Author’s response to the Referees comments on the manuscript ’Retrieval of ozone profiles from OMPS limb scattering observations’ by C. Arosio et al.

We thank the reviewers for the time they spent carefully reading the manuscript and constructively commenting on the paper. In the text below, referees’ comments are shown in italicized font and authors’ responses are highlighted in blue.

1 Anonymous Referee #1

General Comment The overall parts of the paper are written unclearly and illogically. For example, vertical grids where OMPS ozone profiles are retrieved and the unit of ozone should be introduced in the algorithm description section, at once. However, I need to search from.

- In line 8 on page 9, the vertical range between 12 and 60 km
- In line 3 on page 10, unit of ozone: VMR
- In line 13 on page 14, authors described “MLS are converted from VMR vs. pressure into number density vs. altitude, interpolated at the regular altitude grid of OMPS”, in addition, the regular altitude grid is not mentioned before.
- In line 10 on line 16, 2.6 km corresponding to an average vertical resolution of the retrieval scheme.

We agree with the reviewer’s comment, the information has been consolidated and put in the ‘Algorithm implementation’ section together with the altitude grid information. In SCIATRAN the state vector is used in terms of VMR (because the shape of the VMR profile is more suitable for use with smoothing constraints), whereas the retrieval results are provided in terms of both number density and VMR as a function of altitude. We choose to perform the comparisons with the other data sets in terms of number density, because the uncertainty on the number density profile is smaller (due to a less sensitivity to the temperature profile). In addition, plotting profiles in terms of number density is more interesting for the comparison with ozonesondes.

The average resolution of 2.5 km is not related to the retrieval grid but to the resolution of the retrieved profiles as computed using AKs and as shown in Fig. 7 (old Fig. 6).

This article should be checked line-by-line to become more scientific. For example, in abstract, authors mentioned “ozone in the 12-60 km can be retrieved due to using spectral window in the Hartley, Huggins and Chappuis ozone absorption band” In the view of the spectral window, this instrument is optimized to detect ozone over the troposphere including surface rather than the stratosphere. Limb measurements has lack sensitivity to troposphere due to its viewing geometry.

Looking at the weighting functions of ozone at different wavelengths, one sees that the Hartley band is appropriate to retrieve ozone in the upper stratosphere, Huggings (305 and 330 nm) in the middle stratosphere and Chappius band in the lower stratosphere and troposphere (as it is also shown in the NASA’s ATDB document pg. 34). In accordance with the reviewer’s comment about the lack of sensitivity of limb measurements to troposphere, a statement has been added in the introduction: ‘With decreasing altitude the atmosphere becomes more opaque, which results in a decreasing sensitivity of the limb-scatter measurements in the troposphere.’

In addition, authors described the OMPS-LP official algorithm as an inversion scheme with a priori constraints and a Tikhonov regularization, but in OMPS documentation, it is based on an optimal estimation based regulated by a set of a-priori constraints. These two schemes are
Thanks for the remark, we agree with the reviewer and have changed the manuscript text in accordance.

Please change “Level 1” to “Level 1b” because these two product are not same.

The notation L1G has been introduced, i.e. Level 1b gridded data, in accordance with the NASA’s notations.

Insufficient analyses on retrieval/validation were performed, which is commented in the main comment section. I found the text not be precise enough concerning unformatted types, grammatical error, English usage, which is commented in the minor comment section.

Comments in the main section as well minor comments have been addressed as described below. English has been proofread.

The following is the main suggestions for improvements.

0. Abstract

- Remove “this algorithm was originally developed ~~~ to produce a combined data set” in the abstract part and add more about the retrieval related description or results. For example, the vertical resolution of retrievals vary from ~ 2.5 km at lower altitude levels (<~ 30 km) and ~ 1.5 km to upper altitude levels (from 40 km to just below top levels). The theoretical retrieval precisions are estimated to be 1-5 % above 25 km, but rapidly increase to 15 % at 20 km.

In our opinion this statement provides an important introduction about the motivation of this study. This is why it has been kept. As suggested, additional information was added in the abstract about the retrieval characterization.

- “The optimization of the retrieval algorithm ~~~ . → This algorithm use altitude-normalized radiances in the UV and VIS wavelength range.

The sentence has been accordingly changed as: ‘The retrieval algorithm uses altitude-normalized radiances in the UV and Vis wavelength ranges to obtain ozone concentrations in 12-60 km altitude range.’

- indicating a good agreement → specify the altitude range showing a good agreement e.g.) a demonstrating a good agreement from 15 km to 58 km.

Some details about what ‘good agreement‘ means are already in the following sentences: so ‘indicating a good agreement’ was deleted.

- did not mention about the comparison with OMPS/NASA product.

Added without details. Now the sentence, considering also the previous comment, is: ‘OMPS ozone profiles are retrieved for seven months, from July 2016 to January 2017. Results are compared with NASA ozone profile product and validated against profiles derived from passive satellite observations, or measured by balloon-borne in situ sondes.’

1. Introduction
Authors mentioned that the main objective of the study is to create the long-term dataset using OMPS and SCIAMARCH. To do this, how to overcome the discrepancy of two instrument calibration? It is very difficult because of little overlapping period between OMPS and SCIAMARCH. Please add shortly how to overcome the discrepancy of two instrument calibration.

The MLS measurements are planned to be used as transfer function to overcome the calibration discrepancy. A corresponding paragraph was added in the conclusion, as also suggested by the other reviewer: '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 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.'

Authors too much simplified the summery of the previous studies related to your data product compared to the history and importance of ozone chemistry. It might be better to remove the ozone chemistry-related part (this part is unclearly written) and to focus on 1) history of satellite ozone observation using limb instrument, 2) why we need limb instrument compared to nadir instrument for ozone observation 3) why we need solar scattered limb measurements compared to infrared/microwave emission limb measurements for ozone observation, 4) history of SCIAMARCHY limb ozone profile product; algorithm development/validation, the long-term stability of both instrument and ozone dataset, 5)OMPS LP ozone profile product from OMPS science team at least and others if possible (e.g. Daniel et al. 2017 recently submitted to AMT), 6) the effort of this study to optimize the SCIAMARCHY algorithm for OMPS.

Following the reviewer's suggestions, the chemistry-related part has been reduced and more details added about limb observations and OMPS LP products. In our opinion it is not important to explain the history of SCIAMACHY ozone product in this paper, since it would be off-topic.

Line 33-35, page 2: the limb combines the advantage of the other two techniques ∼∼ with relatively high vertical resolution and horizontal coverage; reader who have no idea about satellite instrument could be confused that which instrument has higher vertical (horizontal coverage) resolution compared to Limb.

The sentence has been rewritten to avoid misunderstanding: '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.'

2. OMPS LP instrument
2.1 General features.
- Line 25 (page 3) “The main objective of the mission is to monitor the ozone vertical distribution within the Earth middle atmosphere at high accuracy level” → it is not true because the mission mentioned belongs just to the SNPP.

Corrected: ‘The main objective of OMPS-LP is ∼∼’
- Move line 23-27 to introduction and focus just on OMPS LP.

Done.

- line 1, page 5: the spectral range between 290 nm and 1000 nm → the spectral range of 290 nm to 1000 nm.

Modified to: ‘the spectral range of 280–1000 nm’.

- line 5-8, page 5: The use of such a technology (observation at the same time without vertical scanning and CCD) pose a great challenge as regards the SNR; indeed, scattered solar radiance from the Earth limb decreases by at least five orders of magnitude along the considered vertical range, due to the decrease of atmospheric density. → It is illogically written, about the cause-and-effect.

The sentence has been reworded to be more logical and clear: ‘The use of such a technology [CCD] poses a great challenge as regards the dynamic range: indeed, due to the decrease of atmospheric density, scattered solar radiance from the Earth limb decreases by at least five orders of magnitude along the considered vertical range.’

2.2 Calibration and main issue. - This part should be simplified or removed and then move some parts in other sections. Example, 1) In algorithm description, we can deliver some calibration issues related to the treatment of this algorithm to overcome these issues 2) In lines 8-9 on page 15, authors mentioned the disagreement between OMPS and MLS can be partly related to pointing issues, due to the solar heating of the instrument at high latitudes or stray light in section 4.2. In this paragraph, this paper can provide more detailed calibration issues related to this discrepancy.

The section was simplified. We currently don’t use any other pre-processing steps related to pointing issues in our algorithm and we didn’t split this section into the ‘algorithm description’ and ‘MLS comparison’ ones to avoid confusion.

-Line2 on page 6: Delete “Level 1B data are provided by NASA team” because the data is publicly available.

Deleted at this point.

-Line 24 on page 7: delete “In the preparing time of this paper the new data version was not fully released and only seven consecutive months were available.” This kind of sentence is not suitable in the scientific article. Move or re-mention “Retrievals were performed using data from the central slit of the instrument only because the lateral slits can still suffer from pointing issues” in the algorithm description or in the beginning of 4. Results.

It was deleted at this point and the sentence has been reformulate at the end of the section, where the data version is introduced, and in the ‘Algorithm implementation’ one. The expression ‘at the time of writing this paper’ has been kept since it is related to the chosen period of time and we don’t find it inappropriate.

