

Replies to Referee #1 on the manuscript 'Retrieval of ozone profiles from OMPS limb scattering observations' by C. Arosio et al.

We thank the reviewer for the time he spent commenting on the paper. In the text below, we address the comments from the referee #1. Referee's comments are shown in italicized font and authors' responses are highlighted in blue.

==== General comments

This paper introduces ozone profile retrievals from scattered radiance spectra in the ultraviolet and visible measured by OMPS Limb instrument using a regularized inversion technique. A three kinds of reference data sets (MLS, NASA OMPS-LP O3P, Ozonesonde) are used to assess their retrieval product. The verification results of this product are so interesting and important because this product will be merged with the SCIAMACHY ozone profiles, based on the same algorithm, to create a long-term data set. However, this reviewer would like to comment that the authors should consider deepening strongly the discussion about the OMPS limb Ozone Profile retrievals to convince potential data users of the data quality. Especially, the applied implementations in the retrieval process are mostly adopted from the SCIAMACHY v3.0 ozone retrieval with small modification, this paper should provide reliable results for the verification of the data product to be published. If not, they well show what big efforts they made to optimize/improve the OMPS limb ozone profile retrievals, different from the original algorithm.

Considering a very different spectral resolution of the two instruments and technical differences in the measurement procedure, e.g. in terms of spectral channels, wavelength ranges, atmospheric/scene sampling and radiance collection, it was not possible to apply the SCIAMACHY retrieval scheme to OMPS-LP measurements without significant changes. As a consequence, the algorithm presented in this manuscript has been newly developed starting from the one used for SCIAMACHY. However, the same radiative transfer model (SCIATRAN), a similar retrieval approach and the same spectroscopic and atmospheric parameters databases were used to minimize the systematic errors between the data sets and thus facilitate their merging. We have added a paragraph in the introduction explaining the adjustments of the algorithm in more detail.

To provide a more reliable validation of our product without completely changing the paper structure, we considered the whole 2016 data set, increased the number of latitude bands and updated all the figures in section 4.

Furthermore, we extended the description of the retrieval characterization and of the validation results.

1. Page 3, 21-23: Limb observation cannot see below lower stratosphere due to limited field of view and much strong interference with clouds.

The sentence has been reformulated as: 'The accuracy/sensitivity of limb measurements decreases with the altitude in the lower stratosphere and troposphere, as the increasing optical thickness along the line of sight leads to a saturation of the measured signal. The presence of clouds in the field of view acts as an additional limitation.'

2. Figure 7 (right panel): Why the retrieval errors are maximum at minimum solar zenith angles below 25 km and above 45 km in the retrieved altitude range? This retrieval characterization could be related to the maximum errors in lower stratosphere and upper atmosphere over the tropics compared to middle latitudes, shown in all comparison results.

Fig. 5 (former Fig. 7) has been updated to show in more detail the latitude (i.e. solar zenith angle) dependence of the relative precision and vertical resolution of the retrieval scheme. We notice the degrading precision in the UTLS region, particularly in the tropics. This is related to the low ozone concentration at these altitudes and latitudes, leading to relative errors up to 10-30%. This purely random uncertainty cannot be directly related to the systematic bias we found below 20 km in the comparison with the other data sets, as the random error is expected to be significantly reduced when averaging the profiles. For example, considering 10000 profiles over the validation period in the tropics and a relative precision of 30 % for each single profile, the random uncertainty on the averaged profile is equal to 0.3 %. However, the large standard deviation in the UTLS region shown in the validation section plots reflects a large variability of the ozone profiles and a lower retrieval sensitivity at these altitudes. This explanation has been added to the retrieval characterization section of the manuscript.

3. This author should demonstrate or intensively discuss that this product have the accuracy/precision at least comparable to NASA OMPS-LP O3P product. This point is most interesting part for data users to determine which data set they should use. Especially, the comparisons between IUP-OMPS and NASA-OMPS shows a significant bias of 10 % for most altitude, up to 20 % at the bottom level. I think that this difference is very huge considering the products derived from same satellite measurements and a very good vertical resolution of this instrument. This authors provide a detailed description about NASA-OMPS product, but did not discuss why two OMPS limb products have a big difference, especially in the lower stratospheric region over the tropics. So this paper should apply the comparisons with reference data set to both IUP and NASA OMPS products under the exactly same condition. The NASA v2.5 limb data product is available for the whole period. This comparison could give an insight into the strength/weakness of the retrieval algorithm for a better understanding on the retrievals.

We agree with the reviewer that a thorough comparison with the NASA product would be interesting also for data users. However, the introduction of a triple comparison of IUP and NASA OMPS results with those from MLS, instead of two separate comparisons, would require a complete restructuring of the paper, without contributing significantly, in our opinion, to the scientific value of the manuscript. A dedicated paper devoted to the validation of NASA results and comparison to other OMPS-LP retrievals is currently in preparation by the NASA team and we are also contributing to this work. Including the same results in our paper will cause a double work load without any additional outcome. Since the data quality of NASA product has not yet been assessed in a peer reviewed paper, the reviewer's requirement for our product to 'have the accuracy/precision at least comparable to NASA OMPS-LP O3P product' cannot be directly met at this stage, without performing a full validation of the NASA data set from our side. Furthermore, the main topic of the paper is to present an ozone retrieval algorithm which is optimized for merging with the SCIAMACHY data set. In comparison to the NASA retrieval, this task is achieved to a large extend by providing continuous profiles for the whole altitude range and minimizing systematic errors by using a similar retrieval approach and same data bases for atmospheric and spectroscopic parameters. This is now also clearly stated in the paper. In this respect we do not see us in competition with NASA. This is why we are mainly interested in the absolute accuracy of our retrieval and consider the validation of NASA profiles outside our scientific focus. To our opinion the absolute accuracy of our retrieval is well characterized by comparisons with MLS and sondes: the found agreement within 5-20 %, depending on altitude and latitude, is in a common range achieved in other studies (Mieruch et al., 2012; Tegtmeier et al., 2013; Zawada et al., 2017).

The discrepancies between IUP and NASA profiles, shown in Fig. 6 (former Fig. 8), of about 2-8% above 20 km and up to 20% below 20 km are mainly caused by differences in the used spectral

ranges and in the retrieval approach: NASA algorithm considers spectral points following the triplet method whereas we fit entire spectral windows. In addition, in the NASA product UV and VIS retrievals are kept separated while we try to merge the two spectral ranges around 30-35 km. These facts contribute to a different sensitivity of the retrieval to possible random and systematic errors. Unfortunately, it is not possible to identify and relate each discrepancy at different altitudes to specific settings of the 2 algorithms: it is not feasible to adjust the settings step by step, because the intermediate retrieval versions would result in oscillating or non-converging solutions. From the theoretical point of view, both methods are equally justified and there are no reasons to prefer one to the other, with the exception of the continuity of the IUP profiles.

To meet the reviewer's point about 'comparisons with a reference data set of both IUP and NASA products under the exactly same condition', we considered the same sub-sample of data used for the validation against MLS to produce a plot similar to Fig. 6 (former Fig. 8). That is, only OMPS states collocated with MLS observations were taken into consideration. The reviewer can find the result in Fig. 1. Comparing these two panels with the plots in the paper, no significant differences are found.

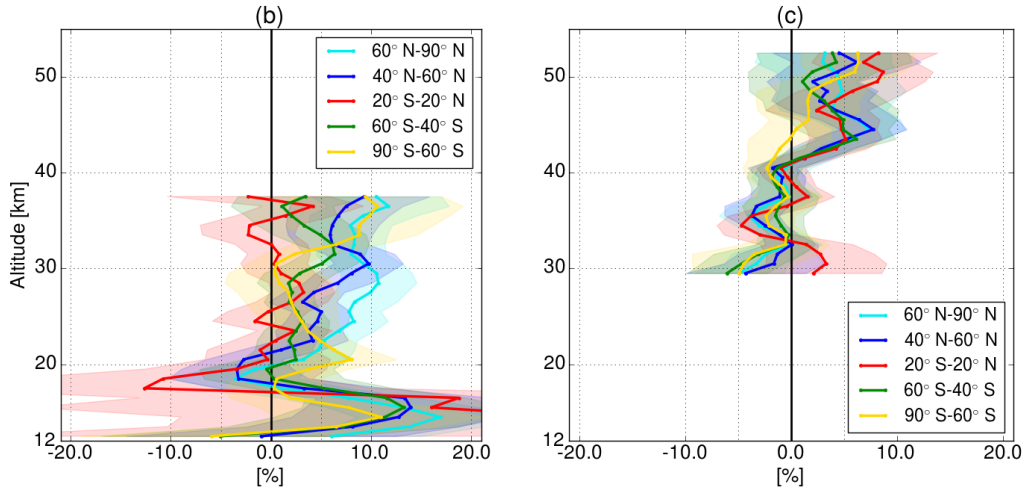


Figure 1: Relative differences between IUP and NASA profiles for the Vis (b) and UV (c) retrievals in five latitudinal bands (60° N-90° N, 40° N-60° N, 20° S-20° N, 60° S-40° S and 90° S-60° S). Only the measurements collocated with MLS are considered.

4. Fig 9: The author just introduce the Fig 9, as following, “ Fig.9 shows the averaged profiles for the tropics and relative differences in the three latitude bands “, but there is nothing related discussion. Please deepen the discussion about the presented figure, which is corresponding to most figures. Generally, this paper tends to provide a huge description about data and methodology used in the comparison and very simple/light discussion about the comparison results.

A discussion of this figure and a comparison with Fig.7 (former Fig.9) have been added. We did our best to extend and improve the descriptions of the other figures as well.

5. Fig 10: The author described that the positive errors above 35 km in NH high latitude during the northern polar summer season are caused due to the presence of the PMC and its sub optimal screening process. If so, why this PMC-induced positive errors are not shown in the SH high latitude during the SH polar summer season (December and January). Based on Bak et al. (2016), OMI UV ozone profiles show systematic PMC-induced errors during both polar summer season and the PMC detection flags systematically works for both Polar areas even though a

relatively weak sensitivity of OMI nadir UV measurements compared to limb UV measurements. This IUP OMPS algorithm should be improved in screening the PMC affected pixels because this PMC-induced biases could impact on the long-term data analysis.

We agree with the referee. The PMC detection flag has been updated to optimize the results in the northern hemisphere. We updated Fig. 8 (former Fig. 10) in the manuscript and its description accordingly.

6.Comparison with ozonesonde: this paper insist that “the lack of stations presents a meaningful comparison over this short time span or validation is less significant because only two ozonesonde stations are available within the considered time span”. If so, this paper should not use the ozonesonde dataset for validating the OMPS dataset or increase the validation period because the OMPS radiance dataset are available for the whole period.

We believe that ozonesondes are a very important validation tool: the high accuracy of these measurements in the troposphere and lower stratosphere is particularly valuable for the comparison of our results over the UTLS region. The sentence quoted by the reviewer referred only to high polar latitudes and mid-latitudes in the southern hemisphere. Considering the extended validation period, the number of available ozonesondes increased significantly and a validation also at northern and southern high-latitudes become possible. We updated the figures and the descriptions accordingly.

7.Please simply the section 2, more maybe within 1 page, focusing on parts required to introduce this algorithm and to discuss the retrieval results. This part contain 5-6 pages among 23 pages. But, this part is rarely referred in other sections.

We see the point of the reviewer and already simplified this section during the first revision of the manuscript. We did our best to get it even shorter, now down to 3 pages (including pictures): we think that an introduction of the instrument, its geometry and the issues related to pointing and stray light is important to understand the retrieval implementation and results.

