the GOME2-MetopB ozone profiles.

The temporal evolution of the Umkehr comparisons per layer with respect to SBUV and GOME2-MetopB observations over Lauder, are shown in Figure 3.16 and Figure 3.17, respectively, for the time period 2017-2020 (blue symbols). The orange symbols show the differences when the AK smoothing is applied.

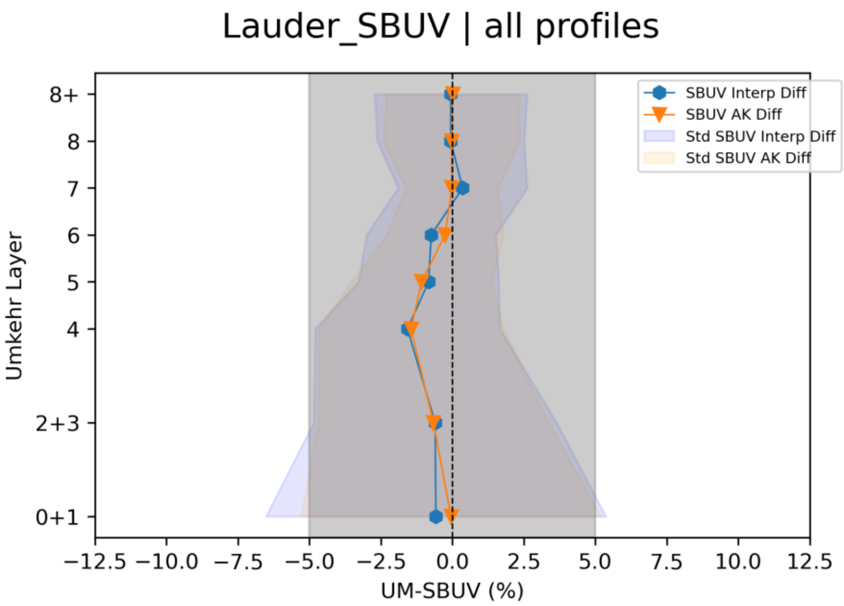


Figure 3.14: : Vertical distribution of the mean profile difference between the Lauder Dobson Umkehr observations and a) SBUV interpolated in the Umkehr analysis (blue square and line) and b) SBUV interpolated in the Umkehr analysis and smoothed with the Umkehr AK and AP (orange triangle and line) for the period 2017 – 2020. The shaded areas show the ±1 standard deviation of the means

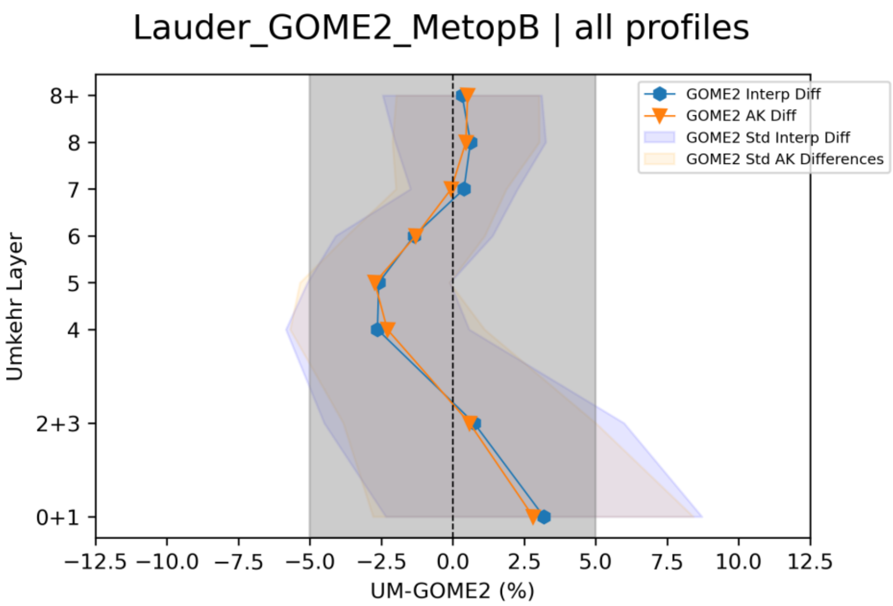


Figure 3.15: The same as Figure 3.14 for the comparison of Umkehr to GOME2-MetopB over Lauder.