2.3 OMPS-LP geometry of observations.
-line 31 on page 7: Azimuth angles could be defined separately as solar azimuth angle and satellite azimuth angle.

For the algorithm only the difference between the two azimuth angles matters. We don’t see the need of two separate definitions.

-line 34 on page 7: positive angles are East of the north, so that values are inside the -180 to 180 range → it is hard to understand this sentence.

'so that values are inside the -180 to 180 range' deleted: not necessary detail.

-Why this paper need this section? The information given in this part is never mentioned in other sections.

We kept the section as the figure shows the latitude coverage of the data set in different seasons and it might be useful to characterize the possible influence of the stratospheric aerosol which is strongly related to the scattering angle. A reference to it has been added also in the aerosol section.

3. Retrieval method
3.1 The retrieval algorithm
-Describe the theoretical inversion scheme first including from line 25 on page 9 to line 18 on page 10, generally and then describe how this algorithm prepare the measurement vector, measurement error vector, forward model vector, and state vector, it might be better to describe them in separated two sections.

The section was re-organized as suggested into two sections: ‘Theoretical basis’ and ‘Algorithm implementation’.

-Move the retrieval characterization and error analysis including Figure 6 in section 4.1 with the changed section title from 4. Satellite data set comparison to 4. Results; 4.1. Retrieval Characterization and Error Analysis 4.2 Comparison with OMPS-LP Ozone Product 4.3 Comparison with MLS 4.4 Comparison with Ozonesonde.

Thanks, this helps the readability. This part was re-organized as suggested.

This study described that “The information content of the measurements as well as the sensitivity of the retrieval can be analyzed using ~ and the covariance of retrieval noise”. It is true for AK, but not true for retrieval error. Sm is generally called “solution error covariance” including random-noise retrieval error covariance and smoothing error covariance. It should be detailed in the paper and an example should be presented in the right panel of Figure 6. It is useful to add the retrieval characterization and error analysis for mid/high latitudes due to the dependence of the sensitivity of solar measurements on solar zenith angles.

In the right panel of Fig. 6 there is already an example of the solution error covariance due to measurements noise, and more examples at different solar zenith angles have been provided. Following (Clarmann, 2014) the smoothing error should not be included in the retrieval error budget.

- The DFS and solution errors of OMPS LP seems to be much better than OMI UV nadir
viewing sensors in the troposphere (Liu et al., 2010). If it is true, we should use OMPS LP measurements for tropospheric ozone retrievals, but it is know that the limb measurements has lack sensitivity to lower troposphere, due to its viewing geometry. I think that the DFS and Retrieval errors are over/under estimated.

We don’t retrieve ozone in the lower troposphere, Fig. 6 vertical axis starts indeed at 12 km. Looking at the paper (Liu et al., 2010), the AK peaks in the stratosphere are actually slightly higher in our case but the relative precision is comparable with the OMI one or worse in the lower stratosphere.

-The definition of normalized radiance is unclear → Measurement vector is defined as the logarithm of the altitude-normalized radiances to an upper TH for canceling calibration errors and reducing the effect of surface/cloud reflectance. Table 1 summarizes ∼∼. In this paragraph, this paper should mention that this algorithm rejects the wavelength between 580 and 670 nm and between 620 and 630.0 to remove the effect of water vapor and O2 absorption when you describe which wavelengths are implemented in this algorithm.

We added equation 4, that explicitly shows the measurement vector. The cutting of the wavelengths was moved as suggested close to the definition of the chosen spectral ranges.

- Describe that ozone profiles are retrieved at which vertical grids; the number of levels, the vertical intervals, the unit of the grid in the same paragraph.

Done: ‘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.’

-Authors described that ozone retrievals are retrieved from 12 and 60 km in the all sections, but analyzed the retrievals from surface and 60 km.

We never show or discuss results at altitudes below 12 km.

-Line 20-24, page 9: “A shift and squeeze correction is applied in the Chappuis band to the modeded spectrum with respect the measured one: this pre-processing is performed for each observation at each TH independently” → a. describe why the wavelength calibration is implemented just for VIS wavelengths. b. Probably the modeled spectrum is high resolution solar reference data?

a) Sentence added to the paper: ‘As the shift and squeeze correction algorithm works with the differential absorption structures, it cannot be applied in the UV range. Furthermore, as the UV retrieval uses either radiances themselves or their slopes, the influence of a possible spectral misalignment is rather small.’

b) No, we mean just the spectrum simulated with the forward model.

- line 23-25, page 10: → surface albedo is simultaneously retrieved with ozone using two spectral fitting windows (∼∼) where ozone absorption is weak.

We still mention the usage of sun-normalized radiance, since it is a new feature of v2.5. Sentence reformulated: ‘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.

4. Satellite data set comparison
4.1 NASA retrieval and comparison

- Line 15: “At the moment of the submission of the paper, only version 2 of Level 2 (L2) NASA product was available, so a comparison with the most recent retrieval could not be performed”. This description is not suitable. This study should use the version 2.5 or should confirm from OMPS science team that there is insignificant difference between v2.0 and v2.5 product. This paper mentioned that OMPS/NASA algorithm is based on an inversion scheme with a prior constraints and a Tikhonov regularization, which should be changed to “an optimal estimation based regulated by a set of a-priori constraints”.

Only recently v2.5 L2 daily files have been produced and are now available, covering the period 2014-2017. As a consequence, following the reviewer’s comment, Fig.8 has been updated, using v2.5 L2 data of NASA.

As above mentioned the explanation of the algorithm has been changed.

- Based on Figure 8, there are significant differences between OMPS/NASA and OMPS/IUP products, which different implementations between algorithms causes these differences? Based on Figure 9, it seems that MLS shows better agreement with OMPS/IUP in the stratosphere (ozone peak layer) and with OMPS/IUP in troposphere. Both OMPS and MLS has lack sensitivity to lower troposphere so the retrievals determine mostly from a priori information, the similarity between two product might come from the similarity of a priori data between two algorithms.

As the retrieval implementations are different, biases at specific altitudes can not directly be linked to the algorithm differences. It is also impossible to ”switch off” the differences step by step as most of the ”mixed” algorithm version will not be stable and able to produce any reasonable results. Yes, the comparison between satellite data sets in the upper troposphere is difficult due to the lower sensitivity to ozone, as we also state in the paper.

- OMPS/NASA should be compared with MLS and ozonesonde to see which one provides better retrieval qualities.

We think that joint comparison between NASA-OMPS, IUP-OMPS and MLS/ozonesondes is not the target of this paper: NASA’s v2.5 just became partially available and our retrieval is still in progress.

4.2 MLS comparison

- change the reference of Waters et al. (2006) to MLS v.2 data quality and description documentation. This doc specifies how to use MLS product as following. This study use this data screening method?

The reference has been added rather than replaced. Yes, the flags reported in this document were used in the comparison between the two data sets: a corresponding sentence has been added.

- In this section, we firstly give a description of the vertical grid and the unit of ozone profile.
used in comparison, but this part should be moved before comparison with OMPS/NASA. I think that this paper create one section to describe the comparison methodology.

The vertical grid has been now described in the retrieval section. However, as the comparison methodology slightly differs for different comparisons it was not moved to a dedicated section.

-This paper mentioned “an increase of the smoothing parameter is expected to partially attenuate the latter problem”, about the large difference between OMPS and MLS profiles around 50 km. This explanation is so vague. Smoothing parameter indicates smoothing errors?

Smoothing parameter means Tikhonov parameter (changed): we were just addressing the oscillations seen at the top levels (58-60 km), not the one around 50 km.

- Figure 10 could be re-analyzed for several months (July and Dec or summer and winter) due to sufficient collocation.

The original plot has been kept but 2 other plots for summer and winter months were added.

-This paper can mention about the validity of OMPS retrievals above ∼15 km and below 58 km based on comparison with MLS.

Added at the end of the paragraph: ‘To summarize, this comparison shows a general validity of IUP-OMPS retrieval between 18 and 58 km, even if during different season the relative bias with respect to MLS exceeds by 10 % in some limited atmospheric regions.’

-Line 4 page 14: What is the modified potential vorticity?

The adjective ‘modified’ has been deleted.

-Line 9 page 15: “not screened polar mesospheric clouds” → based on the cases provided in this paper, it is hard to relate the large difference between OMPS and MLS to polar mesospheric clouds (PMC). That is because the presence of PMC is limited to polar summer season, but your analysis is performed for all seasons. This article did not mention that why the presence of PMC is important for OMPS retrievals and why MLS could be not impacted by PMC, maybe need some reference.

Thanks, this plot has been changed after the implementation of a PMC flag, consequently a short paragraph has been added in the Cloud Filter section, addressing the issues and the flagging. The reference to (Bak et. al 2015) paper was added: the authors use MLS as a reference when OMI detects PMCs.

5. Ozonesonde comparison

-Convolution process of higher resolution profiles with averaging kernels could be described after equation (4).

We think that moving this to the retrieval section would lead to much more confusion: we don’t use smoothing in other parts of the paper.

-This paper mentioned Figure 12 (a) as “averaging kernel smoothing and (b) as “vertical averaging”. Please correct this way to “Comparison of OMPS ozone profiles with ozonesonde
smoothed with OMPS averaging kernel and (b) without smoothing, respectively”.

