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# Umkehr ozone profiles in Thessaloniki and comparison with MLS overpasses

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# Introduction

Regular Umkehr measurements have been carried out in Thessaloniki, Greece (40.634° N, 22.956° E, 60 m altitude) since 1990. Afternoon measurements were performed with a single monochromator Brewer spectrophotometer (serial number 005; B005), type MKII and have been analyzed just partially in the past (Kosmidis et al., 2004). Recently, Thessaloniki's record have been re-evaluated with the modified O<sub>3</sub>BUmkehr processing software (V3.2; www.o3soft.eu), which is based on the UKM04 retrieval algorithm (Petropavlovskikh et al., 2005) and has been modified to take into consideration. In this study, we present analysis of Umkehr ozone profiles covering a 12-year period (2004 – 2015). The Umkehr profiles are compared with profiles from the Microwave Limb Sounder (MLS) instrument aboard the NASA's Aura spacecraft. Furthermore, we examine the dependence of the difference between the Umkehr retrievals and the MLS profiles from various factors, such as the distance of the MLS overpass to the ground station, the quality of the residuals (RMSE) and the measured TOC from the Brewer direct sun measurements. Finally, we investigate some of the parameters that affect the Umkehr retrievals, including the out of band stray-light and the temperature dependence of the ozone absorption coefficients.

# **Umkehr retrievals and comparison with MLS**

During an Umkehr measurement the Brewer records the zenith sky intensity at eight discrete wavelengths. The full set of eight Umkehr wavelengths includes 306.3, 310.1, 313.5, 316.8, 320.1, 323.2, 326.4, and 329.5 nm (nominal wavelengths). These measurements are performed during sunrise and sunset in a number of different solar zenith angles (SZAs), ranging from ~60° to ~92°. The measurements from two selected wavelengths centered at ~310 ("short" wavelength) and ~326 nm ("long" wavelength) form the so-called single-pair N-value (eq. 1) that is used for the ozone profile retrieval.

# **Factors affecting the difference**

Here we examine the dependence of the difference between the Umkehr retrievals and the MLS profiles from various factors, such as the distance of the MLS overpass to the ground station, the quality of the retrieved Umkehr profiles expressed as the root mean squared error of the residuals (RMSE) and the measured TOC from the Brewer direct sun measurements. An example for layer 4 (~20 – 25 Km) is given in Fig. 4. It can be opposed that the difference in this layer has a small dependence from the TOC (~5%/100 DU), which shows that there is a small annual dependence. The difference in the other layers exhibits a similar level of dependence from TOC, ranging from ~-10%/100 DU (layer 2) to ~5%/100 DU (layer 4). Although there is no obvious dependence from the distance of the MLS overpass from the ground-station, it can been seen that the scatter of the difference is higher for distances over 500 Km. However, this high scatter is evident for altitudes lower than ~25 – 30 Km (layer 5 and below), which are the layers that are affected by dynamics.

 $N(\theta) = 100 \times \log\left(\frac{I'(\theta)}{I(\theta)}\right)$ (1), where I' is the intensity at the "long" wavelength and I at the "short" wavelength.

The N-values are 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. The profile retrieval is reported in a 16-layer scheme (from surface to the top of the atmosphere) with each layer being ~5 Km thick. However, not all layers contain independent information (Petropavlovskikh et al., 2005) and here are analyzed in a 9-layer scheme (Table 1).

The Microwave Limb Sounder (MLS) is a limb-viewing spectrometer onboard Aura satellite observing microwave emission of molecules from 118 GHz to 2.5 THz. Ozone mixing ration (ppm) is derived from MLS radiance measurements near 240 GHz. The MLS data are reported in standard pressure levels in the range 261 – 0.02 hPa (Layer 2 and above), with a vertical resolution of ~3 Km (Livesey et al., 2011). The MLS data used in this study is version 3.2 and were obtained from NASA's MIRADOR web database (http://mirador.gsfc.nasa.gov/). Since MLS has a higher vertical resolution from Umkehr, the MLS ozone profiles were smoothed in the Umkehr layers using the Umkehr average kernels and a priori profiles (Miyagawa et al., 2009):

 $X_{sm}(j) = \sum_{k} \left\{ AK(j,k) x \left[ X_{t}(k) - AP(k) \right] \right\} + AP(j)$  (2), where j is the layer number,  $X_{t}(k)$  the MLS ozone profile in layer k, AP(k)the Umkehr a priori in layer k and  $\Sigma_k$  the integral of the smoothed differences in all layers.