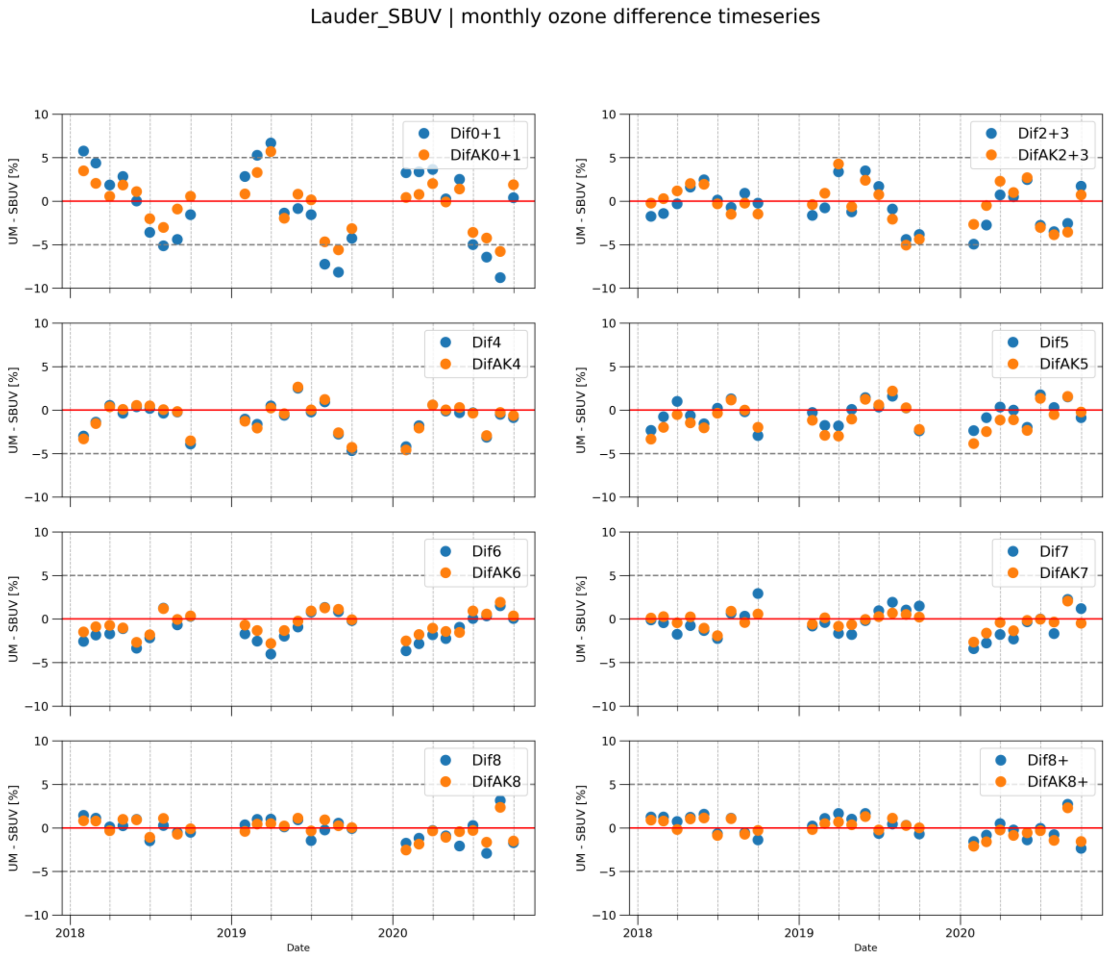


Figure 3.16: The timeseries (per layer) of the monthly mean percentage differences of the comparisons of ground-based Umkehr observations to the SBUV ozone profile overpass data, for Lauder, during 2017-2020 (blue symbols). The orange symbols show the differences when the AK smoothing is applied.

The comparisons of the Umkehr observations to SBUV overpasses (Figure 3.16) are within ±5%, with no abrupt changes for the time span of 2017 to 2020. The seasonal variation is more pronounced in the lower troposphere (layer 0+1) comparisons, with a ~10% peak-to-peak difference, showing positive discrepancies during summer months and negative during winter (Southern Hemisphere). The seasonal variation is reduced for the upper layers showing a minimum of ~± 1% for layers 8 and above.

When GOME2-MetopB ozone profiles are compared to Dobson Umkehr observations at Lauder (Figure 3.17), the timeseries that result for layers 0+1 and 2+3 are noisier. Nevertheless, no abrupt changes are seen in the timeseries and the monthly means show the same behaviour with respect to the seasonal dependence as it was seen with the SBUV comparisons. No particular discontinuities are seen here for any of the layers, while layers 7 and above have a limited variability.

Lauder_GOME2_MetopB | monthly ozone difference timeseries

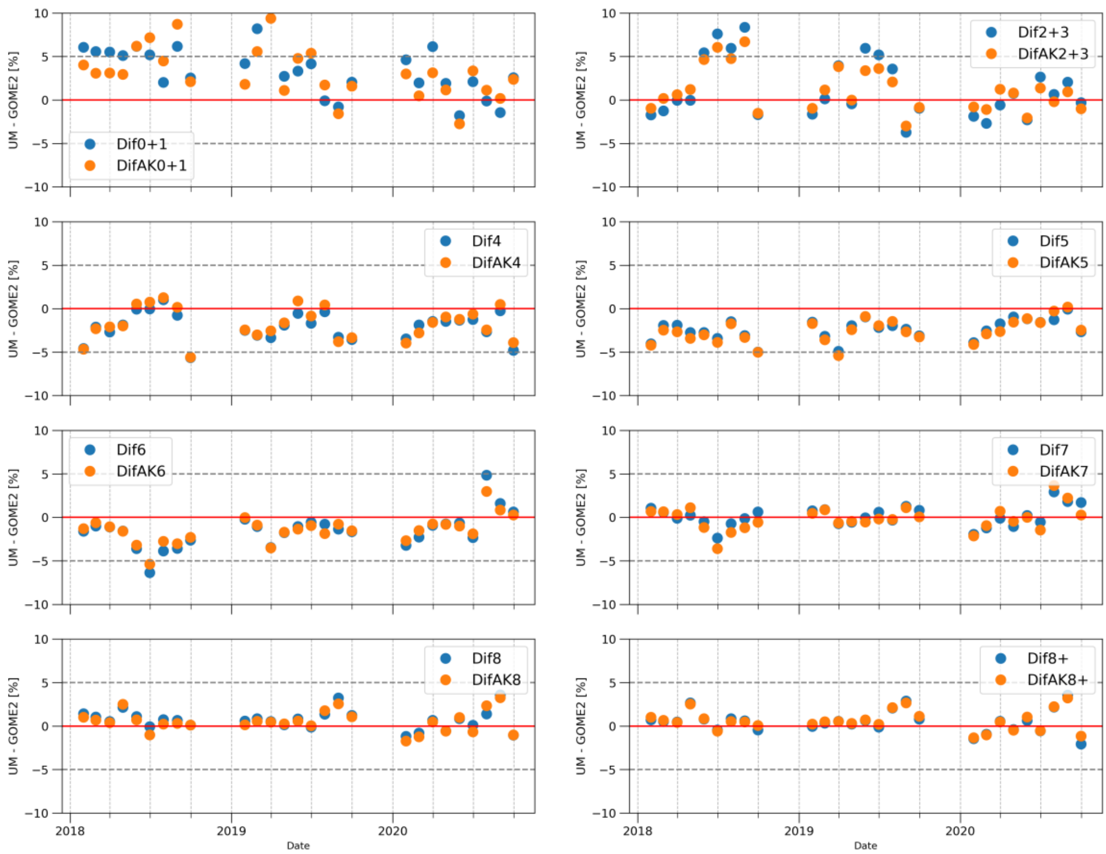


Figure 3.17: The same as Figure 3.16, for the GOME2-MetopB comparisons.