Also the Panel (b) shows smoothed profiles but instead of using the AK to smooth the high resolution sonde measurements, a direct vertical averaging over a range of 2.5 km was performed (kind of box-car averaging kernels).

- This paper can add about insignificant impact of the smoothing of ozonesonde profiles to OMPS vertical resolution on the comparison results in the stratosphere due to the comparable vertical resolution of OMPS LP ozone profile retrievals to ozonesonde, compared to the comparison between nadir UV ozone product and ozonesonde. This fact can emphasize the importance of limb instrument on the stratospheric ozone observation.

A sentence related to panel (a) and (b) of Fig. 12 has been added: ‘Differences between the two panels of this figure show that the smoothing procedure can be critical in the comparison between 15 and 20 km, where the gradient in the ozone profile is usually strong’. We did not stress here the point related to the better resolution of limb sensors in comparison with nadir ones, because not on-topic. In addition, the difference of resolution between ozonesondes and OMPS-LP is still large: for sondes it’s around 10 m, for OMPS in the order of 1 km.

- Should summarize the validation conclusion about the validity of OMPS retrievals above 15 km based on comparison with ozonesonde measurements.

We stressed the point at the end of the paragraph: ‘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.’

- This paper should discuss the difference of comparison results between 2016 and 2013. The comparison with MLS provide same results between 2016 and 2013?

As stated in the paper the two periods were processed using the same settings. Yes, there are no substantial changes in the relative differences IUP-OMPS - MLS between the 2 periods, a sentence was added.

The following is the minor suggestions for technical corrections (I just suggest a few)

1) Please change “facilitate, overarching, exploit” to more proper words.

As the reviewer does not explain why (and where) the words are improper and which words he thinks suit better we did our best to go through all occurrences and use other words instead, if appropriate.

2) Many sentence is unnecessarily formatted like “very long subject” + “passive verb”. e.g) ozone concentrations in the 12-60 km altitude range can be retrieved → ozone concentrations can be retrieved from 12 to 60 km with valid precisions.

   e.g) Observation at altitude where the measurement are contaminated by clouds are rejected by applying a cloud filter → We screen out cloud-contaminated measurements using the color Index ratio of the radiance at 754 and 997 nm.

   e.g) the following molecular specifies with spectral signatures in the selected spectral ranges are
considered. → The radiation calculation take account of NO2 and O4 other than ozone.
e.g) ozonesonde data from WOUDC and SHADOZ archives are used in this analysis → ozonesonde data is collected from WOUDC and SHADOZ archives.

The text has been checked and some sentences changed according to the reviewer’s suggestion, to avoid recurrent ‘very long subject‘ + ‘passive verb’ patterns.

3)Line 3, page 1: SCIAMACHY instrument → SCIAMACHY limb instrument

This statement is incorrect as, unlike OMPS, SCIAMACHY is one instrument working either in limb or in nadir observation mode.

4)Line 10, page 1: Results for seven months ～→ OMPS ozone profile retrievals are validated against both satellite-based and balloon-borne measurements for seven month from July 2006 to January 2007.

Changed as ‘OMPS ozone profiles are retrieved for seven months, from July 2016 to January 2017. Results are compared with NASA ozone profile product and validated against profiles derived from passive satellite observations, or measured by balloon-borne in situ sondes.’

5)Line 14, page 1: those from ozonesondes → ozonesondes or ozonesonde measurements

Done.

6)Line 23, page 1: a stratospheric ozone layer → the stratospheric ozone layer

Line deleted

7)Line 24, page 2: result in the depletion of stratospheric and mesospheric ozone → lead to the destruction of stratospheric ozone.

The statement mentioned by the reviewer is not present in the indicated line/page.

8)Line 25, page 2: both from ground-based instrument and satellite observations → from both A and B.

Done

9)Line 34, page 2: the former instruments point downward while the latter look directly into the solar disk : “whereas” is better than “while”

Done

10)Line 35, page 2: The same geometry of observation can also be → has been

Done

11)Line 1, page 3: ~ limb emission measurements. With this latter technique a day and night coverage of the globe is feasible. → limb emission measurements can be taken during both day and night.
Sentence reformulated: ‘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.’

12) Line 5, page 3: launched in March 2002 → launched in March 2002 on board the ESA ENVISAT satellite. Line 7 page 3: In early 2012 ground communication with the ESA ENVISAT satellite, carrying SCIAMACHY among other ozone science relevant instruments, was lost → SCIAMARCHY ended its operation in early 2012 due to the loss of their platform with ground communication.

Sentence slightly modified: ‘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.’

13) Indents when a paragraph changes. e.g in the lines 3, 22 on page 2, 14 line on page 6

Done

14) Edit the usage of reference: e.g line 5 on page 3, (Burrows et al. (1995, Gottwald and Bovensmann (2011)) → (Burrows et al, 1995; Gottwald and Bovensmann, 2011). These unformatted types are often found in this article.

References were checked.

15) Lines 11-13, page 3 → This paper presents ozone profile retrievals from OMPS limb observations. This algorithm was adapted from the SCIAMACHY v3.0 ozone retrieval algorithm (Jia et al., 2015) developed by the University of Bremen.

Reformulated as: ‘This paper presents ozone profile retrievals from OMPS-LP observations performed at the University of Bremen. The algorithm we use was adapted from the SCIAMACHY v3.0 ozone retrieval (Jia et al., 2015).’


The line was changed accordingly with the previous comment but the citation kept: we want to refer to the SCIAMACHY data set not to the retrieval theory in Rodgers.

17) Line 14, page 3: delete “of this paper” after In sect.2

Done

18) Line 16, page 3: The applied cloud filter, the retrieval of aerosol extinction profiles and of the surface albedo → The applied cloud filter and the retrievals of aerosol extinction profiles and surface albedo

Changed into: ‘A more detailed characterization of the retrieval procedure follows, including the applied cloud filter and the approach to consider aerosol extinction profiles.’

19) Line 20, page 3: In the latter section and in the conclusions → in the conclusions
20) Line 21, page 3: OMPS-LP is not mentioned in the introduction before the title name of OMPS-LP instrument.

In the reviewed version it is mentioned in the introduction.


Done, now in the introduction.

22) Line 9, page 5: slower that → slower than

Done

23) Line 33, page 7: positive angles are East of the North: change from “are” to “represent”

Line deleted

24) Line 11, page 9: get rid of → remove

Done

25) Cross section of these gases are respectively taken from ~ → taken from ~~, respectively.

Done

26) Line 18-19, page 9: delete “used in the radiative transfer mode” and “provided by the NASA team together with OMPS-LP L1 radiances”

‘Provided by the NASA team’ was kept.

27) Line 8, page 14: the geographic distance is required to be whine 1 deg. → limited to be

Done

28) Line 15, page 14: The number is in the order of 5000. → The number is ~ 5000.

Done

29) Line 1, page 15: → the positive difference of larger than 30 % in the tropical lower stratosphere.

Changed as: ‘Starting the discussion form the bottom of the plots, positive differences larger than 30 % are found in the tropical lower stratosphere.’

30) Line 15, page 15: Looser collocation criteria than for MLS → compared to MLS
31) Line 16, page 15: because of the sparseness of the data set → because of the sparseness of ozonesonde station. / In particular → Therefore

Done

32) Line 18, page 15: remove “generally for each sonde profile ∼ found using these loose criteria”

This part of the sentence was deleted and reformulated as: ‘For each sonde profile, all collocated OMPS-LP observations are averaged before the comparison.’


Done

34) Line 14, page 16: for tropical and northern mid-latitude bands, around 120 and 160 sonde profiles, respectively are considered. → , which is ∼ 120 and 160 for tropical and northern mid-latitude bands, respectively.

Done

35) Line 1, page 17: As can be seen also from Fig. 11 → As shown in Fig. 11, the excellent agreement is also found at northern mid-latitudes, with ∼ ∼.

Done: ‘As shown in Figs. 11 and 12, an excellent agreement is found at northern mid-latitudes, with relative differences below 5% between 14 and 30 km.’
2 Anonymous Referee #2

==== General comments
This is a nice paper that does a good job of introducing a new OMPS-LP retrieval approach and
describing the dataset resulting from it. I see this paper as ideally suited to the AMT journal
and a welcome addition to the body of literature. My comments are all pretty minor and mainly
involve requests for further clarification or suggestions of wording changes etc. I’m confident
that, once these are addressed, the paper will be ready for publication.

Before I provide some line-by-line comments and suggestions, just a few “global” thoughts.
In several places the paper presents comparisons between the IUP-OMPS and another dataset
without (that I could readily find) being completely explicit about whether it’s <IUP-OMPS>
minus <other> dataset that’s being presented (as I’m pretty sure it is) or the sign is reversed.
Furthermore, when a percentage or relative difference is shown, you should be clear about what
is in the denominator, is it IUP-OMPS, the other dataset or some combination of the two?

We added an explicit equation (Eq. 8) valid for all the relative differences in the paper and
and corresponding remarks in figure captions, where appropriate.

The abstract and introduction talk about this paper setting the stage for a potential “combined”
dataset linking this new record to the SCIAMACY observations. It would be useful to return
to this point in the conclusions section and briefly discuss the consequences of your findings for
such an activity. Which of the factors uncovered in this analysis might present challenges to
such data fusion?