8.12 page: “As the shift and squeeze correction algorithm works with the differential absorption structures, it cannot be applied in the UV range”. It is hard to understand because the Huggins ozone absorption bands have notable differential absorption structure. The corresponding explanation has been added in the manuscript.

Due to a relatively low spectral resolution of the OMPS Limb Profiler, the differential absorption structure in the Huggins band is largely smoothed out and our algorithm works in the UV range with radiance slope or radiance itself. This explanation has been added to the text.

9.15p page, 24 line: “The aerosol retrieval is particularly important at latitudes where the scattering angle is high”, why ? Please more description using the presented figure 5.

The aerosol scattering phase function has a strong forward peak, so that a correct description of the aerosol scattering is particularly important at high northern latitudes where the scattering angle is small. The sentence has been modified and corrected in the paper as 'Because of the strong forward peak of the aerosol scattering phase function, a correct description of the aerosol scattering is particularly important at high northern latitudes where the scattering angle is small'.

10. *In retrieval characterization, this paper just deals with the retrieval errors related to measurement random-noise errors, but discuss the effect of smoothing errors on the comparisons with high-resolution reference dataset. It is not consistent, so it is good to include the retrieval errors related to smoothing errors in section 4.1*

In section 4.1 we are not dealing with smoothing errors related to the retrieval algorithm and the Tikhonov regularization constraint. The 'smoothing' procedure is applied to the ozonesondes profiles in order to match the vertical resolution of OMPS profiles. In order to avoid confusion, instead of 'AK smoothing' we now call it 'AK convolution': this is what we indeed perform, a convolution of the high-resolution ozonesonde with the AK of the retrieval scheme. Applying this procedure, the error related to the different vertical resolutions of the compared profiles is accounted for.

Minor comments *A few editing correction is suggested and this paper should be more carefully edited.*

The paper has been carefully checked.

P1 14L: below top levels : levels \rightarrow level

The sentence has been partially changed: 'The typical vertical resolution of the retrieved profiles varies from ~ 2.5 km at lower altitudes (< 30 km) to ~ 1.5 km about 45 km and becomes coarser at upper altitudes.'

P2, 9L : it determines the tropopause height : it is partly true, but the contribution of ozone on tropopause determination is not major.

The sentence has been changed to: 'It plays a crucial role in the radiative budget of the stratosphere, determines the stratospheric temperature profile and impacts on atmospheric circulation and climate.'

P2, 14: the discovery of the springtime ozone hole in Antarctica research grew in this field: this sentence is not clearly written.

The sentence has been changed to: 'Because of its relevance to both science and society, ozone-related researches expanded after the discovery of the springtime ozone hole in Antarctica and the subsequent recognition that man-made release of chlorofluorocarbon compounds depletes the stratospheric ozone layer.'

P13, 13 : each iteration \rightarrow i th iteration

Change to 'each i -th iteration'.

P14, 6: The CI is defined as the ratio of

Done.

P 14, 8: delete "an altitude dependent quantity and "

Done.

P15, 3-8: revise this paragraph using "The presence of PMCs can affect limb radiance down to 40 km, causing an interference with ozone retrievals. Therefore, we screen out the PMC contaminated pixels in this study using the PMC detection flag in high latitudes below 50 N and below 50 S where the PMC occurrence is most frequent. PMCS are detected using the radiance profile around 353 nm if the radiance between 40 km and 80 km increases in two consecutive layers at least because radiances decrease monotonically with height in this altitude range under

clear sky condition.”

The paragraph has been accordingly revised and partially updated.

P15: 11-13: revise this sentence using “To be optimized for OMPS aerosol retrieval, the wavelength is changed from 750 nm for SCIAMACHY to 868.8 nm for OMPS because the influence of the O₂ absorption at 750 nm becomes significant due to the OMPS’s coarser spectral resolution.

Sentence reformulated as: ‘As a consequence of a coarser spectral resolution, the radiance measured at 750 nm is affected by the O₂ absorption band. For this reason the OMPS aerosol extinction coefficient retrieval uses the radiance at 869 nm instead of 750 nm, as it was done for SCIAMACHY and OSIRIS.’

P16, 8 : with a peak around 35 km → with a worst resolution around 25 km.

Changed to ‘getting worst around 33 km’.

Figure: the bottom level of y-axis is marked in all figures.

If we understand correctly, the reviewer asked us to put a label at the y-axis lower altitude in all plots. This has been done in the revised manuscript.

References

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Retrieval of ozone profiles from OMPS limb scattering observations

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Abstract. This study describes a retrieval algorithm developed at the University of Bremen to ~~retrieve-obtain~~ vertical profiles of ozone from limb observations performed by the Ozone Mapper and Profiler Suite (OMPS). This algorithm ~~was-is based on~~ the technique originally developed for use with data from the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) instrument. As both instruments make limb measurements of the scattered solar radiation in the Ultraviolet (UV) and Visible (Vis) spectral ranges, an underlying objective of the study is to obtain consolidated and consistent ozone profiles from the two satellites and to produce a combined data set. The retrieval algorithm uses ~~altitude-normalized~~ radiances in the UV and Vis wavelength ranges ~~to-normalized to the radiance at an upper tangent height to~~ obtain ozone concentrations in the altitude range of 12–60 km ~~altitude-range~~. Measurements at altitudes contaminated by clouds in the instrument field of view are identified and filtered out. An independent aerosol retrieval is performed beforehand and its results are used to account for the stratospheric aerosol load in the ozone ~~retrieval~~inversion. The typical vertical resolution of the retrieved profiles varies from ~ 2.5 km at lower altitudes (< 30 km) to ~ 1.5 km about 45 km and becomes coarser at upper altitudes ~~(from 40 to just below top-levels)~~. The retrieval errors resulting from the measurement noise are estimated to be ~~1–5~~1–4 % above 25 km, increasing to ~~10–15 % below 20~~. ~~OMPS ozone profiles are retrieved for seven months, from July 2016 to January 2017.~~ 10–30 % in the upper troposphere. OMPS data are processed for the whole year 2016. Results are compared with ~~NASA ozone profile the NASA~~ product and validated against profiles derived from passive satellite observations, or measured in situ by ~~balloon-borne in situ~~balloon-borne sondes. Between 20 and ~~50~~60 km, OMPS ozone profiles typically agree with data from the Microwave Limb Sounder (MLS) v4.2 within 5–10 %, ~~with the exception of high northern latitudes ($> 70^\circ$ N above 40) and the tropical lower stratosphere~~ whereas in the lower altitude range the bias becomes larger, especially in the tropics. The comparison of OMPS profiles with ozonesonde measurements shows differences within ± 5 % between ~~14~~13 and 30 km at northern ~~mid-latitudes~~mid- and high-latitudes. At southern ~~mid-latitudes~~mid- and high-latitudes, an agreement within ~~5–10~~5–7 % is ~~achieved, although these results are less reliable because of a limited number of available coincidences~~ also achieved in the same altitude range. An unexpected bias of approximately ~~10~~10–20 % is detected in the ~~tropical region at all altitudes~~lower tropical stratosphere. The processing of the 2013 data set using the same retrieval settings and its validation against ozonesondes reveals a much smaller bias; ~~possible reasons~~ a possible reason for this behavior ~~are under investigation~~ is discussed.

1 Introduction

Ozone is one of the most important trace gases in the atmosphere. It is most abundant in the stratospheric ‘ozone layer’, which absorbs strong ultraviolet (UV) radiation, heating this atmospheric region and acting as a protective layer against biologically harmful radiation. It plays a crucial role in the radiative budget of the stratosphere, determines the tropopause height and thus also impacts on climate. After the stratospheric temperature profile and impacts on atmospheric circulation and climate. Because of its relevance to both science and society, ozone-related researches expanded after the discovery of the springtime ozone hole in Antarctica and the subsequent recognition that man-made release of chlorofluorocarbon compounds depletes the stratospheric ozone layer (Molina and Rowland, 1974) and the discovery of the springtime ozone hole in Antaretica (Farman et al., 1985), research grew in this field because of its relevance to both science and society (Molina and Rowland, 1974; Farman et al., 1985). Although nowadays the stratospheric ozone chemistry is generally well understood, there are still several issues to be clarified. These are related to the expected ozone recovery after the adoption of the Montreal protocol, stratospheric responses to changes in tropospheric radiative fluxes and temperatures circulation and temperature responses to the increase of greenhouse gases (Li et al., 2009) as well as long term ozone trends. For example, Solomon et al. (2016) focused the attention on the Antarctic region, investigating possible signatures of an ozone healing. Analyzing observations collected each September since 2000, the authors suggested that the fingerprints of an ozone recovery can be identified in both the increase of its column amount and in the decrease of the areal extent of the ozone hole.

The issues related to changes in the Brewer Dobson Circulation (BDC), possibly linked to climate changes, have been investigated by several studies, which consider the ozone concentration in the lower stratosphere a good proxy to track changes in the stratospheric circulation. Among them, Aschmann et al. (2014) used combined ozone time series from satellite instruments and ozonesondes to investigate changes in the BDC after the beginning of the century and identified an asymmetry in the BDC northern and southern branches. Stiller et al. (2017) suggested a shift of the subtropical mixing barriers as an explanation for this asymmetry.

For all these kinds of studies, reliable long-term data sets are needed from both ground-based and satellite instruments. Recent attempts to consistently merge a large number of different data sets into long-term time series are reported by Froidevaux et al. (2015) and Davis et al. (2016) both including also other species than ozone. Steinbrecht et al. (2017) and Sofieva et al. (2017) focused on ozone trends, revealing a global statistically significant increase in its amount after 2000 above 35 km. Other authors, as Kyrölä et al. (2013), Eckert et al. (2014), Gebhardt et al. (2014) and Nedoluha et al. (2015) pointed out an unexpected decadal negative trend in the ozone abundance in the upper tropical stratosphere.

During the last few decades, several remote sensing observation techniques have been used to derive ozone concentrations from the troposphere up to the mesosphere (Hassler et al., 2014). Following the birth of the space age, instrumentation of different kinds began to be developed. Space-borne remote sensing measurements in the Ultraviolet-Visible (UV-Vis) spectral range have traditionally been of two types: nadir viewing and solar occultation spectrometers; the former instruments point downward and are characterized by a good horizontal coverage, whereas the latter look directly into the solar disk, featuring a good vertical resolution and a strong signal. The limb sounding technique, widely used by more recent satellite instruments,

combines the advantage of these two: the long path through the atmosphere provides a high sensitivity to trace gases and the variation of the observation angle enables a better vertical resolution with respect to the nadir geometry, featuring a much higher horizontal sampling as compared to the occultation measurements. Limb observation geometry has also been used to measure scattered solar radiance and/or atmospheric emission in the InfraRed (IR) and microwave spectral regions. Using the scattered solar light, measurements during daylight only are possible, whereas, using the emission signatures, observations can be performed during both day and night. ~~With decreasing altitude the atmosphere becomes more opaque, which results in a decreasing sensitivity of the limb scatter measurements in the troposphere~~The accuracy/sensitivity of limb measurements decreases with the altitude in the lower stratosphere and troposphere, as the increasing optical thickness along the line of sight leads to a saturation of the measured signal. The presence of clouds in the field of view acts as an additional limitation.