3.3 Extended comparisons at the four optimized NOAA Dobson stations

The optimization methodology of the Umkehr time series was applied at four stations in total: Boulder, MLO, Lauder, OHP and Arosa. Each station record was evaluated against:

- the NASA models M2GMI and GMI-MERRA2 (GMI CTM and GMI in some plots),
- complimentary satellite observations: NASA SBUV aggregated (AGG) version averaged unadjusted SBUV and OMPS records,
- NOAA COH - combined records from the NOAA/2 SBUV and OMPS_NOAA operational ozone profile datasets using correlation-based adjustments to produced coherent long-term record.

Lauder Station

Figure 3.18 shows the comparisons for the Lauder station for two time periods: 2005-2011 and 2012-2018. During the first period we found that the agreement between optimized Umkehr and other records is within ±5 % in the stratosphere. The exception is a larger bias (layers 2, 3, 4) with respect to GMI model, which was reported in Stauffer et al (2019) paper.

During the evaluations, it was decided that Lauder record required additional optimization in 2006 and 2012. Figure 3.18, panels c and d, show the results after the correction was applied in 2006 and 2012, which was associated with the Lauder Dobson calibration in 2006 and the WinDobson automation of the Dobson instrument in 2012 that changed operations and processing of the data. The decision to apply new correction was based on the dis-continuation of the Umkehr record, which was verified by comparisons with other continuous records. The changes are small, but the agreement between most of the records has improved (except for GMI CTM and ozonesonde that show larger biases in the lower layers), while their bias from Umkehr is similar for the two time periods. It was also noticed that the bias between ozonesonde and other records increases in 2012-2020 period as compared to 2005-2011 period. However, the ozonesonde record has not been yet homogenized and could contain step changes.

The time series of Lauder Umkehr data is shown in Figure 3.19. The top panel shows comparisons between COH and Umkehr record in layer 8 (4-2 hPa). The operational Umkehr time series (monthly averaged) is shown in black, the blue line shows optimized Umkehr and the red line show COH data (satellite overpass over Lauder station). The dark green line below shows the difference between operational and COH data, while light green line shows the difference between optimized Umkehr and the COH. The optimized Umkehr version has a reduced bias relative to the COH record.

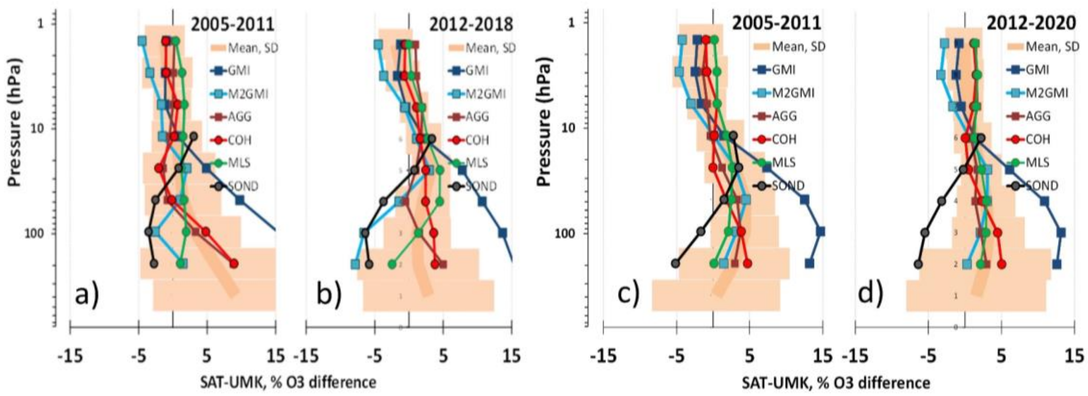


Figure 3.18: Comparisons of models (M2GMI and GMI-MERRA2), satellite (SBUV/OMPS and Aura MLS) and ozonesonde against optimized Umkehr record at Lauder for two periods 2005-2011 and 2012-2018 before (a,b) and after (c, d) the correction.

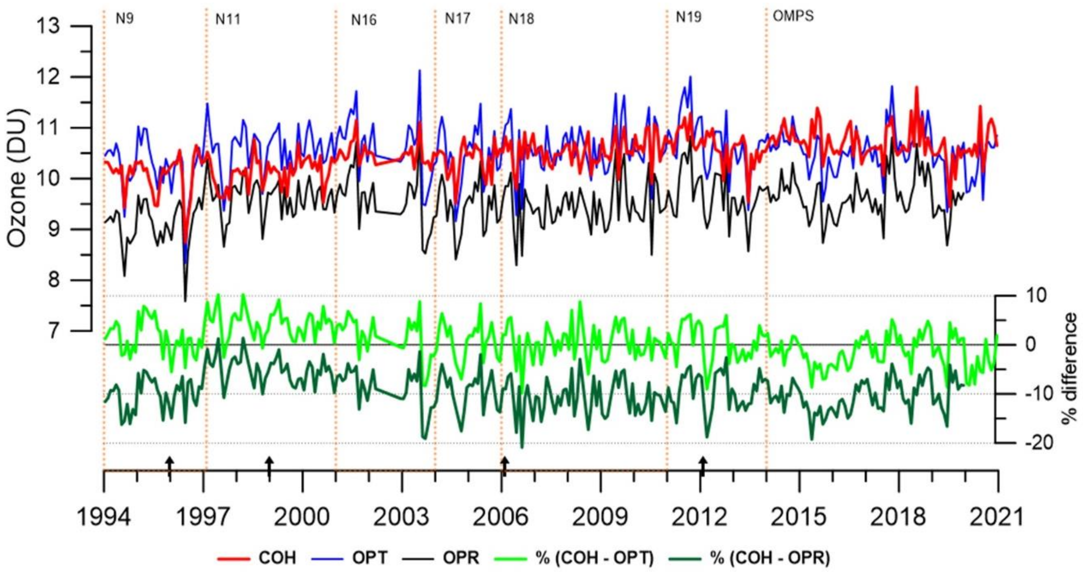


Figure 3.19: Time series of Umkehr ozone in layer 8 derived from operational (black) and optimized (red) versions and COH satellite overpass data (blue) over Lauder. The bottom part of the Figure shows comparisons between COH and operational (dark green) or optimized (light green) version of Umkehr ozone data. Vertical dashed lines represent beginning/end of the SBUV (NOAA/2) or S-NPP OMPS records that are combined in the COH record.