That’s an interesting point: we added a couple of sentences in the conclusions: ‘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
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.’

Finally, I’m aware of at least on other team developing an OMPS-LP data record, that being
the OSIRIS team in Saskatoon. Depending on the availability of data from that team, it’s worth
considering the possibility of expanding section 4.1 (or adding a new section) that at least dis-
cusses their approach and its similarities and differences from yours and the NASA one, and
perhaps even performs an additional data comparison if appropriate.

That’s true, a mention + citation of this other data set was added, however:
1) Also Saskatoon’s paper is currently under discussion, even thought the processing has al-
ready been extensively performed.
2) An inter-comparison with this data set is for us behind the scope of this paper, as the
Saskatoon retrieval is not yet sufficiently validated and differences because of the usage of 2-D
approach are expected. Thus, for now it is unclear how the differences in the results, which are
expected to be identified, should be attributed properly.
3) A dedicated paper about retrieval errors using different algorithms is foreseen by NASA team.

==== Specific comments
It would be good to spell out SCIAMACHY and MLS in the abstract (if space permits)

Done

Odd wording of 2nd sentence. How about "... in the atmosphere. It is most abundant in the stratospheric 'ozone layer', which absorbs..."?

Reformulated as: 'It is most abundant in the stratospheric 'ozone layer', which absorbs...'.


Added

"satellite missions" → "satellite instruments"

Done

This needs rewording. First, OMPS is an instrument not a mission (the Suomi NPP missions has "stated aims" that go far beyond ozone). Secondly, while the OMPS-LP and OMPS-NP components are indeed focused on the vertical distribution, you’ve neglected the OMPS-NM mapping capability which has no vertical resolution and thus a different science focus.

Yes thanks, we reformulated it, addressing the sentence just to OMPS-LP: ‘The main objective of OMPS-LP is to monitor the ozone vertical distribution within the Earth middle atmosphere at high accuracy level.’

"further prior handling" is odd wording (further and prior sound contradictory), how about "additional screening or processing" or something similar?

Reformulated: ‘In this paper, version 2.5 of OMPS-LP L1G data has been used without any additional pre-processing related to stray light and pointing.’

Give a citation or more details on the "another scene-based technique".

We introduced the other acronym as well. The paper Moy et al. has already been introduced.

This reasoning doesn’t actually quite follow. Photons from any altitude can be scattered within the instrument to any other altitude. It so happens that there are more photons in the lower atmospheric views than the upper atmospheric one. The way it’s currently written makes it sound more one way than theoretically can be (though granted, you do start with "For example").

We deleted this part and referred the example to the collection of multiple images on 1 single CCD.

"In the preparation time of this paper” → "At the time of writing this paper"
Done, sentence moved at the beginning of the ‘Results’ section

Line 33: Perhaps delete "the" before "North"?

Done

— Page 8 Lines 10-15: Please be explicit about whether "approximate spherical" is referring to the assumed shape of the Earth (as I assume it is) or to the shape of scattering particles. How does "approximate spherical" (line 12) relate to "pseudo-spherical" (line 14, page 9 line 1). Also how is all of this related to the oblateness of the Earth, are you assuming a spherical Earth surface but with a radius tuned to give approximately the same shape as the Earth ellipsoid along the line of sight?

Clarified in the paper.

— Page 9 Lines 20-24: Please give more details on what this "shift and squeeze" is correcting (some instrumental anomaly?) and why this correction is necessary (also why it is not needed in the UV range).

Sentences added: ‘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.’ and ‘As the shift and squeeze correction algorithm works with the differential absorption structures, it cannot be applied in the UV range. Furthermore, as the UV retrieval uses either radiances themselves or their slopes, the influences off a possible spectral misalignment are rather small.’

— Page 10 Line 12: Typo with Tikhonov

Checked but it was correct.

Also line 12: If gamma linearly increases with height then it’s a vector rather than a scalar surely (or even possibly a diagonal matrix). Please clarify.

True, we address gamma as a diagonal matrix.

Line 24: Insert "Level 1" after "normalized"?

Reformulated: ‘Surface albedo is simultaneously retrieved with ozone using the sun-normalized radiance provided in the L1G data.’

Line 27-29: I’m not quite sure I understand this. It seems like you’re preselecting which wavelength/height subsets of the Level 1 data to use based on the strength of the weighting functions. However, the retrieval factors those strengths in when deciding how much attention to pay to each individual measurement anyway. Why is this additional step, which, in effect, second guesses the retrieval, needed? If including the "weaker" signals has undesirable effects on the result, is it understood why that is? Also, this means that, potentially, each ozone profile was generated by a different "subset" of the instrument, making for a measurement dataset whose properties (precision, resolution etc.) are a moving target, complicating the development of average datasets, long term records, etc. Some discussion of the size of these effects would be good.
This was just a description about what was done at the beginning to adjust the spectral ranges used into the retrieval. Once chosen, the settings are then kept fixed throughout the processing. After the review, we decided to delete this paragraph because it can lead to misunderstandings.

— Page 11 Line 5: suggest "... to reject THs <with radiances> affected by ...”

Changed to ‘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’.

Line 14: Insert "liquid” before ”water”?

Done

— Page 12 Line 5: Start of line: "Aerosol extinction...” → ”An aerosol extinction...”

Changed to ‘The aerosol extinction...’

Line 6: "... has a coarser spectral resolution <than SCIAMACHY>, ...”

Done

— Page 13 Line 1: ”downwards from” → ”below”

We kept ‘downward from’ because we reject also the TH where the cloud has been detected.

Line 15: ”At the moment of submission of the paper” → ”At the time of writing”

Sentence deleted: the section has been updated using the V2.5 of NASA L2 data.

Line 17: ”... Fig. 8, which shows relative ...”

Changed as: ‘. Fig. 8 shows a comparison between NASA-OMPS retrievals and our results’.

— Page 14 Line 2: ”AURA” → ”Aura”

Done

Line 4: ”satellite suite” → ”MLS instrument”

Done

Line 8: Is there a reference or definition for ”modified potential vorticity”.

I just meant potential vorticity, the term came from the ERA Interim extractor we use. ‘Modified’ was deleted.

Lines 11-14: Please state what temperature/height information is used to do the density/height to pressure/vmr conversion?
It is stated in line 13 ‘using MLS geopotential height’: we are aware of possible trend in this variable but we think that it doesn’t have impact on our analysis of few months of data. We are surely going to use ECMWF ERA Interim for the analysis of the whole time series and future merging of the data set.

— Page 15: Line 9: ”... related to impacts of polar mesospheric clouds on the signals that were not successfully screened out of the Level 1 data” or similar wording?

Paragraph partially modified: ‘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...’

— Page 17 Line 16: ”about” → ”into”

Reformulated as: ‘The reasons for this behavior are still under investigation.’

— Figure 1 Wouldn’t hurt to define TH, TP in the caption.

Both acronyms were introduced in the caption.

— Figure 2 Again, make figure more ”stand alone” by defining ”TP”

The acronym was defined in the caption.

— Figures 8 and on: Be clear in each what the sign of the differences shown are. (Do it in both the body text and the figure/caption to allow the figures to ”stand alone”)

References to Eq. 8 have been added.
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 vertical profiles of ozone from limb observations performed by the Ozone Mapper and Profiler Suite (OMPS). This algorithm was originally developed for use with data from the SCIAMACHY—Scanning Imaging Absorption spectrometer for Atmospheric CHartography (SCIAMACHY) instrument. As both instruments make limb measurements of the scattered solar radiation in the ultraviolet and visible spectral range, an overarching Ultraviolet (UV) and Visible (Vis) spectral ranges, an underlying objective of the study is to facilitate the provision of consolidated and consistent ozone profiles from the two satellites and to produce a combined data set. The optimization of the retrieval algorithm for OMPS takes into account the instrument-specific spectral coverage by exploiting information from spectral windows in the Hartley, Huggins and Chappuis ozone absorption bands. Thereby, ozone concentrations in the 12–60 km altitude range can be retrieved. Observations at altitudes where the measurements are contaminated by clouds are rejected by applying a cloud filter in the instrument field of view. Measurements at altitudes contaminated by clouds are identified and filtered. An independent aerosol retrieval is performed beforehand and its results are used to account for the stratospheric aerosol load in the stratosphere during the ozone retrieval. Results. The typical vertical resolution of the retrieved profiles varies from ~2.5 km at lower altitudes (<30 km) to ~1.5 km at upper altitudes (from 40 km to just below top levels). The retrieval errors resulting from the measurement noise are estimated to be 1–5 % above 25 km, increasing to 10–15 % below 20 km. OMPS ozone profiles are retrieved for seven months of data (from July 2016 to January 2017) are compared to January 2017. Results are compared with NASA ozone profile product and validated against independent data sets from both satellite-based and profiles derived from passive satellite observations, or measured by balloon-borne measurements, indicating a good agreement in situ sondes. Between 20 and 50 km, the OMPS ozone profiles typically agree with the MLS data from the Microwave Limb Sounder (MLS) v4.2 results within 5–10 %, with the exception of high northern latitudes (>70° N above 40 km) and the tropical lower stratosphere. The comparison of OMPS profiles with those from ozonesondes shows an agreement in ozonesonde measurements shows differences within ±5 % between 14 and 30 km at northern mid-latitudes. At southern mid-latitudes, an agreement within 5–10 % is achieved, although these results are less reliable because of a limited number of available coincidences. An unexpected bias of approximately 10 % is detected in the tropical region at all altitudes. The processing of the 2013 data set using the same retrieval settings and its validation against ozonesondes reveals a much smaller bias; possible reasons for this behavior are under investigation.
1 Introduction

Ozone is one of the most important trace gases in the atmosphere. This is due to its stratospheric layer. It is most abundant in the stratospheric ‘ozone layer’, which absorbs strong ultraviolet (UV) radiation, heating this atmospheric region and thereby acting as a protective layer against biologically harmful radiation. It is relevant to climate because of its plays a crucial role in the radiative budget of the stratosphere. The presence of a stratospheric ozone layer was first discussed by Hartley (1880) but came to prominence in the late 1960s and early 1970s when it was first recognized that anthropogenic activities could result in the depletion of stratospheric and mesospheric ozone (Molina and Rowland, 1974). Ozone is also of importance in the tropospheric chemistry and it is a greenhouse gas, thus its amount and spatial distribution play a role in the global warming and climate change processes (IPCC 5th report, Pachauri and Meyer (2014)).