The limb scatter technique was for the first time successfully exploited by the LORE/SOLSE (Limb Ozone Retrieval Experiment/Shuttle Ozone Limb Sounding Experiment) instrument launched in 1997 by NASA. Two instruments followed this mission: the Optical Spectrograph and Infrared Imager System (OSIRIS) launched in February 2001 (Llewellyn et al., 1997) and the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY), launched in March 2002 (Burrows et al., 1995; Gottwald and Bovensmann, 2011). SCIAMACHY made observations in the UV, Vis, Near InfraRed (NIR) and Short Wave InfraRed (SWIR) spectral ranges till April 2012, when the platform-to-ground communication was lost. A few aging satellite instruments, such as OSIRIS and the Microwave Limb Sounder (MLS), are still operating, contributing to the task of continuous monitoring the stratospheric ozone. At the end of 2011, just a few months before the end of ENVISAT lifetime, the Ozone Mapping and Profiler Suite (OMPS) instrument was launched on board the Suomi-National Polar-Orbiting ~~Operational Environmental Satellite System Preparatory Project Partnership~~(SNPP) platform and it is still operational (Flynn et al., 2014). The spacecraft has a nominal 13:30 local time ascending sun-synchronous orbit and flies at a mean altitude of 833 km. Scientific data collection started at the beginning of 2012. OMPS comprises three instruments: the Nadir Mapper, Nadir Profiler and Limb Profiler (LP). Only the latter is of interest for our study (see Flynn et al., 2014, for a review of the full suite).

After the launch of the satellite, the NASA team developed a retrieval chain to derive ozone profiles and many by-products from OMPS limb observations, which are publicly available. Besides, at the University of Saskatchewan a 2-D geometry retrieval has been applied to OMPS-LP measurements (Zawada et al., 2017).

This paper presents ozone profile retrievals from OMPS-LP observations performed at the University of Bremen. The algorithm we use was ~~adapted from~~developed based on the SCIAMACHY v3.0 ozone retrieval (Jia et al., 2015). As the two instruments have a very different spectral resolution and the measurement techniques differ in many respects, e.g. in terms of spectral channels, wavelength ranges, atmospheric/scene sampling and radiance collection, a direct application of the SCIAMACHY retrieval scheme to OMPS-LP measurements was not possible. Although the algorithm presented in this manuscript has been newly developed starting from the one used to process SCIAMACHY data, the same radiative transfer model, a similar retrieval approach and the same spectroscopic and atmospheric parameters databases were used to minimize the systematic errors between the data sets. The underlying objective of the study is the creation of a consolidated ~~data-set~~product and the merging of the ~~OMPS~~OMPS-LP and the SCIAMACHY time series, in order to obtain a long-term contin-

uous data set. In Sect. 2, the OMPS instrument is introduced: its geometry of observation, relevant characteristics and issues related to the retrieval of ozone are briefly discussed. The third section is focused on the retrieval methodology, starting with a general description of the inversion algorithm used in this work. A more detailed characterization of the retrieval procedure follows, including the applied cloud filter and the approach to consider aerosol extinction profiles. Sect. 4 presents at first a comparison with NASA ozone profile retrieval algorithm; then MLS and ozonesonde data sets are used for a first-validation of our resultsproduct. Main results, remaining issues and possible future improvements are addressed in the conclusions.

2 OMPS-LP instrument

2.1 General features and main issues

The main objective of OMPS-LP is to monitor the ozone vertical distribution within the Earth middle atmosphere at high accuracy level. It images the Earth atmosphere by viewing its edge (limb) from space. The closest approach of the sensor line of sight to the Earth surface is referred to as Tangent Point (TP) and the altitude of this point above the Earth geoid is called Tangent Height (TH); the limb geometry is schematically drawn in the left panel of Fig. 1.

The OMPS-LP sensor views at the Earth limb backwards with respect to the flying direction, through three vertical slits: the central one is aligned along the nadir track, whereas the other two are cross-track, separated horizontally by 4.25° , which corresponds to 250 distance between the TPs. With respect to the satellite. As shown in the right panel of Fig. 1, the TPs are located on the East, around about 25° latitude South of the sub-satellite point. The geometry is drawn in Fig. ?? The spacecraft completes 14–15 orbits per day and the instrument performs normally 180 limb observations (referred to as states) per orbit, around 160 of which with solar zenith angle less than 80° .

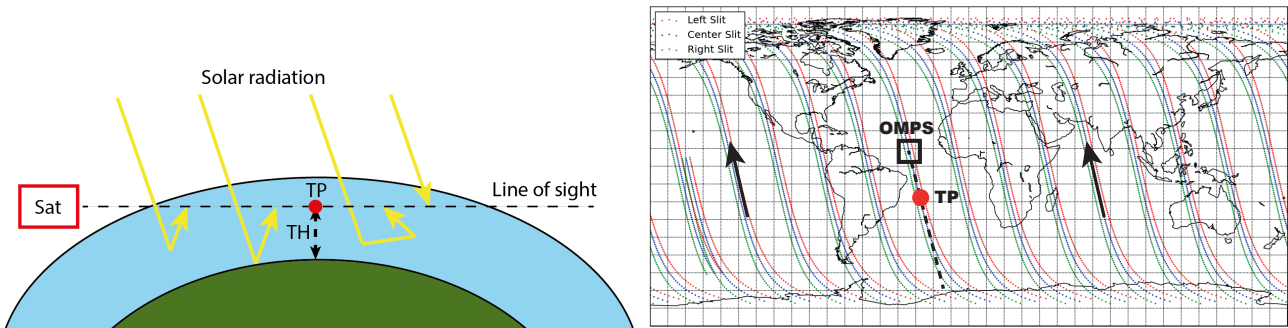


Figure 1. Left panel: schematic diagram of the viewing geometry of a satellite limb observation, showing the so called Tangent Point (TP) and its height above the Earth, or Tangent Height (TH). Right panel (adapted from Bhartia et al., 2013): OMPS daily orbits and observation geometry sketch; black arrows indicate the satellite flight direction and the red dot approximately locates the Tangent Point (TP). Adapted from Bhartia et al. (2013).

OMPS-LP measures limb scattered radiance in the spectral range of 280–1000 nm. A particular characteristic of this instrument is the use of a prism spectrometer instead of a grating disperser. The employed prism provides a spectral resolution that

degrades with the wavelength, from 1 nm in the UV region up to 40 nm in the NIR. OMPS-LP observes the full altitude range at the same time, without vertical scanning: each, and radiance is collected by means of a Charge-Coupled Device (CCD). Each slit covers a vertical range of 112 km, with an instantaneous the instantaneous vertical field of view of each detector pixel is about 1.5 km and a sampling of the vertical sampling is 1 km at TP (Jaross et al., 2014). Radiance is collected by means of a Charge-Coupled Device (CCD). The use of such a technology the CCD detector poses a great challenge as regards the dynamic range: indeed, due to the decrease of the atmospheric density, scattered solar radiance radiation from the Earth limb decreases by at least five orders of magnitude along the considered vertical range. Therefore, in order to cover the required dynamic range, four images at a 2-D physical CCD are taken for each slit: the full atmosphere is imaged at two integration times (that differ by a factor 30) and through a large and a small aperture (Jaross et al., 2014). Since the down-link rate is by far slower than the data collection rate, only a selected number of pixels from these four images can be transferred. Then, ground processing is Ground processing is then needed to select unsaturated signals and combine down-linked pixels from different images in a single radiance file. The combined image features a non-uniform wavelength and TH grid (spectral and vertical smile), therefore it is, that is finally re-sampled and mapped onto a regular grid. Left panel of Fig. 2 shows examples of radiance profile, displaying the large dynamic range of measured values. The gridding procedure is performed using a bi-linear interpolation and pixel-to-pixel calibration errors linked to this consolidation procedure are estimated to be around 1%. As radiance measured at large and small aperture can differ by several percent, radiance profiles at a specific wavelength are derived from one aperture only; on the contrary, a better consistency is found between long and short integration time, so that they are combined at different altitudes to get each radiance profile. Fig. ?? shows, whereas the right panel depicts examples of spectral signal-to-noise ratio (SNR) at different altitudes. Jumps in this plot are related to changes of the sampled image the switch between the sampled images: for example, the jump between large and small aperture that occur at 450 nm (fixed threshold). In the retrieval scheme we were careful take care not to consider spectral ranges crossing this fixed boundary.

2.2 Calibration and main issues

One of the most important issues that affects the quality of the limb scattering technique is the TH registration. In order to retrieve reliable ozone profiles, the TP altitude has to be known with high precision: in fact, a 200 uncertainty in the TP height translates into a 5 % error in the ozone profile. Such a high The required high pointing accuracy cannot be directly reached for OMPS-LP sensor, because the star-tracker on board the SNPP satellite is mounted on a distant position from the instrument, so that thermal effects and mis-alignments of the instrument focal plane play an important role.

To solve this problem, two methods called Rayleigh Scattering Altitude Sensing (RSAS) and Absolute Radiance Residual method (ARRM) are implemented by the NASA team in the several pointing corrections are established during the level 1b gridded (L1G) data processing (Moy et al., 2017), as described in Moy et al. (2017):

1. Fixed adjustments between 1 and 2 km are applied independently for each slit, meaning that the instrument points at altitudes higher than expected. A, depending on the slit.

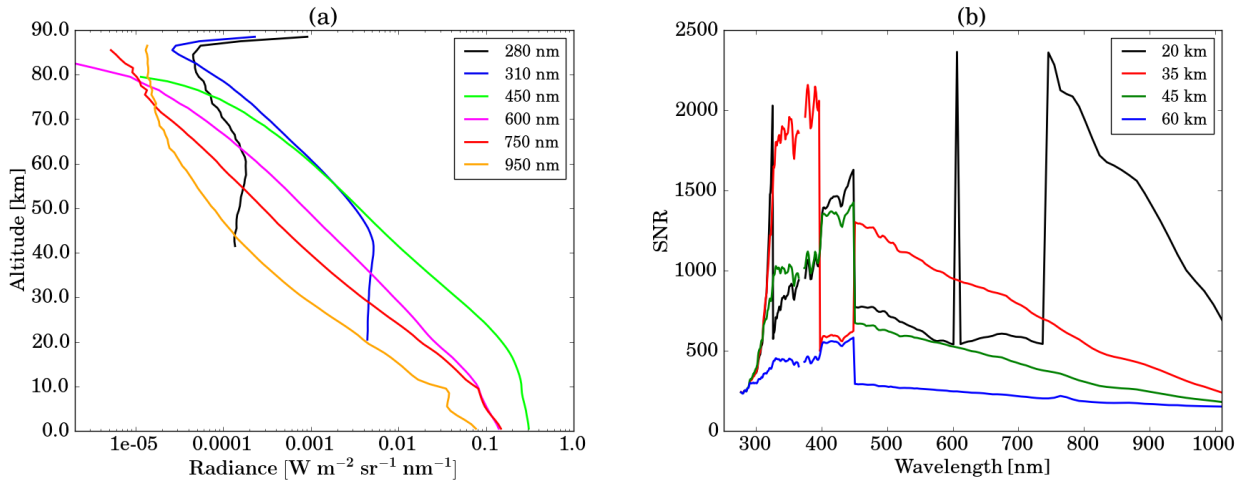


Figure 2. ~~Example~~ Left panel: ~~example~~ of OMPS-LP radiance profiles at some selected wavelengths; right panel: OMPS-LP signal-to-noise ratio (SNR) at different tangent heights.