For each day with available Umkehr retrieval, the closest (within an effective radius of 1000 Km) to the ground-based station daytime MLS profile was selected for the comparison. The comparison between Umkehr and MLS profiles is based on the period 2004 – 2015, with a total of 1057 coincident profiles. Fig. 1 shows the time series of the retrieved Umkehr profile for layer 4 (~20 – 25 Km) and the corresponding layer amount from MLS (upper panel, left), alongside with the annual cycle for the specific layer (upper panel, right), the frequency distribution of the layer ozone amount (lower panel, left) and the mean monthly bias between Umkehr and MLS (lower panel, right). It is obvious that the agreement between Umkehr and MLS for the specific layer is very good.



*Table 1.* Umkehr layers and their typical altitude range

Layer	Layer Boundary (km)	Pressure limits (hPa)
1	0-10	1013 – 253.25
2	10 - 15	253.25 – 126.63
3	15 – 20	126.63 - 63.31

3.96 – 0



Fig 4. Scatterplot of the difference between Umkehr and MLS for layer 4 as a function of the TOC (upper panel, right), of the RMSE of the residuals (upper panel, right) and the distance between the satellite overpass and the ground-based station (lower panel).

### **Effect of stray light and ozone effective temperature**

In order to investigate the Umkehr retrievals for the effects of stray light a whole year (2008) was analyzed with a previous version of the O<sub>3</sub>BUmkehr (V2.7) that didn't include a stray light correction. In V3.2 the measured slit function of B005 (Fig. 5) was modelled to include the effect of the stray light (wings) and was incorporated in the algorithm. An extra step of analysis includes the retrieval of the Umkehr profiles using the ozone effective temperature are calculated from the overpass MLS ozone and temperature profiles, instead of the climatological ones used in the retrieval algorithm. As can be seen in Fig. 6, the "actual" ozone weighted temperature (MLS) for Thessaloniki is on average 5-10°C lower than the one calculated from the climatological ozone and temperature profiles.

Fig 1. Upper panel: Time series of the ozone amount in Layer 4 from Umkehr and MLS (left) and annual cycle (right). Lower panel: Frequency distribution of the layer ozone amount from Umkehr and MLS (left) and mean monthly bias between Umkehr and MLS (right). The vertical error bars represent ±1 standard deviation of the mean.

Fig. 2 shows the mean bias for the whole period between Umkehr and MLS as a function of altitude (layer), while Fig. 3 shows the seasonal bias. The highest variability appears in UTLS (layers 2 and 3, between 10 and 20 Km), where both the Umkehr method and the MLS retrievals have some issues in their quality. Layers 4 and 5 (between 20 and 30 Km), where also the bulk of the ozone absorption occurs, shows the higher consistency with differences less than ±5%. Layers 6 and 7 shows a strong negative bias (~10%) for the Umkehr retrieval, which is possibly connected with not the complete rejection of the out-of-band stray light. The main conclusions are the same for each season.







Fig 6. Yearly evolution of — Umke MLS effective ozone temperature from the Umkehr ozone profiles climatological and temperature profiles and calculated (blue) from the MLS ozone and temperature profiles (red). 008 2008.1 2008.2 2008.3 2008.4 2008.5 2008.6 2008.7 2008.8 2008.9 2009

It is obvious (Fig. 7) that the stray light correction improves the agreement with the MLS profiles (from ±20% initially to ±10%). While the stray light correction effect is evident in all layers, it is less pronounced in layers 4 and 5. For most months the bias in the lower layers (2, 3 and 4, from ~10 to ~25 km) is negative, while in the upper layers (5, 6 and 7, ~25 to ~40 km) is positive. The difference in the layers 6 and 7 remains significant high negative, which possible indicates that the empirical correction for the stray light effect doesn't reject all the out of band stray light. The correction for the temperature dependence of the ozone absorption coefficients with the "actual" effectiv e temperature instead of the one based on the climatol ogical profiles has a minor effect.

**Fig 7.** Monthly mean difference (%) between the derived ozone profiles and the MLS with (blue) and without (red) including correction for the stray light, and additionally with correction for the "actual" ozone effective temperature (green). The dashed lines show the  $1\sigma$  limits.

Fig 2. Vertical distribution of the mean profile difference between Umkehr and MLS for the period 2004 – 2015. The dashed lines show the  $\pm 1$ standard deviation

## Conclusions

- Quite good agreement overall with MLS (±10%)
- Best agreement for layers 4 and 5 (between ~20 and 30 km)
- Highest variability in ULTS (layers 2 and 3)
- Negative bias in layers 6 and 7. Possible connected with no full rejection of the whole out of band stray light.
- The difference between Umkehr and MLS has small dependence from TOC
- Very important the effect of the stray light (between -14 and 8%, depending on the layer), which is in accordance with Petropavlovskikh et al. (2011)
- Minor effect of the effective temperature, similar with Petropavlovskikh et al. (2011)

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