The vertical dashed lines indicate the beginning of the new satellite record (the satellite name is marked at the top of the plot). The arrows at the bottom of the plot indicate the dates when the Dobson instrument was inter-compared against the Dobson standard. The data between arrows (dark green line) are adjusted to homogenize the record. The light green line shows that there are no discontinuities before/after the dates indicated by arrows and therefore the record is homogenized.

Arosa/Davos station

The optimized Umkehr record at Arosa was also compared against models (M2GMI, GMI CTM) and satellite station overpass records (NASA SBUV aggregated, COH, SAGE III, S-NPP OMPS Nadir and Limb profilers, and Aura MLS) for verification of the Umkehr bias corrections (Figure 3.20). In addition, the vertical resolution of Aura MLS, S-NPP OMPS LP and SAGE III/ISS observing systems is high in comparisons to Umkehr profile and therefore the AK-smoothing is applied prior to comparisons with Umkehr data. In general, the agreement is good (±-5 %) in the upper and middle stratosphere (above 50 hPa) and larger biases (up to 10 %) are found in the lower stratosphere in comparisons of Arosa Umkehr against the SAGE III/ISS and GMI CTM.

The scatter plots of the monthly mean data compare the optimized Umkehr ozone and the NASA AGG satellite (and Ozonesonde) at Arosa/Davos (seen in Figure 3.21**)**. When Umkehr Averaging Kernels (AKs) smoothing is applied, both the ozonesonde and satellite AK-smoothed profiles shows better agreement with Umkehr data.

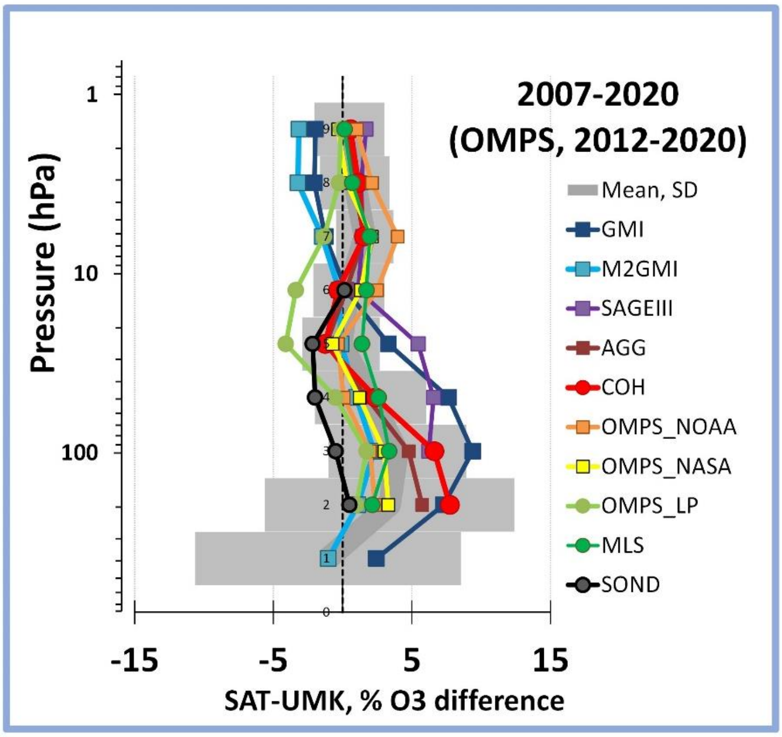


Figure 3.20: Bias between Umkehr and the station overpass data from satellites, i.e. SAGE III, SBUV (AGG), OMPS/LP NASA, OMPS NOAA and Aura MLS at Arosa. Comparisons against two models (GMI CTM and M2GMI are also shown)