After the 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 Antarctica (Farman et al., 1985), the field of stratospheric chemistry and physics researches expanded. This resulted in the mechanism of the production and loss of stratospheric ozone being much better explained. Research grew in this field because of its relevance to both science and society. 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 Montreal protocol adoption, long term ozone trends and adoption of the Montreal protocol, stratospheric responses to changes in tropospheric radiative fluxes and temperatures 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, are have been investigated by several studies, that 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 O_3 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 of 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 to study trends 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 the ozone 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. The occurrence of strong ozone loss events over the Arctic during spring after particularly cold stratospheric conditions, as occurred in 2011 and 2016, drew the attention of scientists and public concern to the possible consequences for human health (Manney et al., 2011).
Current predictions of a long-term impact of global warming coupled with the removal of ozone depleting species indicate a
colder stratosphere and an increase in stratospheric ozone, a so-called super recovery of ozone (WMO (2014)). For all these
kinds of studies, reliable long-term data sets are needed both from ground-based instruments and satellite observations: for
example, recent discussions have shown the importance of multi-decadal time series in order to detect trends in the ozone
concentration and the possible recovery of the ozone layer in the Antarctic region (Stolarski and Frith, 2006).

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, UV–Vis)
spectral range have traditionally been of two types: nadir viewing and solar occultation spectrometers; the former instruments
point downward while and are characterized by a good horizontal coverage whereas the latter look directly into the solar disk.
A more recent technique, the limb scater of sunlight, combines the advantages of the other techniques and provides vertical
profiles of ozone density with relatively high vertical resolution and horizontal coverage. The same geometry of observation
can also be exploited to collect measurements 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) or and microwave spectral regions, the so-called limb emission measurements. With this latter technique
the scattered solar light, measurements during daylight only are possible, whereas, using the emission signatures,
observations can be performed during both day and night coverage of the globe is feasible.

One of the instruments capable of performing With decreasing altitude the atmosphere becomes more opaque, which results
in a decreasing sensitivity of the limb-scatter observations in the UV, VIS, Near-InfraRed (NIR) and Short Wave InfraRed
(SWIR) spectral ranges was measurements in the troposphere.

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)). In early (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 (ground communication with the European Space Agency ENVISAT satellite, carrying SCIAMACHY among
other ozone science relevant instruments, when the platform-to-ground communication was lost. A few aging satellite
missions instruments, such as the Optical Spectrograph and InfraRed Imager System (OSIRIS) 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) in-
strument was launched on board the Suomi-National Polar-Orbiting Operational Environmental Satellite System Preparatory
Project (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).

In this paper the retrieval algorithm developed 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 Bremen to retrieve vertical ozone profiles from OMPS limb observations is discussed. An overarching objective for 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 the SCIAMACHY v3.0 ozone retrieval (Jia et al., 2015). The underlying objective of the study is the creation of a consolidated data set and the merging of the OMPS and the SCIAMACHY time series, in order to obtain a long-term continuous data set. For a description of SCIAMACHY v3.0 ozone retrievals refer to Jia et al. (2015).

In Sect. 2 of this paper, 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, the retrieval of and the approach to consider aerosol extinction profiles and of the surface albedo. In Sect. 4 presents first a comparison with NASA ozone profile retrieval algorithm is shown; then MLS and ozonesonde data sets are used for a first validation of our results. Main results, remaining issues and possible future improvements are addressed in the latter section and in the conclusions.

2 OMPS-LP Instrument

2.1 General features

The Suomi-National Polar-Orbiting Operational Environmental Satellite System Preparatory Project (SNPP) platform carrying the OMPS instrument was launched in October 2011 and OMPS data collection started in January 2012. The spacecraft has a nominal 13:30 local time ascending sun-synchronous orbit and flies at a mean altitude of 833 km. The main objective of the mission—OMPS-LP is to monitor the ozone vertical distribution within the Earth middle atmosphere at high accuracy level. OMPS comprises three instruments: a Nadir Mapper, a Nadir Profiler and a Limb Profiler (LP). Only the latter is of interest for our study (see Flynn et al. (2014) for a review of the full suite). OMPS-LP 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 the 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 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, while whereas the other two are cross-track, separated horizontally by 4.25°, which corresponds to 250 km distance between the TPs. Each slit covers a vertical range of 112 km, imaging the atmosphere
Figure 1. 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).

Without scanning, OMPS-LP was designed to measure ozone vertical distributions in the upper troposphere and stratosphere with an instantaneous field of view of about 1.5 and a sampling of 1 at TP (Jaross et al., 2014). The orbit is inclined, so that the TP is located on the East with respect to the satellite, around 25° latitude South of the sub-satellite point. The geometry is drawn in Fig. 2. OMPS-LP 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°, and completes 14–15 orbits per day.

Figure 2. 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).
The instrument measures limb scatter OMPS-LP measures limb scattered radiance in the spectral range between 280 of 280–1000 nm and 1000. 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. The full atmospheric range is observed OMPS-LP observes the full altitude range at the same time, without vertical scanning, and radiance: each slit covers a vertical range of 112 km, with an instantaneous field of view of about 1.5 km and a sampling of 1 km at TP (Jaross et al., 2014). Radiance is collected by means of a Charge-Coupled Devices Device (CCD). The use of such a technology poses a great challenge as regards the Signal to Noise Ratio (SNR) dynamic range: indeed, due to the decrease of the atmospheric density, scattered solar radiance from the Earth limb decreases by at least five orders of magnitude along the considered vertical range, due to the decrease of atmospheric density. So, Therefore, in order to cover the required dynamic range, four images at two physical CCDs 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). Then, since 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. Ground Then, ground processing is 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), so therefore it is re-sampled and mapped onto a regular grid. Example of radiance profiles that show Fig. 3 shows examples of radiance profile, displaying the large dynamic range of measured values are shown in Fig. 3. 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. Jumps in the SNR plot (Fig. 4 Jumps in this plot) shows examples of spectral signal-to-noise ratio at different altitudes. Jumps are related to changes of the sampled image: for example, the jump between large and small aperture that occur at 450 nm (fixed threshold). In the retrieval scheme we were careful not to consider spectral ranges crossing this fixed boundary.

2.2 Calibration and main issues

Level 1 (L1) data used in this study are provided by NASA team (Jaross et al., 2014) and used without any further prior handling. 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 m uncertainty in the TP height translates into a 5% error in the ozone profile. Such a high accuracy cannot be directly reached for OMPS-LP sensor. This is because the star-tracker on board the SNPP satellite is mounted on a distant position from the instrument, so that thermal effects and errors in mis-alignments of the instrument focal plane alignment increase the uncertainty. play an important role.

To solve this problem, a technique two methods called Rayleigh Scattering Altitude Sensing (RSAS) is and Absolute Radiance Residual method (ARRM) are implemented by the NASA team in the L1-level L1b gridded (L1G) data processing (Moy et al., 2017). This technique exploits the fact that at 350 the atmosphere at low altitudes becomes opaque enough not
Figure 3. Example of OMPS-LP radiances profiles at some **selected** wavelengths.

![Figure 3](image)

**Figure 3.** Example of OMPS-LP radiances profiles at some selected wavelengths.

Figure 4. Example of OMPS-LP **SNR**-signal-to-noise ratio at different tangent heights.