2. TH variation related to the heating up of the instrument ~~is detected when the instrument, as it~~ approaches northern mid-latitudes. ~~It is accounted for in L1G data applying a latitudinal dependent correction on the order of 500 for every orbit. This correction remains the same for every orbit. A further dynamic TH variation was detected~~
3. Dynamic TH variation within each orbit, ~~with~~ characterized by an almost linear dependence with ~~latitude. The current estimate is around 400 change between the South and the North Pole. A state number.~~

While the first two are implemented in the current v2.5 version of L1G data, a satisfactory explanation for this the latter variation still has to be found and this effect is not currently corrected neither in L1G data nor in our retrievals currently not accounted for. However, following NASA recommendations in (DeLand et al., 2017), we implemented a linear TH adjustment as a function of latitude, with values ranging from +300 m at the South Pole till -100 m at the North Pole.

- 10 The second important issue that affects the accuracy of the limb radiance is the so-called stray light. The general phenomenon of stray light describes photons that are registered by the detector at wavelengths or altitudes which they do not belong to. ~~There are several causes of the stray light.~~ For example, with multiple images on a single detector, photons from the IR part of one slit can be scattered into the UV part of the neighboring image. This problem was reduced with both a thorough study of the point spread function during the pre-launch operations and the careful application of cutoff filters at the focal plane (Jaross et al.,
- 15 2014). Stray light is mainly an issue at high altitudes, with levels that are usually less than 10 % of the measured value ~~and tend to increase with the altitude for the same wavelength.~~

~~The CCD used for detection of photons for OMPS-LP operates at -45 °C to minimize dark current and other noise sources. Dark current and non-linearity of the sensor are corrected accurately and introduce minor errors in the reported radiance.~~

Transient events can affect the instrument reliability: energetic charged particle can penetrate through the CCD shielding and cause transients in pixel signal. Such events are frequent in the so-called South Atlantic anomaly.

~~In this paper, version 2.5 of OMPS-LP LIG data has been used without any additional pre-processing related to stray light and pointing. The treatment of stray light has been improved with respect to the previous version and pointing corrections implemented as discussed above. In addition, both sun-normalized and absolute radiances are provided.~~

2.2 OMPS-LP observation geometry

Several angular coordinates are needed in the retrieval algorithm to correctly describe the observation geometry; satellite azimuth (φ), solar azimuth (φ_0) and solar zenith angle (ψ_0) at the TP are reported for three THs (25, 35 and 45 km) in the LIG data files and are used to define the geometry of the observation. The solar zenith angle (ψ_0) is defined as the angle between the local vertical at the TP and the sun pointing vector. The azimuth angles (φ and φ_0) are defined as the angles between the direction to North Pole and the projections of the solar beam and the instrument line of sight, respectively, on the plane orthogonal to the normal vector at the TP.

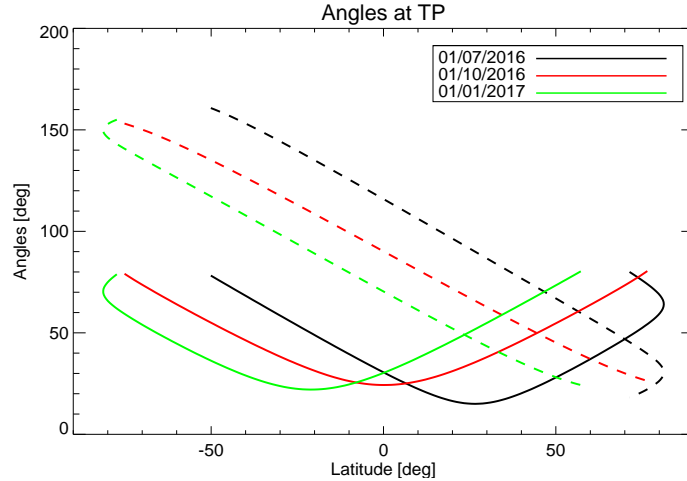


Figure 3. Solar zenith angles (solid lines) and scattering angles (dashed lines) at the TP along three OMPS orbits on the following dates: Jul 1, 2016, Oct 1, 2016 and Jan 1, 2017.

Combining azimuth and zenith angles, the scattering angle θ at the TP can be computed as:

$$\cos(\theta) = \sin(\psi_0) \cos(\varphi - \varphi_0) \quad (1)$$

This is an important quantity that defines the scattering geometry. In Fig. 3 values of scattering angles together with solar zenith angles are plotted as a function of latitude for three OMPS orbits in different seasons. Solar zenith angles are shown as solid lines, with symmetric values with respect to the equatorial region, whereas scattering angles are plotted as dashed lines. Only solar zenith angles less than 80° are plotted and the ozone retrieval is run only for the corresponding states, usually 140 per orbit, to avoid high stray light levels. The latitude coverage in different seasons can be assessed from the figure.

3 Retrieval method

3.1 Theoretical basis

The retrieval of ozone profiles is performed using the regularized inversion technique with the first order Tikhonov constraints (Tikhonov, 1963; Rodgers, 2000). The non-linearity of the inverse problem is accounted for using an iterative approach. The forward modeling takes into consideration atmospheric multiple scattering in the framework of the approximate spherical solver of the SCIATRAN radiative transfer model (Rozanov et al., 2014). Thereby, the CDI (Combined Differential-Integral) approach is employed to solve the radiative transfer equation: first, the entire radiation field is calculated in the pseudo-spherical approximation for a set of solar zenith angles using the finite difference method. Pseudo-spherical approximation means that the ~~single scattering contribution is calculated~~ direct solar beam is traced in a fully spherical geometry while a plane parallel atmosphere is assumed to calculate the ~~multiple scattering contribution (Rozanov et al., 2000)~~ scattered light. Then, an integration along the line-of-sight is carried out in a spherical geometry, i.e. intersecting a spherical shell atmosphere, accounting also for the atmospheric refraction. Thereby, ~~the pseudo-spherical radiative field calculated at the first step is used to approximate the~~ the single scattering contribution is calculated fully-spherically while the multiple scattering contribution at each point along the line of sight. ~~The weighting is approximated by an angular integration of the pseudo-spherical radiative field calculated at the first step (Rozanov et al., 2000).~~ Weighting functions are calculated using the same method as for the radiance, but considering only the single scattering contribution.

Linearizing the forward model around an initial guess state x_0 , the general equation that has to be solved can be written as:

$$y = y_0 + K(x - x_0) + \epsilon \quad (2)$$

where y is the measurement vector, y_0 is the simulated spectrum, K is the linearized forward model operator represented by the weighting function matrix, x is the state vector and ϵ represents errors of any kind. Following (Rodgers, 2000), the solution of Eq. (2) can be estimated iteratively. Taking into consideration that in our algorithm the retrieval is performed from a zero a priori profile, the iterative step $i + 1$ can be expressed as:

$$x_{i+1} = (K_i^T S_\epsilon^{-1} K_i + S_0 + S_1^T \gamma S_1)^{-1} K_i^T S_\epsilon^{-1} (y - y_i + K_i x_i) \quad (3)$$

Here, S_ϵ is the measurement noise covariance matrix. S_0 is the diagonal matrix optimized to constrain the solution within physically meaningful values and minimize a possible negative bias caused by the use of a zero a priori profile. The effect of the chosen matrix is significant only at tropical low altitudes and globally at high altitudes, where the ozone concentration is very small. Finally, S_1 is the first order derivative matrix ($S_1^T \gamma S_1$ is the first order Tikhonov term). ~~It is multiplied by the~~ The diagonal matrix γ ~~which~~ contains altitude dependent weights, used to constrain the smoothness of the retrieved profile. In the following, the sum $S_0 + S_1^T \gamma S_1$ will be named as S_r .

3.2 Algorithm implementation

For the ozone vertical profile retrieval from OMPS-LP, four spectral segments are selected: three in the UV spectral region (Hartley and Huggins bands) and one in the visible range (Chappuis band); the former ranges are sensitive to the upper stratospheric ozone, whereas the latter to the lower stratospheric region, where the peak of the number density occurs. In order to avoid strong absorption bands of water vapor and O₂, wavelengths in the ranges 580.0–607.0 nm and 620.0–635.0 nm are rejected. A complete treatment of these absorption features requires line-by-line calculations, that are computationally expensive. The altitude range over which the retrieval is performed spans between 12 and 60 km above the sea level. The vertical grid is fixed throughout the processing and covers the retrieval range at evenly spaced steps of 1 km. To prepare the measurement vector, limb radiance in each spectral interval is normalized with respect to a limb measurement at an upper TH, in order to provide a self calibration of the instrument and reduce the effect of surface/cloud reflectance. In addition, for longer wavelength intervals, a polynomial is subtracted from the logarithm of the normalized radiance in order to remove ~~slowly-variable~~ slowly variable spectral features, e.g. caused by Rayleigh or aerosol scattering (Rozanov et al., 2011). Eq. Equation (4) explicitly shows the measurement vector at the ~~i-th~~ j-th TH and details about spectral segments and TH normalizations are listed in Table 1. The last column provides the information about the subtracted polynomial in the measurement vector: first order in the visible range, zeroth order or no polynomial in the UV region.

$$y_j = \log \left(\frac{I_{TH_i}}{I_{TH_{norm}}} \frac{I_{TH_j}}{I_{TH_{norm}}} \right) - P_n \quad (4)$$

Table 1. List of the spectral segments considered for the ozone retrieval with corresponding altitude ranges, THs used for the normalization and the order of the subtracted polynomial (- means that no polynomial is subtracted).

Altitude range [km]	Spectral segment [nm]	Normalization TH [km]	Polynomial order
46-60	285-300	63-63.5	-
35-46	305-313	52-52.5	-
31-36	322-331	47-47.5	0
12-33	508-660 †	42-42.5	1

† 580.0–607.0 and 620.0–635.0 nm ranges are rejected.

In the forward model, the radiation is calculated taking into account O₃, NO₂ and O₄, which have spectral signatures in the selected spectral ranges. Cross sections of these gases are taken from Serdyuchenko et al. (2014), Bogumil et al. (2000) and Hermans (2011), respectively. Cross sections are beforehand convolved to the OMPS-LP spectral resolution. Ancillary pressure and temperature profiles are taken from the Global Modeling and Assimilation Office (GMAO) interpolated data set, provided by the NASA team together with OMPS-LP L1G radiances.

Before the main retrieval procedure, a shift and squeeze correction is applied in the Chappuis band to the modeled spectrum with respect to the measured one. This pre-processing is performed for each observation at each TH independently and is

introduced to account for issues related to the spectral calibration and possible thermal expansion of the detector. Typical values for the spectral shift are inside the range $[+1,+4]$ nm for the first point of the interval and $[-2,+1]$ nm for the last spectral point. ~~As the shift and squeeze correction algorithm works with the differential absorption structures, it cannot be applied in the UV range. Furthermore, as~~ Due to the relatively low spectral resolution of the instrument, the differential absorption structure

5 in the Huggins band is largely smoothed out and the UV retrieval uses either normalized radiances themselves or their slopes. As a consequence, the influence of a possible spectral misalignment is rather small and the shift and squeeze algorithm is not applied in the UV. In the pre-processing procedure, we obtain the S_e matrix from the fit residuals, fitting absorption features of all relevant gases in the selected spectral windows.

The inversion scheme is then iteratively run employing the Eq. (3). The state vector x_{i+1} , containing the retrieved ozone
10 vertical distribution at each i-th iteration, is expressed in terms of the Volume Mixing Ratio (VMR), which is more suitable for use with smoothing constraints. The smoothing weights, i.e. square roots of the diagonal elements of γ , linearly increase with the height above 45 km and remain constant below.

Surface albedo is simultaneously retrieved with ozone using the sun-normalized radiance provided in the L1G data. Two spectral fitting windows at THs around 38 km are employed: 355–365 nm and 455–470 nm, where ozone absorption is weak.