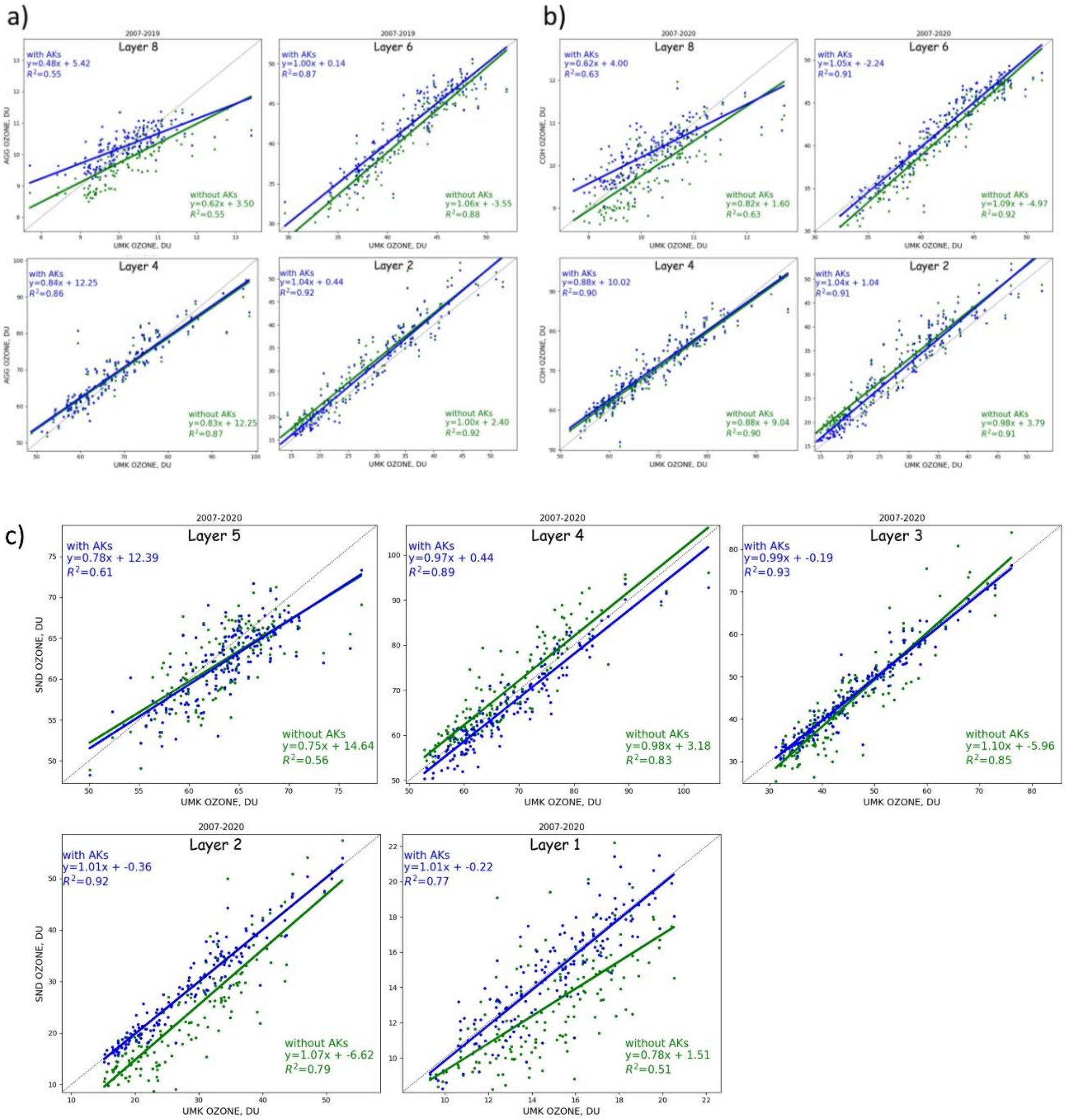


*Figure 3.21: **a)** The scatter plot of MM compared the optimized Umkehr ozone and the NASA AGG satellite at Arosa/Davos. The blue symbols are smoothed to AGG ozone using Umkehr AK. **b)** Same as Figure 5a, but with NOAA COH satellite. **c)** Same as Figure 5a, but with ozonesonde at Payeren. Each altitude is based on ten Umkehr layers.*

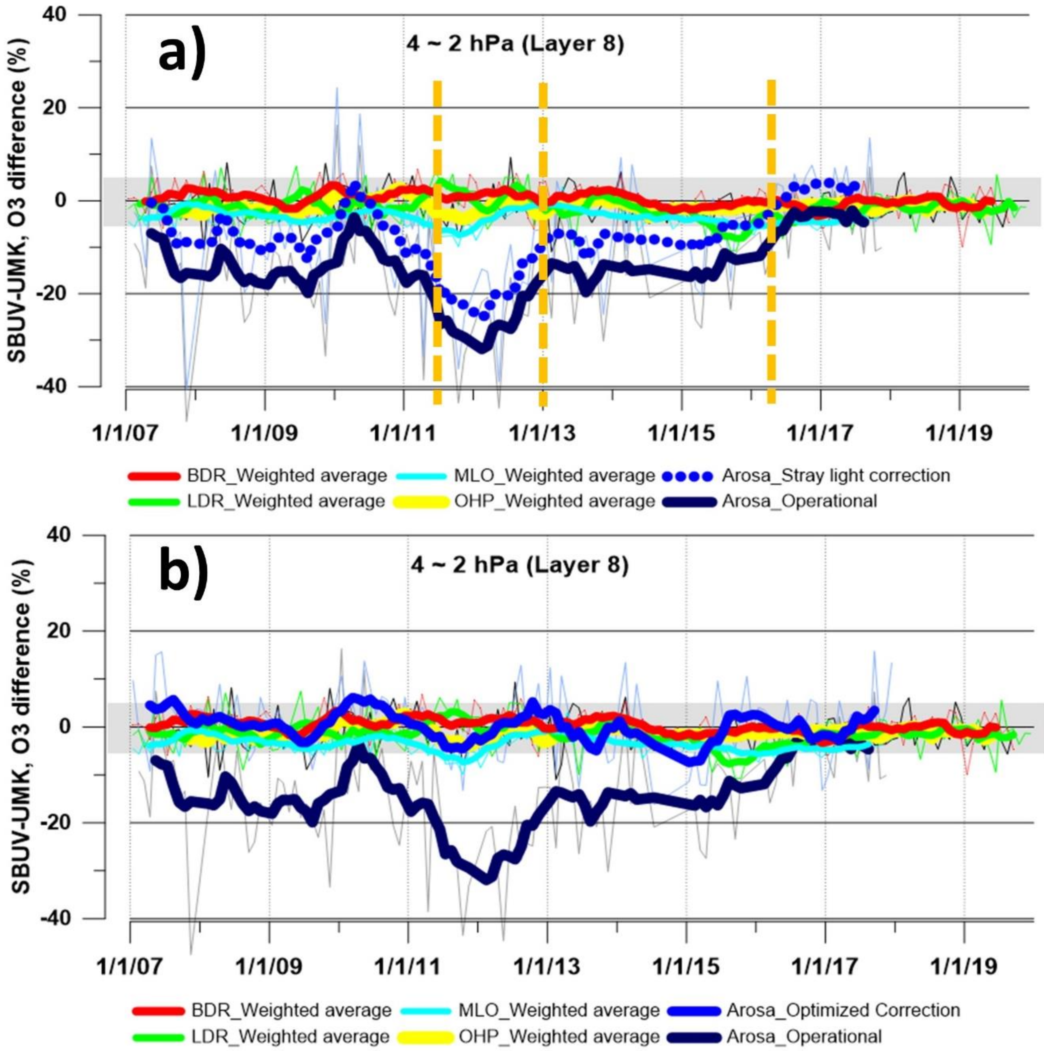


Figure 3.22: Time series of Umkehr monthly mean records of ozone partial column at 4-2 hPa pressure are compared against the co-incident SBUV satellite records. The thin lines represent ozone variability from month-to-month and thick lines show 13-months running smoother. ***a)*** *Bias between station overpass data from satellite (AGG). The step change by instrument calibration is assumed (A vertical orange dotted line). Arosa data prior to optimization is shown as the dark blue line. The step change caused by instrument artifact is identified in time series (A vertical orange dotted line).* ***b)*** *Results for Arosa (light blue solid line) are shown after optimization.*

3.4 Comparison of Umkehr with Ozonesonde for Arosa/Payeren

Balloon-borne ozonesondes in Payeren, Switzerland, provide accurate observations of atmospheric ozone with a long-term record. Payeren and Arosa are in a close distance. In this section the Ozonesonde record from Payeren, downloaded from NDACC, was compared with the Arosa Umkehr data, which were corrected for the stray light (SLC) and optimized. The Payeren ozonesonde data are combined from three records available in different type/format for the following periods.