![Figure 4](image)

**Figure 4.** Example of OMPS-LP **SNR**-signal-to-noise ratio at different tangent heights.

to let the TP be seen; on the contrary, above 30° limb scattered radiation decreases accordingly with the atmospheric density. So, a comparison between measured and simulated 30°/20° radiances ratio yields an estimate of the applicable tangent altitude correction. Averaged values of the TH corrections span between **Fixed adjustments between** 1 and 2 km (respectively for
are applied independently for each slit, meaning that the instrument points at altitudes higher than expected. Fixed adjustments are applied independently for each slit. Another issue that was discovered after the satellite launch concerns the thermal drift - A TH variation related to the heating up of the instrument - during each orbit, as it is detected when the instrument approaches northern mid-latitudes, sunlight directly hits the limb sensor causing its rapid heating up. As a consequence, both spectral and spatial shifts occur, affecting the three slits in different ways. The related average TH variation is. It is accounted for in L1G data applying a latitudinal dependent correction on the order of 500 m and fixed but latitudinal dependent corrections are actually applied for every orbit, the largest uncertainty of this correction is at northern latitudes, where the solar heating is the greatest. In addition, a This correction remains the same for every orbit. A further dynamic TH variation was detected within each orbit has been detected: intra orbital TH error varies almost linearly, with an almost linear dependence with latitude. The current estimate is around 400 m change from the South to between the South and the North Pole, but a A satisfactory explanation for this variation still has to be found - Currently, and this effect is not corrected for. Finally, long-term drifts and seasonal variations in pointing with a magnitude of 200 have been detected using RSAS results and another scene-based technique. These may also result from errors in the used temperature profile and are not currently corrected currently corrected neither in L1G data nor in our retrievals.

The second important issue that affects the accuracy of the limb radiances 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, as limb scattering is proportional to air density, photons from lower altitudes can be scattered within the instrument to detector areas associated with different altitudes or wavelengths. Furthermore, 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 with the careful application of cutoff filters at the focal plane (Jaross et al., 2014). The full detector response to several point sources was extensively studied during ground testing: a stray light matrix was created, providing the basis for subtracting the stray light contribution from the measured Earth limb radiances. 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. The instrument uses a diffuser in the field of view in order to measure the extraterrestrial solar spectrum and maintain the spectral registration. 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. A related quality flag is reported in L1 data and used in this study for the comparison with NASA retrieval (Kahn and Kowitt, 2015): so-called South Atlantic anomaly.

In this paper, version 2.5 of OMPS-LP L1 gridded L1G data has been used the 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 the RSAS technique for pointing corrections fully implemented (corrections were discussed above) pointing corrections implemented as
discussed above. In addition, both sun-normalized and absolute radiances are provided. In the preparation time of this paper the new data version was not fully released and only seven consecutive months were available, from July 1, 2016 till January 31, 2017. Retrievals were performed using data from the central slit of the instrument only because the lateral slits can still suffer from pointing issues.

2.3 OMPS-LP observation geometry of observations

Several angular coordinates are needed in the retrieval algorithm to correctly describe the observation geometry; satellite azimuth \((\varphi)\), solar azimuth \((\varphi_0)\) and solar zenith angle \((\psi_0)\) at the TP are reported for three THs (25, 35 and 45 km) in the L1-L1G data files and are used to define the geometry of the observation. The solar zenith angle \((\psi_0)\) is defined as the angle between the local vertical at the TP and the sun pointing vector. The azimuth angles \((\varphi \text{ and } \varphi_0)\) are defined as the angles between the direction to the 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; by convention, positive angles are East of the North, so that values are inside the \(-180, 180^\circ\) range. Looking at the OMPS-LP observation geometry and considering only solar zenith angles less than \(80^\circ\) to avoid high stray light levels, the satellite azimuth angle is always negative while the solar azimuth angle changes sign along the orbit. Combining \((\varphi \text{ and } \varphi_0)\) azimuth and zenith angles, the scattering angle \(\theta\) at the TP can be computed as:

\[
\cos(\theta) = \sin(\psi_0) \cos(\varphi - \varphi_0)
\]

This is an important quantity that defines the scattering geometry. In Fig. 5 values of scattering angles together with solar zenith angles are plotted as a function of latitude for three OMPS orbits in different seasons. The 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 \(80^\circ\) are plotted and the ozone retrieval is run only for the corresponding states to avoid high stray light levels. The latitude coverage in different seasons can be assessed from the figure.
Figure 5. 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.

3 Retrieval method

3.1 The retrieval algorithm

The retrieval of ozone profiles is performed using the regularized inversion technique with the first order Tikhonov constraints \( (\text{Tikhonov} \ (1963); \ \text{Rodgers} \ (2000)) \). The non-linearity of the inverse problem is accounted for using an iterative approach. The forward modeling is performed taking into consideration atmospheric multiple scattering in the framework of the approximate spherical mode solver of the SCIATRAN radiative transfer model (Rozanov et al., 2014). The-Thereby, the CDI (Combined Differential-Integral) model-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. Then, an integration along the line-of-sight is carried out calculating the pseudo-spherical approximation means that the single scattering contribution is calculated in a fully spherical geometry and using the pseudo-spherical radiation field to account for while a plane parallel atmosphere is assumed to calculate the multiple scattering contribution (Rozanov et al., 2000). The-Then, an integration along the line-of-sight is performed 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 multiple scattering contribution at each point along the line of sight. The weighting functions are calculated using the same method as for the radiance, but in this case considering only the single scattering contribution only is considered.~
For the OMPS-LP retrieval, linearizing the forward model around an initial guess state \( x_0 \), the general equation that has to be solved can be written as:

\[
y = y_0 + K (x - x_0) + \epsilon
\]  

(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 \( \epsilon \) 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:

\[
x_{i+1} = (K_i^T S_\epsilon^{-1} K_i + S_0 + S_i^T \gamma S_1)^{-1} K_i^T S_\epsilon^{-1} (y_i + K_i x_i)
\]  

(3)

Here, \( S_\epsilon \) 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 (\( S_i^T \gamma S_1 \) is the first order Tikhonov term). It is multiplied by the diagonal matrix \( \gamma \) which contains altitude dependent weights, used to constrain the smoothness of the retrieved profile. In the following, the sum \( S_0 + S_i^T \gamma S_1 \) will be named as \( S_\gamma \).

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 Chappuis band (Chappuis band); the former ranges are sensitive to the upper stratospheric ozone, while whereas the latter to the lower stratospheric region, where the peak of the number density occurs. Details are listed in Table 1. In order to avoid strong absorption bands of water vapor and \( \text{O}_2 \), 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. Limb-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 first 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 the visible range in order to get rid of order to remove slowly-variable spectral features, e.g. caused by aerosol scattering (Rozanov et al., 2011). Eq. (4) explicitly shows the measurement vector at the \( i \)-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.

\[
y_i = \log \left( \frac{I_{TH_i}}{I_{TH_{norm}}} \right) - P_n
\]  

(4)
Table 1. List of the spectral segments considered in for the ozone retrieval with respective corresponding altitude ranges and THs used for the normalization and order of the subtracted polynomial (- means that no polynomial is subtracted).

<table>
<thead>
<tr>
<th>Altitude range [km]</th>
<th>Spectral segment [nm]</th>
<th>TH normalization Normalization TH [km]</th>
<th>Polynomial order</th>
</tr>
</thead>
<tbody>
<tr>
<td>46-60</td>
<td>285-300</td>
<td>63</td>
<td>3</td>
</tr>
<tr>
<td>35-46</td>
<td>305-313</td>
<td>52</td>
<td>3</td>
</tr>
<tr>
<td>31-36</td>
<td>322-331</td>
<td>47</td>
<td>0</td>
</tr>
<tr>
<td>12-33</td>
<td>508-660 †</td>
<td>42</td>
<td>1</td>
</tr>
</tbody>
</table>

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

In the forward model, the following molecular species with radiation is calculated taking into account O₃, NO₂ and O₄, which have spectral signatures in the selected spectral ranges are considered and. Cross sections of these gases are respectively 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. In order to avoid absorption lines of water vapor and of wavelengths between 580.0 and 607.0 and between 620.0 and 635.0 are rejected. A complete treatment of these absorption features requires line-by-line calculations, that are computationally expensive. Ancillary pressure and temperature profiles used in the radiative transfer model are taken from the Global Modeling and Assimilation Office (GMAO) interpolated data set, provided by the NASA team together with OMPS-LP L1G radiances.

At a pre-processing step 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. In the UV range no As the shift and squeeze correction is applied. Linearizing the forward model around an initial guess state \(x_0\), the general equation that has to be solved can be written as:

\[
y = y_0 + K(x - x_0) + \epsilon
\]

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 containing the retrieved ozone vertical distributions in terms of Volume Mixing Ratio (VMR), and \(\epsilon\) 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, algorithm works with the differential absorption structures, it cannot be applied in the UV range. Furthermore, as the UV retrieval uses either normalized radiances themselves or their slopes, the iterative step \(i+1\) can be expressed as:

\[
x_{i+1} = (K_i^T S_{\epsilon}^{-1} K_i + S_0 + \gamma S_i^T S_1)^{-1} K_i^T S_{\epsilon}^{-1} (y - y_i + K_i x_i)
\]

Here, influence of a possible spectral misalignment is rather small. In the pre-processing procedure, we obtain the \(S_{\epsilon}\) is the measurement noise covariance matrix. It is obtained matrix from the fit residuals after the pre-processing procedure, assuming
that absorption features from gases other than H2O, fitting absorption features of all relevant gases in the selected windows are negligible, while is fitted. $S_0$ is the diagonal matrix optimized to constrain the solution within physically meaningful values and minimize the 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 VMR is very small. Finally, $S_1$ is the first order derivative matrix ($S_1^T S_1$ is the first order Tikhonov term), weighted by a parameter $\gamma$ that linearly increases with height above 45 km, used to constrain the smoothness of the retrieved profile. In Eq. (7), the sum $S_0 + \gamma S_1^T S_1$ will be named $S_1$. The information content of the measurements as well as the sensitivity of the retrieval can be analyzed using the averaging kernels ($A$) and the covariance of retrieval noise ($S_m$) obtained respectively as (Rodgers, 2000):

$$A = (K^T S_\epsilon^{-1} K + S_r)^{-1} K^T S_\epsilon^{-1} K$$

$$S_m = (K^T S_\epsilon^{-1} K + S_r)^{-1} K^T S_\epsilon^{-1} K (K^T S_\epsilon^{-1} K + S_r)^{-1}$$

The square root values of spectral windows.