15 3.3 Cloud filter

A cloud filter is applied during the ozone retrieval to reject THs at which a cloud is present in the field of view of the instrument. The applied algorithm is based on the Color Index Ratio (CIR) concept (Eichmann et al., 2016), using OMPS-LP radiance at 754 nm and 997 nm. The ~~so-called~~ Color Index (CI) is ~~obtained calculating~~ defined as the ratio of the radiance at the two chosen wavelengths for the same OMPS-LP spectrum. The CI ~~is an altitude dependent quantity and~~ can be used to detect the
20 presence of scattering particles in the field of view, since we know the expected ratio for a cloud-free atmosphere. First, the CI is calculated at all THs, then the CIR is obtained as:

$$CIR(z_{TH}) = \frac{CI(z_{TH})}{CI(z_{TH} + \Delta z_{TH})} \quad (5)$$

where Δz_{TH} is the vertical grid step of 1 km. An example of the results for simulated clouds is reported in Fig. 4: cirrus clouds consisting of hexagonal crystals with an optical depth between 0.01 and 0.15 are taken into consideration. Since the ozone
25 retrieval is run above 12 km, we are generally not interested in liquid water clouds.

The chosen threshold to flag a TH as cloudy is 1.25. This technique was also applied to SCIAMACHY measurements with a different threshold (Eichmann et al., 2016). At the considered wavelengths the measured radiation is related to the scattered light from molecules, aerosol or cloud particles. A question may arise regarding the inability of such an approach to distinguish between high aerosol loads and cirrus clouds. Future investigations will focus on a comparison between the CIR
30 filter and aerosol profiles retrieved as described in the next subsection.

A different approach was used to detect Polar Mesospheric Clouds (PMC). The presence of ~~these clouds~~ PMCs can affect limb radiance down to 40 km, ~~leading to a bias in the ozone concentration at these altitudes. In clear conditions radiance in the upper stratosphere decreases monotonically with height. To detect the PMC presence, radiance profile around 353 is considered~~

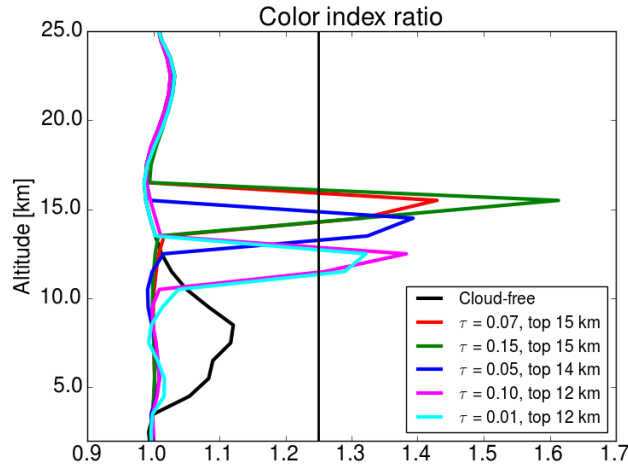


Figure 4. Example of Color Index Ratios for different simulations of ice clouds. Top of the cloud and optical depth (τ) ranges are chosen to simulate the impact of thin cirrus clouds in the upper troposphere.

for each observation causing an interference with ozone retrievals. Therefore, we screen out the PMC contaminated profiles in this study using the PMC detection flag at high latitudes above 50° N and below 50° S where the PMC occurrence is most frequent. PMCs are detected using the radiance profile at 353 nm and several conditions on radiance and its gradients. In absence of PMCs, radiance is expected to decrease monotonically with height above 40 km. As a consequence, the ozone profile is flagged if the radiance between 40 km and 80 km increases for with altitude or its gradient increases more then 50% between at least two consecutive layers, than the observation is flagged as affected by a PMC. These profiles are rejected throughout all the comparisons with independent data sets.

3.4 Aerosol treatment

The aerosol extinction coefficient is retrieved employing the general approach as used for SCIAMACHY v1.4 stratospheric aerosol extinction product (Rieger et al., 2017). Since OMPS-LP has a As a consequence of a coarser spectral resolution than SCIAMACHY, the retrieval, the radiance measured at 750 nm as used for SCIAMACHY is sub-optimal because of the influence of the is affected by the O_2 absorption band. Instead, a wavelength of 868.8 For this reason the OMPS aerosol extinction coefficient retrieval uses the radiance at 869 nm is chosen instead of 750 nm, as it was done for SCIAMACHY and OSIRIS. Stratospheric aerosol extinction is retrieved in the altitude range from 10.5 km to 33.5 km. The spectrum measurement at 34.5 km is used as the reference; the effective Lambertian albedo is simultaneously retrieved using the sun-normalized spectrum at 34.5 km. In order to smooth spurious oscillations, the first order Tikhonov regularization is employed. Scattering phase functions are calculated using Mie scattering theory. Thereby, the The particle size distribution is assumed to be lognormal with the median radius (r_g) of $0.08 \mu m$, and distribution width parameter (σ) of 1.6. This distribution is described The corresponding

probability distribution function is given by the following equation:

$$\frac{n(r)}{dr} = \frac{N}{\sqrt{2\pi} \ln(\sigma) r} \exp\left(\frac{(\ln(r_g) - \ln(r))^2}{2 \ln^2(\sigma)}\right) \quad (6)$$

The aerosol particles are assumed to be sulfuric droplets with 0 % relative humidity in the surrounding atmosphere. Below 10 km and above 46 km the aerosol load is set to zero. The refractive indexes are calculated using the Optical Properties of Aerosols and Clouds (OPAC) database (Hess et al., 1998). Before using the retrieved aerosol product, altitudes downwards from the detected cloud top height are rejected and each profile is extrapolated by the scaled a priori. The scaling factor is derived by averaging three altitude levels above the cloud. ~~The aerosol retrieval-~~

Because of the strong forward peak of the aerosol scattering phase function, a correct description of the aerosol scattering is particularly important at high northern latitudes where the scattering angle is high ~~(small (refer to Fig. 3)).~~

10 4 Results

~~OMPS ozone profiles are retrieved for seven months, from July 2006 to January 2007, limited by the availability of v2.5~~ In this section we present the results of the processing, for the whole year 2016. Version 2.5 of OMPS-LP L1G data at the time of writing this paper has been used, which, in comparison to the previous version, features an improved stray light treatment and pointing corrections as described in Sect. 2.1. Retrievals were performed using data only from the central slit of the instrument only because the lateral slits ~~can still~~ are still considered to suffer from pointing issues.

4.1 Retrieval characterization and error analysis

The information content of the measurements as well as the sensitivity of the retrieval can be analyzed using the averaging kernels (\mathbf{A}) and the covariance of the retrieval noise (\mathbf{S}_m) obtained respectively as (Rodgers, 2000):

$$\mathbf{A} = (\mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} + \mathbf{S}_r)^{-1} \mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} \quad \mathbf{S}_m = (\mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} + \mathbf{S}_r)^{-1} \mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} (\mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} + \mathbf{S}_r)^{-1}$$

20

$$\mathbf{A} = (\mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} + \mathbf{S}_r)^{-1} \mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} \quad (7)$$

$$\mathbf{S}_m = (\mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} + \mathbf{S}_r)^{-1} \mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} (\mathbf{K}^T \mathbf{S}_\epsilon^{-1} \mathbf{K} + \mathbf{S}_r)^{-1} \quad (8)$$

The square root values of the diagonal elements of the retrieval noise covariance matrix \mathbf{S}_m will be referred to as the theoretical precision of the retrieval. Following von Clarmann (2014), we do not include smoothing errors in the retrieval error budget. The vertical resolution of the retrieved profile is computed as the inverse of the diagonal elements of the averaging kernel matrix, multiplied by the altitude layer width. Examples of averaging kernels, vertical resolution and theoretical precision are plotted in Fig. 5.

The left panel shows AKs for an example profile at 30° N. For the sake of clarity, only each fourth AK is plotted. Middle and right panels show the latitudinal dependence of the vertical resolution and precision, respectively, for one day of OMPS

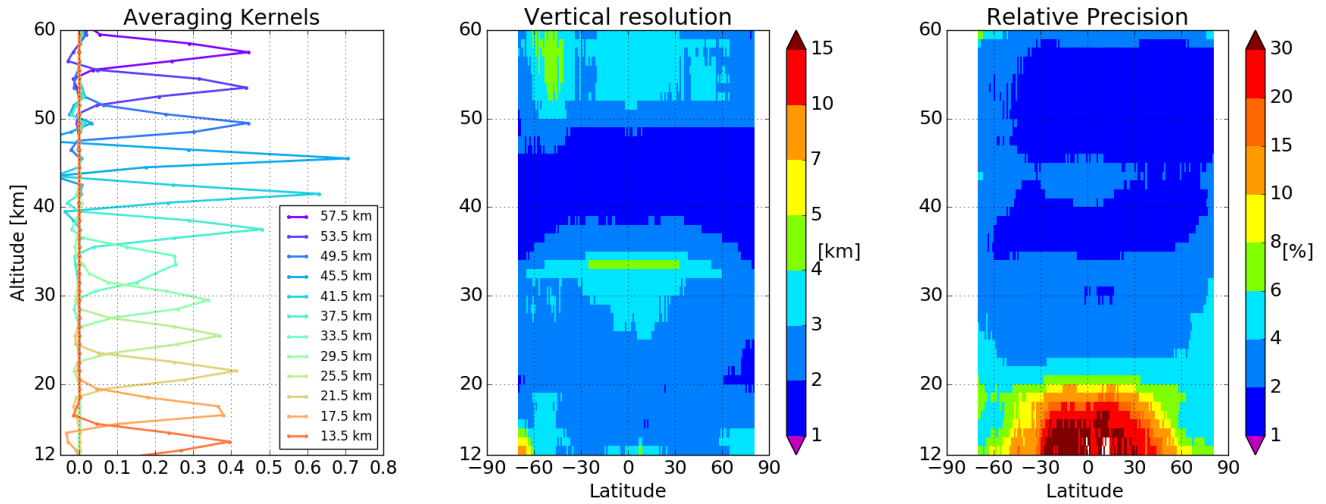


Figure 5. From left to right, examples of averaging kernels (plotted every 4 km for sake of clarity), vertical resolution and theoretical precision of the retrieval scheme. AKs are plotted for a measurement at 30° N, whereas vertical resolution and theoretical precision are shown as a function of latitude, i.e. solar zenith angle, for one day (15 September 2016).

measurements (15 September 2016). Below 30 km the actual vertical resolution of the retrieval scheme is typically about 2–3 km with a peak around 35 getting worst around 33 km, where the transition between UV and Vis spectral ranges occurs. The best vertical resolution of the profiles is achieved around 45 km, whereas above 50 km it gets coarser, due to the increasing Tikhonov parameter. The theoretical precision of the retrieved ozone profiles doesn't show a strong any significant dependence on the solar zenith angle (or latitude) above 25 km. It lies in the range 1–5 % between 25 and 50 of 1–4 % up to 60 km and tends to increase in the upper stratosphere and in the at lower altitudes, particularly in the tropical Upper Troposphere - Lower Stratosphere (UTLS) region: at these levels, the ozone concentration drops significantly and the retrieval precision gets lower, with relative errors up to 10–30 %. This purely random uncertainty is expected to be significantly reduced when averaging several profiles, as it is done in the validation section of this paper. For example, considering 10000 profiles and a relative precision of 30 % for each single profile, the random uncertainty on the averaged profile is equal to 0.3 %. Therefore, the random noise error is rather negligible when analyzing the validation results.

