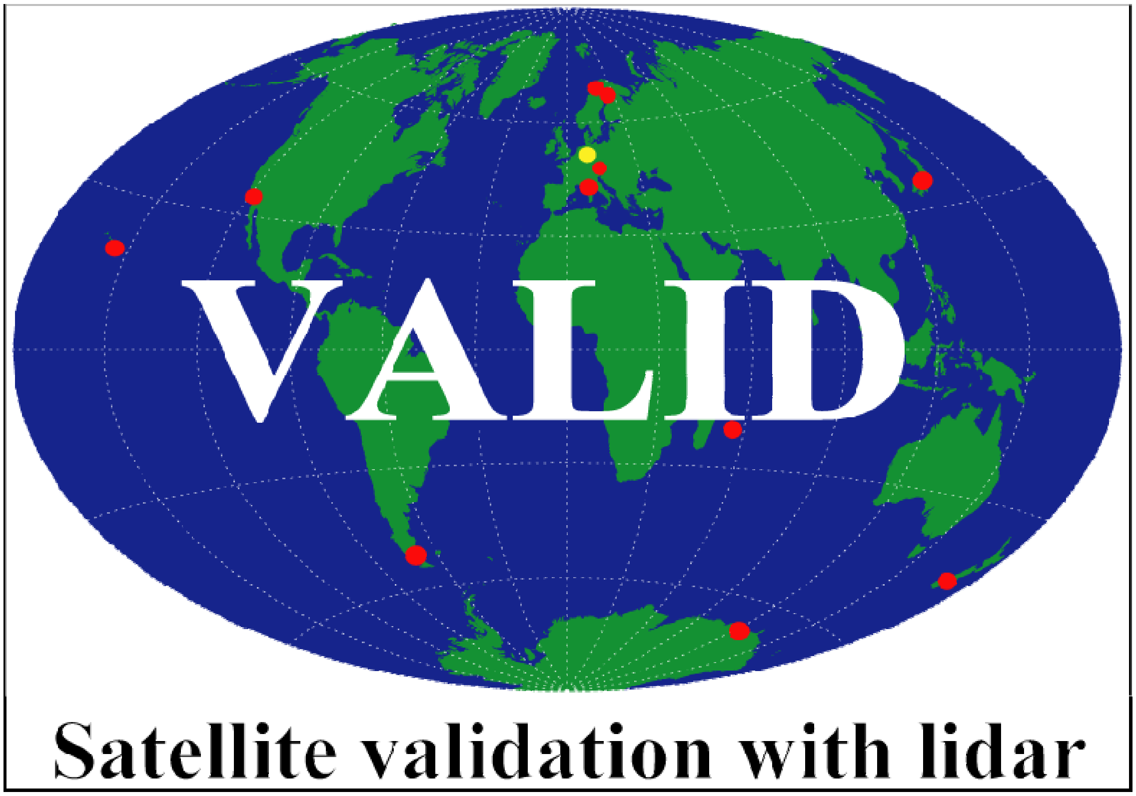
Validation of GOMOS version 6.01 ozone profiles using ground-based lidar observations



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Introduction

In this study we have compared GOMOS IPF version 6.01 ozone profiles for the years 2002 to 2011 with lidar profiles. Simultaneously, the GOMOS data of the previous version (IPF 5.00) of the same period were also compared to the validation data. Although the processing and selection procedure (e.g. maximum allowed error) results in a different extent of the finally selected GOMOS data for the two versions, the majority used should to correspond to the same occultations. Recommendations from the GOMOS quality working group have been taken into consideration where possible.

Methodology

GOMOS data have been read with BEAT version 6.6. For GOMOS version 6.01 ozone error profiles, the data were converted as following the implementation in GOPR 7. In parallel, data from version 5 for the same years were also acquired to allow for a comparison between the two versions.

Data were grouped into different selections based on observation characteristics (such as obliquity) and data quality (reported error). This results in a slightly different selection for the two versions of GOMOS data as the uncertainties are calculated differently.
A maximum allowed error in both the lidar data and the GOMOS data of 30% was chosen in accordance with previous studies. Furthermore, the retrieved GOMOS data had to have a ozone concentration flagged valid. Note that reported errors from the lidars have distinct meaning amongst the different PIs. The lidar data have been used in the altitude range 18 to 45 km for ozone comparisons.

Collocations had to fulfil the following requirements: a maximum difference between GOMOS and validation observations of 800 km in space and 20 hours in time. All datasets were interpolated to a common altitude grid.

In an additional analysis, equivalent latitudes have been calculated from ECMWF era-interim potential vorticity data (475K) to allow for collocations in more similar air masses. Adding such a requirement reduces the number of collocations substantially (~factor 2) and therefore validation results have also been presented without specifying a maximum difference in equivalent latitudes condition.

Illumination conditions (following solar zenith angle).