- 1990 - 2002.AUG: Brewer Mast -Ozone number density (molecules/cm^3)
- 2002.SEP - 2013: EnSci 2Z - Ozone number density (molecules/cm^3)
- 2014 - 2020: EnSci 2Z - Ozone partial pressure [mPa]

The amount of ozone above the balloon burst was calculated from Sonde using SBUV climatology.

The TOC that results from the ozonesondes shows several biases and noise fluctuation as seen in Figure 3.23a, where the blue dashed lines on 1999.11.1, 2002.9.1 and 2014.1.1 are placed. Also, as seen in panel d, a bias was detected at the ozonesonde profiles in layers 4 and 5. The issue of the shift in 2014 may be related to the drop-off currently seen at the global ozonesonde stations (Stauffer, et al., 2020).

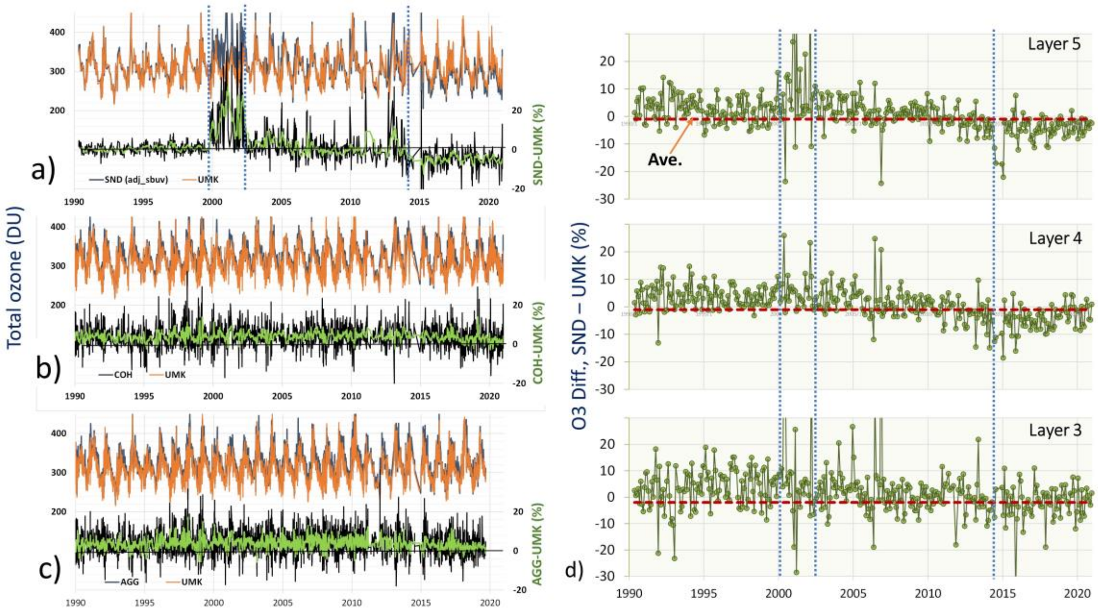


Figure 3.23: TOC comparison with ozonesonde and two different SBUV satellite datasets, a) Ozonesonde , b) COH and c) AGG. d) The percentage difference of Ozonesonde and a Umkehr for layers 3, 4 and 5 is shown.

3.5 Umkehr Ozone Profile and Satellite Validation in Africa

An operational Umkehr retrieval error is shown by comparing the biases between the stray light correction (SLC) and ozone measurements satellite overpass. The validation of Umkehr ozone profiles against NASA SBUV Aggregated overpass (AGG) was performed for 6 African stations, shown in Figure 3.24.

As shown in Figure 3.25, the stray light correction has improved the operational retrieval ozone profiles. The systematic ozone profile error after the Stray light correction was applied is similar to the observations of NOAA's network in Africa. The summary of comparisons between AGG satellite overpass and Umkehr at five stations is shown in Figure 3.26. Umkehr records I corrected for stray light and AGG profiles are smoothed with Umkehr AKs. The Umkehr ozone is lower in the layers 7-10, and higher in the layers 0 to 4 in comparisons to the AGG record. The Springbok Umkehr records is available only over a short time period, however Umkehr and AGG records agree within 5%, and the bias in lower Umkehr layers is less than is found for other stations.