From left to right, examples of averaging kernels (plotted every 4 for sake of clarity), vertical resolution and theoretical precision of the retrieval scheme. AKs and vertical resolution are plotted for a measurement at 30° N, whereas theoretical precision is shown for several observations in the same orbit but at different solar zenith angles (the black line lies behind the green one below 25).

4.2 Comparison with NASA OMPS-LP ozone product

To retrieve ozone profiles from OMPS-LP observations, the NASA team implemented the Environmental Data Record algorithm, based on the Optimal Estimation approach with a priori constraints. In this procedure, a series of secondary parameters such as surface albedo, cloud height and TH correction are derived before the main retrieval of ozone profiles (Rault and Loughman, 2013). Two spectral ranges are used for the latter task: UV wavelengths between 29.5 and 52.5 km and wavelengths in the Chappuis band between 12.5 and 37.5 km (~~the bottom height depends on the detected cloud top altitude~~). The normalization of the radiance is performed with respect to high altitude TH measurements: 55.5 km in UV and 40.5 km in Vis. The measurement vector is obtained using the doublet and triplet method respectively for the Hartley-Huggins and Chappuis bands; more details are given in Table 2. An additional TH correction is applied by NASA team on L1G data, with values that follow an approximate linear decrease along the orbit, as described in the Release Notes of Level 2 (L2) data (DeLand et al., 2017). The quality flag related to the South Atlantic Anomaly is taken into consideration for the following comparison (Kahn and Kowitt, 2015).

Table 2. Wavelengths used in the NASA-OMPS ozone retrieval, according to DeLand et al. (2017)

Parameters	Values
Doublet λ_0	353 nm
Triplet λ_l	510 nm
Triplet λ_r	675 nm
Wavelength used in UV (nm)	302, 312, 322
Wavelength used in Vis (nm)	600

In version 2.5 of NASA L2 data, independent profiles for the Vis and UV ~~retrieval~~ retrievals are provided. ~~Fig~~ Figure 6 shows a comparison between NASA-OMPS retrievals and our results (in the following called IUP-OMPS), considering the two retrieved profiles independently. Panel (a) presents an example of averaged profiles in terms of the number density for the tropics. In panels (b) and (c), relative differences are shown for the tropical region, southern and northern ~~mid-latitude~~ mid- and high-latitude bands. Throughout the paper, relative differences are computed as:

$$\text{Rel diff} = \frac{2 * (\text{IUP-OMPS} - \text{Reference data set})}{(\text{IUP-OMPS} + \text{Reference data set})} * 100 \quad (9)$$

Considering the discrepancies with the NASA Vis retrieval, in panel (b), ~~the agreement is particularly good for an excellent agreement within 3 % is achieved in~~ the tropical region above 20 km, ~~as it is also in panel (a). Looking at . At northern mid-latitudes , IUP-OMPS values are generally higher with respect to the NASA product, especially between 22 and 32 the agreement is slightly worse with differences up to 5 % between 18 and 27 km and 5–9 % above 28 km. This positive bias slightly increases towards northern polar regions. The differences at southern mid-latitudes show a similar altitude behavior as those in the northern hemisphere but have a smaller magnitude. Towards the South Pole, we notice the worst agreement above 30 km. These discrepancies are possibly related to the merging of the spectral information from UV and Vis ranges at~~

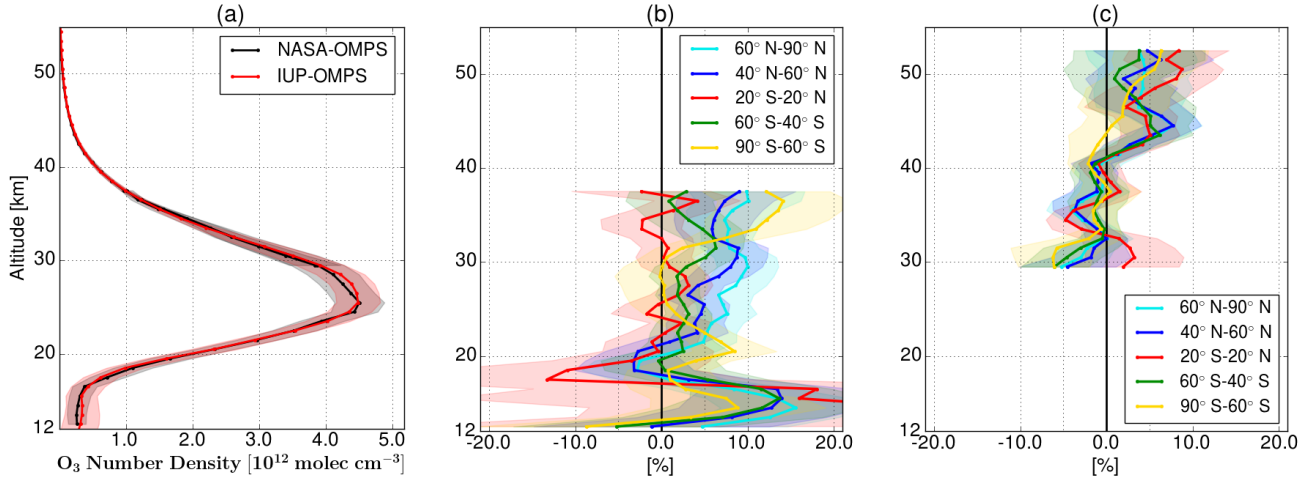


Figure 6. Panel (a): IUP-OMPS and NASA-OMPS retrieved number density profiles averaged in the tropical region. Panel (b) and (c): the relative differences (Eq. 9) for the Vis and UV retrievals, respectively, are shown in five latitudinal bands (60° N–90° N, 40° N–60° N, 20° S–20° N, 60° S–40° S and 90° S–60° S), with corresponding standard deviations as shaded areas.

these altitudes in IUP retrievals. In the ~~lower stratosphere we can~~ UTLS region we notice larger differences between the two profiles especially in the tropics: at these altitudes the ozone concentration and, thus, the retrieval accuracy gets lower. As a consequence, specific settings of the two retrievals such as spectral ranges, a priori values, aerosol and cloud retrievals play a larger role and are the most probable reason for the observed disagreement. Unfortunately, it is not possible to identify and relate each discrepancy at different altitudes to specific settings of the 2 algorithms; a stepwise adjustment of the settings is not always feasible, because the intermediate retrieval versions would result in oscillating or non-converging solutions.

Considering the NASA UV retrieval, the differences shown in ~~all latitude bands. Considering the UV NASA retrieval in~~ panel (c) are very similar for all latitude bands and an agreement within ± 5 % is found in almost all the cases, even if higher values are shown by IUP-OMPS around observed at most altitudes, except around 50 km in the tropics and at 45 km at northern mid- and high-latitudes, where the relative differences increase to 5–8 %. This may be related to the different usage of UV spectral ranges or TH normalization.

The jump between Vis and UV retrievals, evident when comparing panels (b) and (c), especially at northern mid-latitudes, is also reported by the NASA team in the corresponding Release Notes (DeLand et al., 2017): a preliminary comparison of their results with MLS assesses that values retrieved in the Vis range in the overlapping region (29.5–37.5 km) are systematically lower at mid- and high-latitudes.

4.3 Comparison with MLS

The MLS instrument was launched on board the Aura satellite in July 2004 to observe the thermal emission from atmospheric trace gases in the millimeter/sub-millimeter spectral range. It scans the Earth limb 240 times per orbit, providing retrievals of ~~daytime-day-~~ and nighttime profiles of several gases. For a detailed description of the MLS instrument refer to Waters et al. (2006). In this paper, the version 4.2 of MLS L2 data is used for the validation. Quality flags and recommendations reported in Livesey et al. (2017) are taken into consideration for the following analysis. Because of the large amount of available data, tight ~~collocation~~-criteria are applied to ~~find-collocated-collocate~~ measurements. The geographic distance between the centers of the two instrument footprints is limited to be within 1° latitude and longitude and the time difference is required to be within 6 h. In addition, the difference in the potential vorticity at 20.5 km is required to be less than 5 PVU, in order to avoid collocation of measurements inside and outside the polar vortex. Information about potential vorticity is taken from the European Center Medium Weather Forecast (ECMWF) database (ERA interim). OMPS-LP states affected by the presence of PMCs and observations at altitudes flagged as cloudy are rejected. In case of multiple MLS collocations for the same OMPS-LP measurement, only the closest one is taken into consideration. To be consistent with NASA and sonde comparisons, MLS profiles are converted from VMR vs. pressure into number density vs. altitude (using MLS geopotential height), interpolated at the regular altitude grid of IUP-OMPS retrieved profiles and finally zonally averaged. ~~Three-Five~~ latitudinal bands are selected for the comparison: ~~60° N–90° N, 40° N–60° N, 20° S–20° N and, 60° S–40° S and 90° S–60° S~~. Fig. 7 shows the averaged profiles for ~~the-tropics-and-tropics and northern mid-latitudes and the~~ relative differences (Eq. 9) in the ~~three-five~~ latitudinal bands. Standard deviations are reported in the plots as shaded areas. The number of collocations per band is $\sim 5000-10000$. The zonally averaged relative differences of IUP-OMPS with MLS are found to be generally within 5% between 20 and 58 km for all latitude bands. In the tropics a fairly constant positive bias of 2–4% is observed at all altitudes above 28 km. At northern mid-latitudes we notice a negative discrepancy of about 6–7 % around 28–30 km, which becomes more evident towards polar regions; up to 58 km the relative difference exceeds 3 % only at 45 km. At southern mid-latitudes IUP-OMPS shows about 5 % higher ozone number density around 25 km, whereas at other altitudes between 20 and 58 km an agreement within 3 % is achieved. Below 20 km, the agreement with MLS gets worse, with relative differences above 20% in the tropics, even though the absolute difference is rather small (see panel a).

Fig. 8 shows the relative differences between IUP-OMPS and MLS zonal means ~~binned~~-in 2.5° ~~wide~~-latitude bins as a function of altitude. Three time periods are considered in the panels. In panel (a), showing ~~all-6-months-of-data~~the whole year 2016, we can see that between 20 and ~~5060~~ km the differences are ~~generally-mostly~~ within $\pm 5\%$ ~~and never exceed 10 % at all latitudes~~. Starting the discussion of the discrepancies from the bottom of the plots, ~~positive-oscillating~~ differences larger than 30 % are found in the tropical UTLS region. This large discrepancy can be related to ~~multiple-several~~ factors such as ~~different vertical-resolutions-of-the-instruments~~a high dynamic variability of ozone, generally low sensitivity ~~to-ozone~~ in the lowermost retrieval altitude range or issues with the cloud filtering. ~~At mid-latitudes around 25~~As already mentioned, in this region the ozone concentration gets very low and the accuracy of the retrieved profiles degrades. Around 28–33 km a positive difference of 5–10 % is observed. This bias can be related to the water-vapor treatment inside the retrieval scheme: the intensity of the