The inversion scheme is then iteratively run employing the Eq. (3). The state vector $x_{i+1}$, containing the retrieved ozone vertical distribution at each 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 the retrieval noise covariance matrix $S_m$ are commonly referred to as the theoretical precision of the retrieval. The vertical resolution of the retrieved profile is computed as the inverse of the diagonal elements of the averaging kernel matrix, scaled by the altitude grid width. Examples of averaging kernels, vertical resolution and theoretical relative precision are plotted in Fig. 7. One can notice that below 35 km, linearly increase with the height above 45 km the actual vertical resolution of the retrieval scheme is about 2.3 with a peak around 35 where the transition between UV and VIS spectral regions occurs. The relative uncertainty of the ozone profiles is in the range 1.5% above 25 km and increases up to 10-20% below 20 km, remain constant below.

From left to right, examples of averaging kernels (plotted every 4 for sake of clarity), vertical resolution and theoretical relative precision of the retrieval scheme, for a measurement at 30°N.

Simultaneously with the ozone retrieval, surface albedo in UV and VIS spectral ranges is estimated exploiting the sun normalized product: the two spectral intervals between 355 and 365 nm and between 455 and 470 nm are used, where ozone absorption has a minimum, and three. 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 considered employed: 355–365 nm and 455–470 nm, where ozone absorption is weak.

In order to tailor the retrieval scheme to OMPS LP data, a three-way approach is followed: 1. An evaluation of ozone weighting functions is performed. Each selected spectral interval contains information originating from a range of altitudes that could be estimated analyzing the ozone weighting functions. Each of these spectral segments is used at those THs where it provides most information on ozone VMR. 2. An analysis of spectral fits is carried out, to detect spectral ranges where the model fit is not satisfactory. During the test phase, spectral ranges are adjusted looking at fit residuals and at the structure of the retrieval profile: oscillations or unexpected jumps between different altitude regions are avoided. 3. An evaluation of the averaging kernels is done. As we mentioned above, the worst values of the vertical resolution of the retrieval are found around...
which is in the transition region between dominating contributions from VIS and UV ranges. The choice of the spectral interval for this altitude is aimed at optimizing the vertical resolution of the retrieval.

3.3 Cloud Filter

A cloud filter is applied during the ozone retrieval to reject THs affected by the presence of clouds 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 the ratio of the radiance at the two chosen wavelengths for the same OMPS-LP statespectrum. The CI is an altitude dependent quantity and can be used to detect the 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:

\[
CIR(z_{thTH}) = \frac{CI(z_{th})}{CI(z_{th} + \Delta z_{th})} \frac{CI(z_{TH})}{CI(z_{TH} + \Delta z_{TH})}
\]

where \(\Delta z_{TH}\) is the vertical grid step of 1 km. An example of the results for simulated clouds is reported in Fig. 6: cirrus clouds consisting of hexagonal crystals with an optical depth between 0.01 and 0.15 are taken into consideration. Since the ozone retrieval is run above 12 km, we are generally not interested in liquid water clouds.

![Figure 6](image)

**Figure 6.** Example of Color Index Ratios for different simulations of ice clouds. Top of the cloud and optical depth (\(\tau\)) ranges are chosen to simulate the impact of thin cirrus clouds in the upper troposphere.

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 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 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 nm is considered for each observation above 50° N and below 50° S; if the radiance between 40 km and 80 km increases for 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

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 coarser spectral resolution than SCIAMACHY, the retrieval at 750 nm as used for SCIAMACHY is sub-optimal because of the influence of the O₂ absorption band. Instead, a wavelength of 868.8 nm is chosen. Stratospheric aerosol extinction is retrieved in the altitude range from 10.5 km to 33.5 km. The spectrum at 34.5 km is used as the reference; the 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 particle size distribution is assumed to be lognormal with the median radius \( r_\varnothing \) of 0.08 µm, and distribution width parameter \( \sigma \) of 1.6. This distribution is described by the following equation:

\[
 n(r) = \frac{N}{\sqrt{2\pi} \ln(\sigma) r} \exp \left( \frac{\ln(r_\varnothing) - \ln(r))^2}{2 \ln^2(\sigma)} \right)
\]  

(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 averaging three altitude levels above the cloud. The aerosol retrieval is particularly important at latitudes where the scattering angle is high (Fig. 5).

4 Satellite data set comparisons

OMPS ozone profiles are retrieved for seven months, from July 2006 to January 2007, limited by the availability of v2.5 L1G data at the time of writing this paper. Retrievals were performed using data from the central slit of the instrument only because the lateral slits can still suffer from pointing issues.

4.1 NASA retrieval Retrieval characterization and comparison error analysis
The information content of the measurements as well as the sensitivity of the retrieval can be analyzed using the averaging kernels \( A \) and the covariance of retrieval noise \( S_m \) obtained respectively as (Rodgers, 2000):

\[
A = (K^T S_e^{-1} K + S_r)^{-1} K^T S_e^{-1} K \quad \quad S_m = (K^T S_e^{-1} K + S_r)^{-1} K (K^T S_e^{-1} K + S_r)^{-1}
\] (7)

The square root values of the diagonal elements of the retrieval noise covariance matrix \( S_m \) will be referred to as the theoretical precision of the retrieval. 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. 7. One can notice that below 35 km the actual vertical resolution of the retrieval scheme is about 2–3 km with a peak around 35 km where the transition between UV and Vis spectral ranges occurs. The theoretical precision of the retrieved ozone profiles doesn’t show a strong dependence on the solar zenith angle. It lies in the range 1–5 % between 25 and 50 km and tends to increase in the upper stratosphere and in the Upper Troposphere - Lower Stratosphere (UTLS) region.

**Figure 7.** 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 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 km).

### 4.2 Comparison with NASA OMPS-LP ozone product

To retrieve ozone profiles from OMPS-LP observations, the NASA team has implemented the Environmental Data Record algorithm that processes L1 together with the provided ancillary data, in, 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 exploited for the latter task: UV wavelengths are used between 30 and 60\(\) between 29.5 and 52.5 \(\) km, while wavelengths in the Chappuis band (520 and 650 between 12.5 and 37.5 \(\) km is used between 6 and 40 \(\) km (the bottom height depends on the detected cloud top altitude). The NASA retrieval algorithm is based on an inversion scheme with a priori constraints and a Tikhonov regularization. The normalization of the radiances is performed with respect to high altitude TH measurements: 6555.5 \(\) km in UV and 4540.5 \(\) km in VISVis. 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. Comparison between NASA-OMPS retrieval and our results (in the following called IUP-OMPS) is reported in Fig. 8 for the tropical region. Only measurements at solar zenith angles less than 80\(\) have been considered to avoid stray light issues. At the moment of the submission of the paper, only version 2 of Level 2 (L2) NASA product was available, so a comparison with the most recent retrieval could not be performed. An additional TH correction is applied by NASA team on L1G data, as described in the Release Notes (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 Rault and Loughman (2013) DeLand et al. (2017)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Doublet (\lambda_0)</td>
<td>355353 nm</td>
</tr>
<tr>
<td>Triplet (\lambda_t)</td>
<td>500510 nm</td>
</tr>
<tr>
<td>Triplet (\lambda_r)</td>
<td>680675 nm</td>
</tr>
<tr>
<td>Wavelength used in UV (nm)</td>
<td>289.3, 303.0, 308.9, 311.6, 318.0, 312.7, 302, 312, 322</td>
</tr>
<tr>
<td>Wavelength used in VISVis (nm)</td>
<td>522.8, 526.3, 549.9, 554.3, 572.1, 576.9, 602.5, 608.1, 613.4, 619.6, 621.8, 637.4, 643.4, 649.7, 7600</td>
</tr>
</tbody>
</table>

A direct comparison between NASA and IUP-OMPS retrieval products is reported in In version 2.5 of NASA L2 data, independent profiles for the Vis and UV retrieval are provided, Fig. 8, showing relative differences 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 number density for the tropics. In panels (b) and (c), relative differences are shown for the tropical region, southern and northern mid-latitude bands. Differences are generally within \(\pm 10\%\). Throughout the paper, relative differences are computed as:

\[
\text{Rel diff} = \frac{2 \times (\text{IUP-OMPS} - \text{Reference data set})}{(\text{IUP-OMPS} + \text{Reference data set})} \times 100
\]

Considering the Vis NASA retrieval in panel (b), the agreement is particularly good for the tropical region above 20 km; in, as it is also in panel (a). Looking at mid-latitudes, IUP-OMPS values are generally higher with respect to the NASA product. The peak values around 25, especially between 22 and 32 km are generally lower than in the IUP results in all the latitude bins. In the lower stratosphere we can also note a disagreement between the two profiles, with the IUP data showing lower values in all latitude bands. Considering the UV NASA retrieval in panel (c), an agreement within \(\pm 5\%\) is found in almost all the cases, even if higher values are shown by IUP-OMPS around 45 km at mid-latitude.
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 and nighttime profiles of several gases. For a detailed description of the **satellite suite** 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 measurements. The geographic distance between the centers of the two instrument footprints is required to be within 1° latitude and longitude and the time difference is required to be within 6 h. Only measurements at solar zenith angles less than 80° are considered and In addition, the difference in the modified 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 form 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 latitudinal bands are selected for the comparison: 40° N–60° N, 20° S–20° N and 60° S–40° S. Fig. 9 shows the averaged profiles for the tropics.
and relative differences (Eq. 8) in the three latitudinal bands. Standard deviations are reported in the plots as shaded areas. The number of collocations per band is in the order of $\sim 5000$.