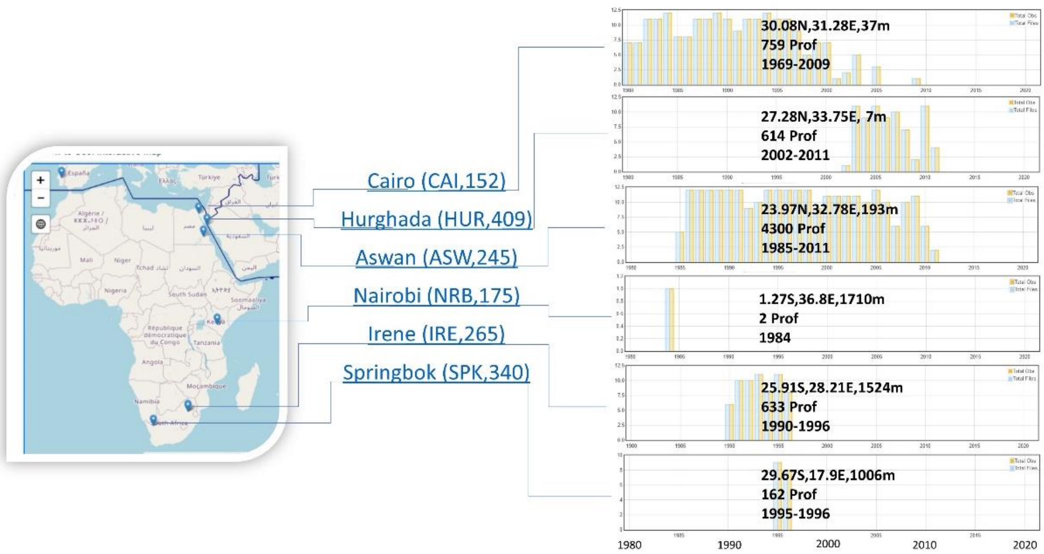


Figure 3.24: The number of profiles since Umkehr observations started in six African stations.

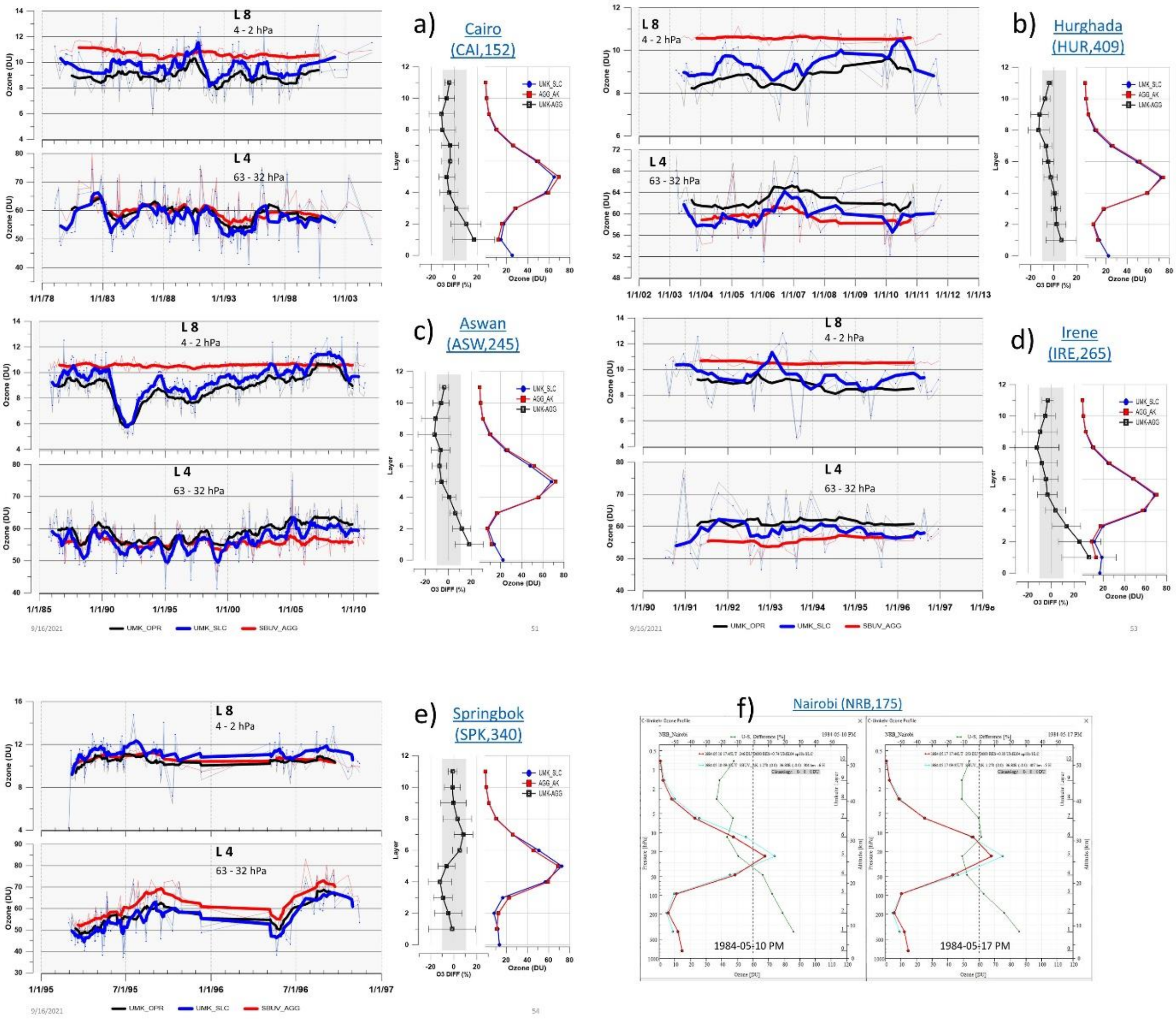


Figure 3.25: Comparisons of Umkehr ozone profiles and NASA SBUV Aggregated record, selected as overpass for six African stations. The time series plot show comparisons between AGG profiles (red solid line), Umkehr retrievals after SLC (blue), as well as operational Umkehr retrievals (black line). Selected, AK-smoothed AGG (red) and SLC Umkehr (blue)profiles are shown for Aswan (c) Irene (d), Springbok (e) and Nirobi (f) stations. The black line shows the difference and grey envelope represents +/- 5 % limits.