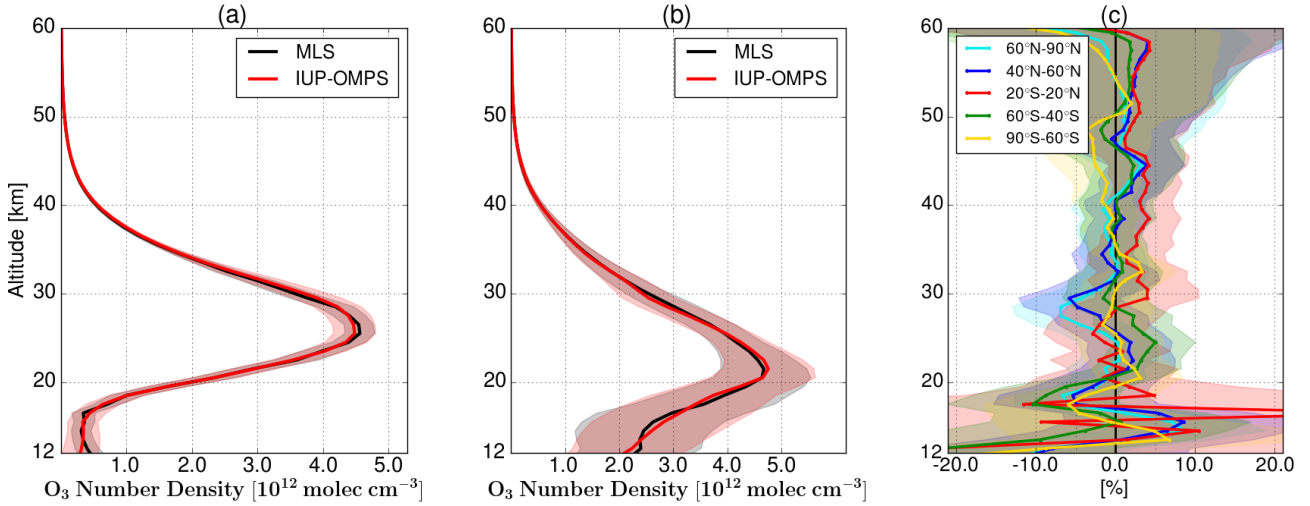


Figure 7. Panel (a) and (b): collocated IUP-OMPS retrieved profiles and MLS ozone product in the tropical region and at northern mid-latitudes, respectively. Panel (c): relative difference profiles (Eq. 9) in three-five latitudinal bands (60° N–90° N, 40° N–60° N, 20° S–20° N and, 60° S–40° S and 90° S–60° S), with standard deviations shown as shaded areas.

ozone-number-density peak is found to be sensitive to the choice of the spectral points that are skipped in the Chappuis band, where has non-negligible absorption a dip in IUP-OMPS ozone values is visible towards the northern high-latitudes, especially during winter months (panel c), whereas higher values are found in the tropics: this altitude range corresponds to the overlap region between the contributions from UV and Vis spectral windows and their merging can lead to some inconsistencies. In addition, an non-optimal albedo retrieval could cause biases during winter at northern polar latitudes. Around 45 km, higher values are shown by IUP-OMPS in tropics and at northern mid-latitudes, especially during winter months (panel c). This issue, already found in Fig. 6 panel (c), can be related to a problem in the junction between the spectral ranges in the Hartley and Huggins bands, that occurs indeed at 46 km. We In panel (c), we also notice a significant discrepancy towards northern latitudes ($>70^\circ$) above 40 discrepancy in the equatorial region and towards the North Pole above 50 km; this disagreement can be partly related to the stray light affecting the TH normalization at 63. Looking at panel (b) we notice that the discrepancy increases: these are months when PMCs are expected. This is an indication of a sub-optimal screening of these clouds in IUP-OMPS data, while MLS observations are found not to be affected by the presence of PMCs (Bak et al., 2015). Above 50 lower values than those from MLS are found in the southern hemisphere: this can be related to a pointing issue of the instrument as described in Sect. 2.2. Furthermore, a dip around 50 can be noticed, which is most probably related to the TH normalization chosen for the Huggins band, and artificial oscillations appear evident at the two uppermost levels. An increase of the Tikhonov parameter is expected to attenuate the latter problem, used for the normalization.

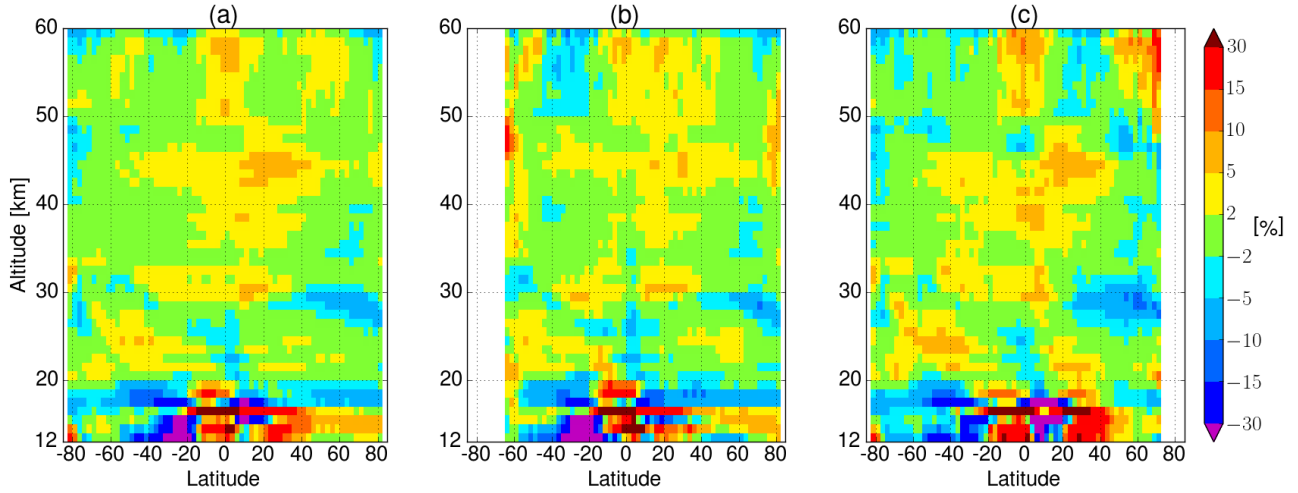


Figure 8. Relative differences (Eq. 9) averaged over 2.5° latitude bins, plotted as a function of altitude. Panel (a) whole year, panel (b) June, July and August, panel (c) January, February and December.

To summarize, this-the presented comparison shows a general validity of IUP-OMPS retrieval between 18-20 and 58 km in the tropics and down to 15 km at mid-latitudes, even if during different seasons the relative bias with respect to MLS exceeds by-may exceed 10 % in some limited atmospheric regions.

4.4 Comparison with ozonesondes

- 5 In order to provide a more reliable validation of our product at altitudes below 30 km, we are taking into consideration ozonesonde measurements. Ozonesonde data are obtained from WOUDC (World Ozone and Ultraviolet Radiation Data Center) and SHADOZ (Southern Hemisphere ADditional OZonesondes, Thompson et al., 2007) archives. We selected looser collocation criteria compared to MLS, because of the sparseness of ozonesonde measurements. Therefore, OMPS-LP measurements are required to be within 5° in latitude and 10° in longitude from the ozonesonde station and within ± 12 h time
- 10 span around the sonde launch. For each sonde profile, all collocated OMPS-LP observations are averaged before the comparison. Ozonesonde profiles are smoothed to the In order to account for the different vertical resolution of the OMPS-LP retrieval grid, by using the AKs as follow compared profiles, ozonesonde measurements are convolved with the AKs of the IUP-OMPS retrieval scheme as follows. First, we calculate the linear interpolation matrix \mathbf{L} to map the low resolution OMPS profile onto the fine sonde grid. Then this matrix is inverted using the pseudo-inverse formulation (Rodgers, 2000), obtaining \mathbf{L}^* as:

$$15 \quad \mathbf{L}^* = (\mathbf{L}^T \mathbf{L})^{-1} \mathbf{L}^T \quad (10)$$

The ozonesonde high resolution profile x_{fine} is smoothed-then-then convolved as follows:

$$x_{coarse} = \mathbf{A} \mathbf{L}^* x_{fine} \quad (11)$$

The upper altitude of the ~~smoothed-convolved~~ profile is chosen at the OMPS-LP grid level whose corresponding AK altitude range is fully covered by the sonde profile. An approach alternative to the AK ~~smoothing-convolution~~ assumes a simple vertical average, considering 2.5 km (i.e. ± 1.25 km) ranges around each grid point (value corresponding to an average vertical resolution of the retrieval scheme below 30 km, refer to Fig. 5). The altitude where a cloud is detected and all altitudes below are screened out. Latitude bins are selected ~~as-for-in the same manner as in~~ the previous comparisons.

Fig. 9 shows averaged collocated profiles in the tropical and northern mid-latitude bands with corresponding standard deviations. On the left side of these plots, the number of available collocations at each altitude is reported, which is about ~~120 and 160-220 and 370~~ for tropical and northern mid-latitude bands, respectively. Overall, 37 ozonesonde stations were considered, corresponding to over 1300 single collocated profiles.

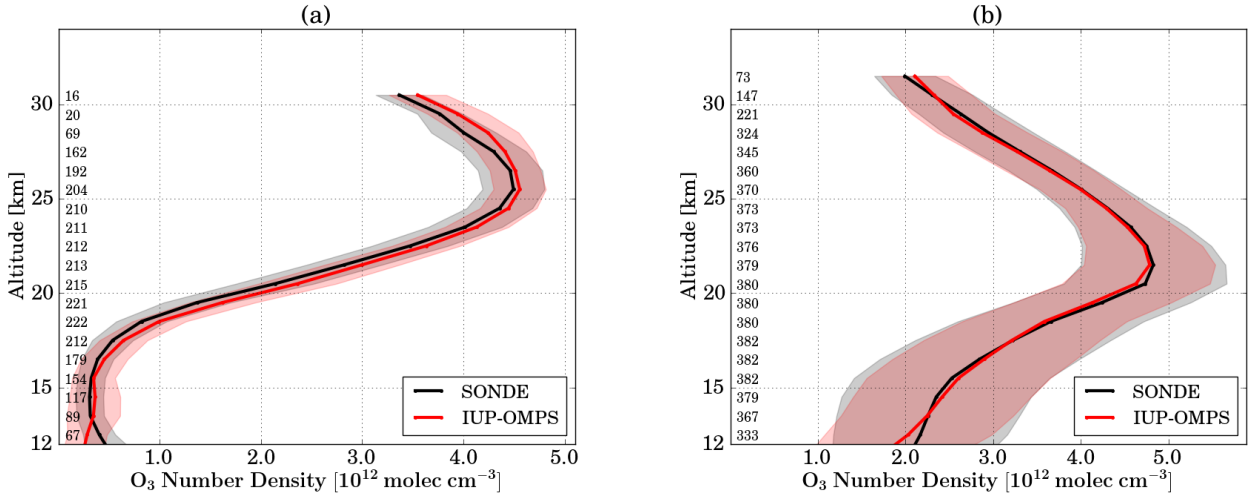


Figure 9. Comparison between collocated IUP-OMPS profiles and ozonesonde measurements in the latitudinal bands 20° S–20° N in panel (a) and 40° N–60° N in panel (b); standard deviations are shown as shaded areas.