**Figure 9.** Panel (a): collocated IUP-OMPS retrieved profiles and MLS ozone product in the tropical region. Panel (b): relative difference profiles (Eq. 8) in the three latitudinal bands (40°N–60°N, 20°S–20°N and 60°S–40°S), with standard deviation deviations shown as shaded areas.

In Fig. 10 shows the relative differences between IUP-OMPS and MLS are shown 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, we can see that between 20 and 50 km the differences are generally within ±10%. An exception is the positive difference (meaning that OMPS shows higher values) found in the lower tropical stratosphere, with values that locally exceed 30%.

Starting the discussion from the bottom of the plots, positive differences larger than 30% are found in the tropical UTLS region. This large discrepancy can be related to multiple factors such as the different vertical resolution. Different vertical resolutions of the instruments, the generally low sensitivity to ozone in the lowermost retrieval altitude range or issues with the cloud filtering. At mid-latitudes around 25 km a positive difference of 5–10% is found observed. This bias can be related to the water vapor treatment inside the retrieval scheme: the intensity of the ozone number density peak is found to be sensitive to the choice of the spectral points that are skipped in the Chappuis band, where H$_2$O has non-negligible absorption. Around 45 km, higher values are shown by IUP-OMPS at northern mid-latitudes, especially during winter months (panel c). This issue, already found in Fig. 8 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 also notice a significant discrepancy towards northern latitudes (> 70°) above 40 km; this disagreement can be partly related to pointing issues, due to the solar heating of the instrument at high latitudes, or stray light. A similar deviation was also found comparing the stray light affecting the TH normalization at 63 km. 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
Figure 10. Relative differences between IUP-OMPS and MLS (Eq. 8) averaged over 2.5° wide-latitude bins, plotted as a function of altitude. 
Panel (a) 6 months, panel (b) July and August, panel (c) December and January

screening of these clouds in IUP-OMPS and NASA retrievals at these high latitudes above 40 data, while MLS observations are found not to be affected by the presence of PMCs (Bak et al., 2015). Above 50 km (not shown) 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. This points out possible issues in our retrieval settings, related to not screened polar mesospheric clouds, the spectral range considered in the Hartley band or to the TH normalization at 63. Furthermore, a dip around 50 km 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 smoothing-Tikhonov parameter is expected to partially attenuate the latter problem. To summarize, this comparison shows a general validity of IUP-OMPS retrieval between 18 and 58 km, even if during different seasons the relative bias with respect to MLS exceeds by 10 % in some limited atmospheric regions.

5 Ozone sondes comparison

4.1 Comparison with ozone sondes

Ozone sondes data are obtained from WOUDC (World Ozone and Ultraviolet Radiation Data Center) and SHADOZ (Southern Hemisphere ADDitional OZonesondes, Thompson et al., 2007) archives are used in this analysis. Looser collocation criteria than for MLS are selected (Southern Hemisphere ADDitional OZonesondes, Thompson et al., 2007) archives. We selected looser collocation criteria compared to MLS, because of the sparseness of the data set. In particular, ozone sondes measurements. Therefore, OMPS-LP measurements are required to be within 5° in latitude and 10° in longitude from the ozone sondes station and within ±24 ±12 h time span about around the sonde launch. Generally, for each sonde profile more than one
all collocated OMPS-LP measurement is found using these loose criteria; therefore, all the collocated retrieved profiles observations are averaged before the comparison. Ozone profiles are smoothed to the vertical resolution of the OMPS-LP retrieval grid, by using averaging kernels. For each collocated sonde profile, first the AKs as follow. First, we calculate the linear interpolation matrix $L$ 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 $L^\ast$ as:

$$L^\ast = (L^T L)^{-1} L^T$$  \hspace{1cm} (9)

Then the ozone profile $x_{fine}$ is smoothed as follows:

$$x_{coarse} = A \times L^\ast \times x_{fine}$$ \hspace{1cm} (10)

The upper point altitude of the smoothed profile is set chosen at the OMPS-LP grid point whose respective averaging kernel level whose corresponding AK altitude range is fully covered by the sonde profile. An alternative approach to this smoothing consists in approach alternative to the AK smoothing assumes a simple vertical average, considering 2.5 km (i.e $\pm 1.25$ km) ranges around each grid point (value corresponding to an average vertical resolution of the retrieval scheme below 30 km, refer to Fig. 7). The altitude where a cloud is detected by the cloud filter algorithm and all the and all altitudes below are screened out. Latitude bins are selected as for the previous comparisons. Averaged collocated profiles over Fig. 11 shows averaged collocated profiles in the tropical and northern mid-latitude bands are shown in Fig. 11, with respective with corresponding standard deviations. On the left side of these plots, the number of available collocations at each altitude is also reported, which is about 120 and 160 for tropical and northern mid-latitude bands, around 120 and 160 sonde profiles, respectively, are considered respectively.

Fig. 12 shows the relative differences (Eq. 8) in the three latitudinal bands, in panel (a) using the averaging kernel smoothing approach and in panel (b) the vertical averaging. Differences between the two panels of this figure show that the smoothing 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 can be seen also from Figs shown in Figs. 11, the agreement and 12, an excellent agreement is found at northern mid-latitudes is remarkably good, with relative differences below within $\pm$ 5 % between 14 and 30 km. Focusing on the tropical region, a bias between the two data sets is clearly visible, with differences around 5–15$\%$ between 20 and 32 km. This positive bias is unexpected considering the good agreement found when comparing to MLS data in the same region. In the lower stratosphere 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 % between 20 and 30 km 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 over within the considered time span.

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 latitudinal bands are shown in
Figure 11. 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.

Figure 12. Relative differences between collocated IUP-OMPS profiles and ozonesonde measurements in the three latitudinal bands (40° N–60° N, 20° S–20° N and 60° S–40° S), using in panel (a) averaging kernel smoothing and in panel (b) vertical averaging. Respective corresponding standard deviations are shown as shaded areas.

Fig. 13, following the averaging kernel smoothing approach. Since most of the sondes considered over the period Jul 2016–Jan 2017 come from the SHADOZ archive, we also take only measurements from the same archive for the 2013 validation: over the whole year, around 140 collocations are available from 10 stations. In Fig. 13, focusing the attention on the
differences in the tropical region, we can see that at least between 20 and 30 km the bias is within 5%; larger discrepancies are still evident in the lower stratosphere. Further investigations about a comparison with MLS shows a very similar pattern to the one found for the 2016 data set. Further investigations of possible reasons for the observed behavior are ongoing. 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 v2.5 L1-gridded L1G data were processed, analyzed and validated. 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, with discrepancies within 10 ± 5% between 20 and 58 km in all considered latitude bins. The, and a bias of about 10% at 30 and 45 km at northern mid-latitudes. We presented the results of the validation against MLS v4.2 ozone profiles and ozonesonde measurements from SHADOZ and WOUDC archives were presented. A good agreement was found with the MLS ozone product: relative differences were generally within ± 5% between 15 and 48 km. On the other hand, we observed a larger discrepancy between
IUP-OMPS retrievals and MLS in the tropical lower stratosphere was observed UTLS region, related most probably to the decreasing sensitivity of limb retrievals from both instruments in this region. A strong discrepancy above 10 % in the upper stratosphere beyond 70° N can be related to different issues: problems in the pointing of the instrument or high-altitude stray light, disturbance from polar mesospheric clouds, or is related to a sub-optimal normalization at the upper THPMC screening. In regard to the comparison with ozonesondes, at northern mid-latitudes differences within ± 5 % were found between 14 and 30 km. Focusing on the tropical region, a consistent positive bias with SHADOZ measurements was detected, unexpected after the good agreement observed with MLS data. However, the processing and validation of the 2013 data set, using the same retrieval settings, revealed a much better agreement consistency. The reasons for this behavior are still under investigation. 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 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 L2-v2.5 L1G OMPS-LP data were downloaded from https://ozoneaq.gsfc.nasa.gov/data/omps/, where v2.5 L1 gridded data are now 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, 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 from https://tropo.gsfc.nasa.gov/shadoz/Archive.html. Our results are available upon request to at 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.

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