		NH			SH	
	Layer	CAI ,152	HUR, 409	ASW, 245	IRE, 265	SPK, 340
Underestimated Umkehr retrieval ozone	11	-3.6	-3.5	-3.6	-3.2	-2
	10	-5.5	-7.6	-5.5	-4.9	-3.6
	9	-9.2	-11.8	-9.2	-9.5	-4.5
	8	-8.5	-12.2	-8.5	-11.9	-2.5
	7	-3.0	-6.2	-3.0	-10.5	1.8
	6	-4.0	-4.7	-4.0	-3.2	0.3
	5	-6.9	-2.9	-6.9	-0.9	-5.9
Overestimated Umkehr retrieval ozone	4	-4.4	0.4	-4.4	2.7	-7.2
	3	2.5	1.5	2.5	9	-3.8
	2	10.9	3.3	10.9	17	0.3
	1	17.6	8.4	17.6	26	5.3
	0	20.3	8.2	20.3	27.7	6.3

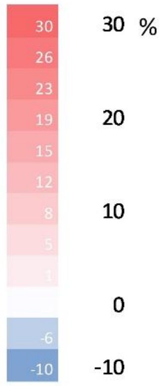


Figure 3.26: The mean % difference between the SLC Umkehr profile and AGG satellite overpass ozone record at 5 African stations

4 Conclusions

Within this work, Dobson and Brewer Umkehr retrieval methods for the years 2017-2020 have been optimized and applied to Umkehr ozone profile measurements for four Brewer and five Dobson stations, namely:

- Brewer stations: Thessaloniki, Greece; Hradec Kralove, Czech Republic; Madrid, Spain and Warsaw, Poland
- Dobson stations: Boulder, USA; Mauna Loa, Hawaii; Haute Provence, France, Lauder, New Zealand and Arosa, Switzerland.

The optimization methodology of the Brewer Umkehr observations at this stage includes the re-evaluation of the profiles using (a) post-corrected total ozone column, (b) a calculated, more representative, effective temperature calculated from the combination of local radiosonde temperature profiles and climatological ozone profiles and (c) the standard deviation of the residuals as the error covariance values in the O3BUmkehr algorithm.

The Dobson Umkehr records were fully homogenized at 4 NOAA stations. The Umkehr record at Arosa was also fully optimized. The NOAA optimization methodology for the Umkehr measurements is based on evaluation of Umkehr instrument-related step-changes with a reference to the M2GMI modeled continuous ozone record. The homogenization process reduced Umkehr biases relative to co-located ozone-sonde, SBUV/OMPS, MLS, SAGE III/ISS station-overpass satellite records to less than +/- 5 % in the middle and upper stratosphere. The largest difference between the optimized Umkehr and the GMI CTM simulated ozone is found over Lauder in the lower stratosphere. However, this bias was discussed in other publications and in comparisons with the M2GMI (Stauffer et al, 2018).

Optical characterization of Dobson instruments in the Umkehr mode is not performed regularly at the Dobson intercomparison campaigns. The measurement of the stray light in the instrument requires special equipment (i.e., lasers) and therefore is not practical. Besides, it is hard to find any information about the optical characterization of instruments that were used a long time ago at the station. Therefore, it was decided the simulated ozone timeseries (M2GMI and GMI-MERRA-2) to be used as a reference record to test the consistency of the Umkehr ozone time series across the period of the instrumental change. This information is used to create corrections to the Umkehr curve before and after the instrumental change and homogenize the record. Several homogenized Dobson Umkehr records were validated against alternative ozone observations.

The Brewer and Dobson Umkehr observations resulted in the updated datasets demonstrated as timeseries per layer in Figure 3.6 and Figure 3.8, respectively. The ground-based Umkehr datasets were afterwards compared to the ozone profiles provided from (a) the SBUV merged satellite ozone dataset and (b) GOME2-MetopB. The comparison results for two stations, one Brewer (Thessaloniki, Greece) and one Dobson (Lauder, New Zealand), were used as case studies, in order to show the level of agreement between ground and satellite data. The main conclusions were the following:

- The agreement between the Umkehr profiles and the satellite ozone profile products is always within ± 5%, for all layers of observation. In the lower stratosphere, some biases remain, possibly due to wide AKs of the Umkehr retrieval.
- The best agreement (~±1%) occurs for layers 2+3, 4 and 5, i.e. for the tropopause and the lower half of the stratosphere, were the bulk of the ozone amount is located. Higher discrepancies, up to -5% are seen for the layers 6 and 7, i.e. between 30 and 40 km.
- No particular discontinuities were seen in the timeseries of the comparisons for any of the layers. On the contrary, they were all very stable temporally, with no abrupt changes present for the time span of 2017 to 2020.
- The seasonal variations of the comparisons between ground and satellite data, were more pronounced in the lower troposphere (layer 0+1), with a peak-to-peak amplitude of ~ 5 - 10%.
- We found that occasionally the change of the instrument at the station or optical refurbishing or repairing of the instruments can create a step change in the continuous ozone profile time series. The step-change in an Umkehr curve is caused by the difference in the stray light that is specific for each Dobson or Brewer instrument, and it is depicted in the altitude-dependent bias in the Umkehr profile, if that change is not accounted in the data processing.

- In this work, the step changes in the reported Umkehr records were minimized and the long-term difference from other records is within the measurement noise of compared Umkehr record. Some step-changes were however identified in 5 African Umkehr records when compared with the AGG (SBUV/OMP) overpass records. Therefore, to proceed with optimization of these records the history of the Dobson instrument calibrations needs to be acquired from station operators.

There are several more Dobson and Brewer Umkehr records that can be homogenized and used for satellite validations. Although Umkehr profiles are not highly resolved profiles like ozonesondes or lidar observations, they are performed more frequently than the once-a-week ozonesonde launches and they are performed during the day, when most of the satellite observations take place.

Plans for future work

Following the work completed within this project, we are planning on applying the Dobson optimization methodology to Brewer Umkehr observations in order to significantly reduce the observed biases in layers 6 and above. The Dobson Umkehr records in Africa can be also homogenized and provide ground-based reference for satellite validation over the region that has very limited ground-based observations.

Additionally, within the frame of a possible future QA4EO project, we are planning to use the Brewer and Dobson optimized datasets for the validation of the TROPOMI/S5P ozone profile product, that is expected to be released soon.

5 The Umkehr database

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 (please contact Dimitris Balis: balis@auth.gr and the PI of the instrument)

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- *BREWER #207 (Warsow, Poland):* Janusz Jarosławski, Institute of Geophysics, Polish Academy of Sciences, Department of Atmospheric Physics, Poland
- *BREWER #184 (Hradec Kralove, Czech Republic):* Martin Stanek, Solar and Ozone Observatory, Czech Hydrometeorological Institute, Hradec Kralove, Czech Republic

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