Fig. 10 shows the relative differences (Eq. 9) in ~~the-three-five~~ latitudinal bands, in panel (a) using the averaging kernel ~~smoothing-convolution~~ approach and in panel (b) the vertical averaging. Differences between the two panels of this figure show that the ~~smoothing-averaging~~ procedure can be critical in the comparison between 15 and 20 km, where the gradient in the ozone profile is usually strong. ~~The-lack-of-stations-at-northern-and-southern-high-latitudes-prevents-a-meaningful-comparison-over-this-short-time-span.~~ As shown in Figs. 9 and 10, an excellent agreement is found at northern mid-latitudes, with relative differences mostly within ± 53 % between ~~14-13~~ and 30 km. Towards northern polar regions, a similar agreement is found, with a positive bias of 3 % down to 12 km. At southern mid-latitudes, we notice a fairly constant positive difference between 20 and 30 km, with values of 4–6%. A similar positive bias at southern mid-latitudes is also visible in Fig. 7. At southern polar latitudes the agreement gets slightly worse, with a discrepancy up to 7 % above 13 km. Focusing on the tropical region, a bias between the two data sets is clearly visible, with differences around ~~5–20 % between 18 and 322–20 % above 13 km.~~ This

~~positive bias~~ The positive bias above 17 km is unexpected considering the good agreement found when comparing to MLS data in the same region. In the UTLS region we also notice a peak of deviation; at these altitudes, ozone is hard to retrieve due to its decreasing concentration and the smoothing procedure may also introduce artifacts in the sonde profiles. Finally, at southern mid-latitudes, we notice a difference around 10 %, even though a positive anomaly is also visible in Fig. 8 about 18–20 km between 20 and 30 and a better agreement below. However, in this case, the validation is less significant because only two ozonesonde stations and about 25 comparisons are available within the considered time span° S and 0° S.

Looking at panel (b) of Fig. 10, the same patterns are depicted but stronger oscillations below 20 km are found, due to the smaller vertical range over which the sonde profiles are averaged.

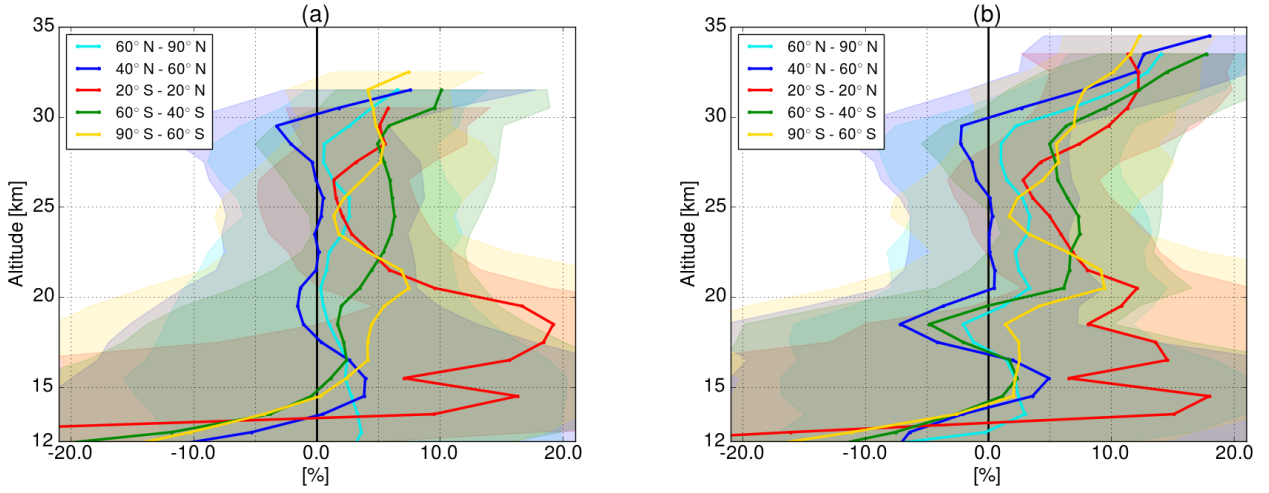


Figure 10. Relative differences between collocated IUP-OMPS profiles and ozonesonde measurements in ~~three-five~~ latitudinal bands (~~60° N-90° N~~, 40° N-60° N, 20° S-20° N ~~and~~, 60° S-40° S ~~and~~ 90° S-60° S), using in panel (a) averaging kernel ~~smoothing convolution~~ and in panel (b) vertical averaging. Corresponding standard deviations are shown as shaded areas.

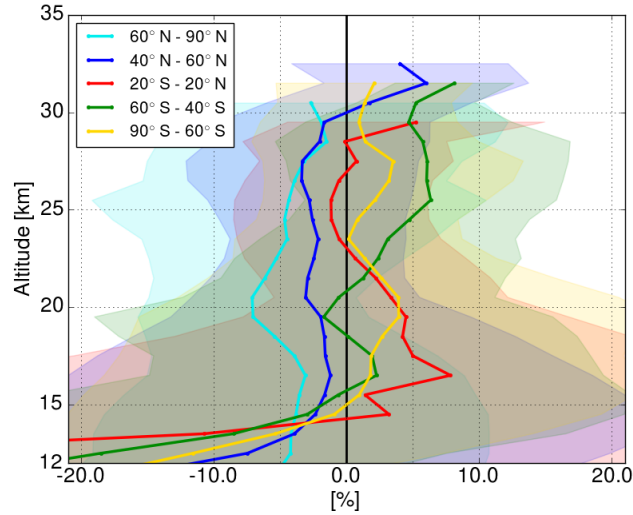


Figure 11. Relative differences between collocated IUP-OMPS profiles and ozonesonde measurements in ~~three-five~~ latitudinal bands (60° N-90° N, 40° N-60° N, 20° S-20° N and 60° S-40° S and 90° S-60° S) for the 2013 data set, with corresponding standard deviations as shaded areas.

With respect to the bias found in the tropical region, the processing of the OMPS-LP 2013 data set is also performed using the same retrieval settings. The analysis of these results and their validation against ozonesondes reveal a much smaller bias in the tropics. Relative differences between IUP-OMPS and sonde profiles in the same ~~three-five~~ latitudinal bands are shown in Fig. 11, following the averaging kernel ~~smoothing-convolution~~ approach. Since most of the ~~tropical~~ sondes considered over the ~~period Jul-2016-Jan-2017-year 2016~~ come from the SHADOZ archive, we also take only measurements from the same archive for the 2013 validation: over the whole year, around ~~140-200~~ collocations are available from 10 stations in the tropics and around 1000 collocations from 30 stations at mid and high-latitudes. In Fig. 11, focusing the attention on the differences in the tropical region, we can see that ~~at least between 20 between 14 and 30 km the bias is mostly within 5 %; larger discrepancies are still evident in the lower stratosphere, although a discrepancy of about 8 % is still evident at about 16 km.~~ Considering all the latitude bands, an agreement within 8% is seen at all altitudes above 14 km, as found in Fig. 10, panel (a). A comparison with MLS shows a very similar pattern to the one ~~found-observed~~ for the 2016 data set. ~~Further investigations of possible reasons for the observed behavior are ongoing. A possible reason for this difference between the data from 2013 and 2016, might be a jump of about 100 m in the pointing of the instrument that the NASA team detected in September 2014 and that was not corrected in L1 data. The effect of this small jump would be particularly evident at altitudes where ozone profile shows the strongest gradient, that is around 18-22 km in the tropics, and it is in agreement with the slight shift of the two profiles visible in panel (a) of Fig. 9, even though this is not found in the comparison with MLS.~~ Concluding, we find a general consistency of IUP-OMPS retrieval results with ozonesonde measurements in all considered latitude bands, except for the 12-20 km altitude range in the tropics, where the agreement with SHADOZ ozonesondes is ambiguous.

5 Conclusions

The retrieval algorithm originally developed at the University of Bremen to obtain vertical distributions of ozone from SCIAMACHY limb measurements was tailored and applied to OMPS-LP observations. ~~Seven months (Jul-2016–Jan-2017) of The~~ v2.5 L1G data ~~were set from the whole year 2016 was~~ processed, analyzed ~~and validated~~, validated and the results were
5 presented here. Ozone profiles were retrieved between 12 and 60 km, considering only the central slit of the instrument and observations at a solar zenith angle less than 80° . A comparison with NASA v2.5 L2 official product was carried out, ~~showing a~~
~~general good agreement in the tropics~~; we found an overall good agreement with the UV product at all latitude bands, with discrepancies typically within $\pm 5\%$ ~~between 20 and 52~~, except around 45 km and 50 km, ~~and a bias of about 10 % at 30 and 45~~.
10 The comparison with the Vis product above 20 km showed generally good consistency, even though a discrepancy of 7–12 %
was observed above 27 km at northern mid-latitudes and polar regions. We presented the results of the validation against MLS v4.2 ozone profiles and ozonesonde measurements from SHADOZ and WOUDC archives. A good agreement was found with the MLS ozone product: relative differences were generally within $\pm 5\%$ between ~~15 and 48~~ 20 and 58 km. On the other hand, we observed a larger discrepancy between IUP-OMPS retrievals and MLS in the tropical UTLS region, related most probably to smaller ozone amounts, larger dynamical variations and the decreasing sensitivity of limb retrievals from both instruments
15 in this region. ~~A discrepancy above 10 % in the upper stratosphere beyond 70° N is related to a sub-optimal PMC screening~~. In regard to the comparison with ozonesondes, ~~at northern mid-latitudes we found at northern mid- and high-latitudes~~ differences within $\pm 5\%$ ~~were found between 14~~ between 13 and 30 km and at southern mid- and high-latitudes a positive bias about
5–7 % for the same range. Focusing on the tropical region, a ~~consistent~~ significant positive bias with SHADOZ measurements was detected, unexpected after the good agreement observed with MLS data. However, the processing and validation of the
20 2013 data set, using the same retrieval settings, revealed a much better consistency. The reasons for this behavior are still under investigation, ~~but are possibly related to a jump in the pointing of the instrument occurred in 2014~~. In light of the results presented here, an additional work for tuning of some retrieval settings is needed before processing the whole data set and attempting the merging with the SCIAMACHY time series. Since the same 1-D retrieval approach has been used for both data sets, we expect this to ease the merging. Unfortunately, only a couple of overlapping months between the two instruments
25 are available, so that a third product must be used for the merging. After the good agreement found in the comparison of our retrievals with MLS, we are considering the use of the latter instrument as a transfer function to handle calibration issues in the merging procedure.

6 Data availability

Ancillary information and v2.5 L1G OMPS-LP data were downloaded from <https://ozoneaq.gsfc.nasa.gov/data/omps/>, where
30 L2 data are also available.

For the validation sections, MLS L2 data were taken from <https://disc.gsfc.nasa.gov/datasets>. WOUDC data were retrieved on ~~May 18, 2017~~ Feb 5, 2018, from <http://woudc.org>; a list of all contributors is available on the following website: doi:10.14287/10000001.

SHADOZ were retrieved on ~~April 6, 2017~~ Feb 5, 2018 from <https://tropo.gsfc.nasa.gov/shadoz/Archive.html>. Our results are available upon request ~~at~~ from the University of Bremen.

Author contributions. CA adapted the retrieval algorithm to OMPS-LP observations, processed the data set, performed the validation of the results and wrote the manuscript. AR provided the retrieval algorithm exploited in this study, supervised and guided the retrieval process and reviewed the paper. EM provided retrieved aerosol extinction profiles. K-UE contributed with the algorithm for cloud filtering that was adapted to OMPS-LP observations. TvC contributed to the discussion of the regularization matrices for the retrieval scheme and the proper use of averaging kernels to smooth the ozonesonde profiles and reviewed the paper. JPB, who proposed the research and leads the project, analyzed the results and contributed to the writing of the manuscript and the scientific outcomes.

Competing interests. The authors declare that they have no conflict of interests. TvC is associated editor of AMT but is not involved in the reviewing of this particular paper.

Acknowledgements. This work was partially funded by ESA within the Ozone CCI project and was supported by the University and State of Bremen. We would like to acknowledge NASA OMPS SIPS team (in particular G. Jaross, N. Kramarova and P.K. Bhartia) for the support provided during the data analysis as well as for the concession of the new v2.5 of OMPS-LP L1G data before its official release. Part of the data processing has been done on the German HLRN (High Performance Computer Center North). The GALAHAD Fortran Library was employed in the retrieval scheme.

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