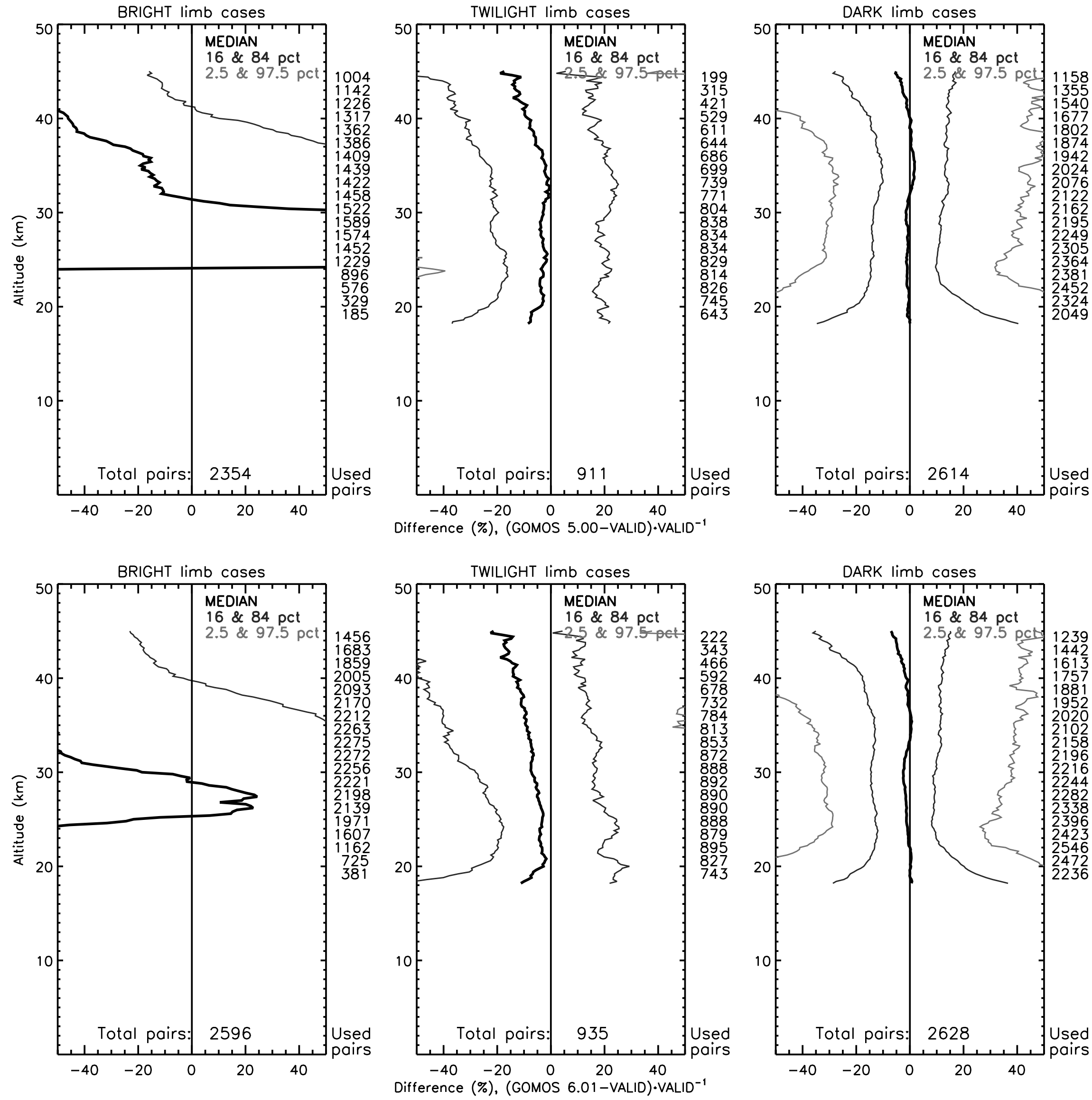

Figure 1. Validation results for GOMOS version 5.00 (top) and version 6.01 (bottom) in comparison to lidar data, grouped by solar zenith angle (sza): left panels – bright limb (sza = [0°,90°]); middle panels – twilight limb (sza = <90°, 108°>; right panels – dark limb (sza = [108°, 180°]). Shown are the 2.5th, 16th, 50 (median), 84th and 97.5th percentiles of the relative difference (lidar data as the reference) as a function of altitude. On the right side of each panel is listed the number of used collocations at a given altitude and the total number of pairs used is listed at the bottom of each panel.

Figure 1 shows the comparison of lidar ozone profiles with GOMOS version 5.00 (top) and version (6.01) grouped by the solar zenith angle of the GOMOS limb. More collocations are available for version 6.01 under all illumination conditions and over all altitudes. The bright limb retrieval of the operational processor is still not producing usable data. The retrievals in twilight show a negative bias that is increasing with altitude and that is somewhat stronger in version 6.01. The spread between the 16th and 84th percentiles has increased, especially the lower boundary is indicating a higher presence of too low ozone concentrations.

In contrast, the spread has reduced for version 6.01 data acquired with solar zenith angles of 108° or greater. Here we also observe a small change of a few percent of the bias towards the negative above 25 km.

Illumination conditions (following flag in product).
Inside the operational products are also flags for the illumination condition following a different set of criteria (see the GOMOS handbook).

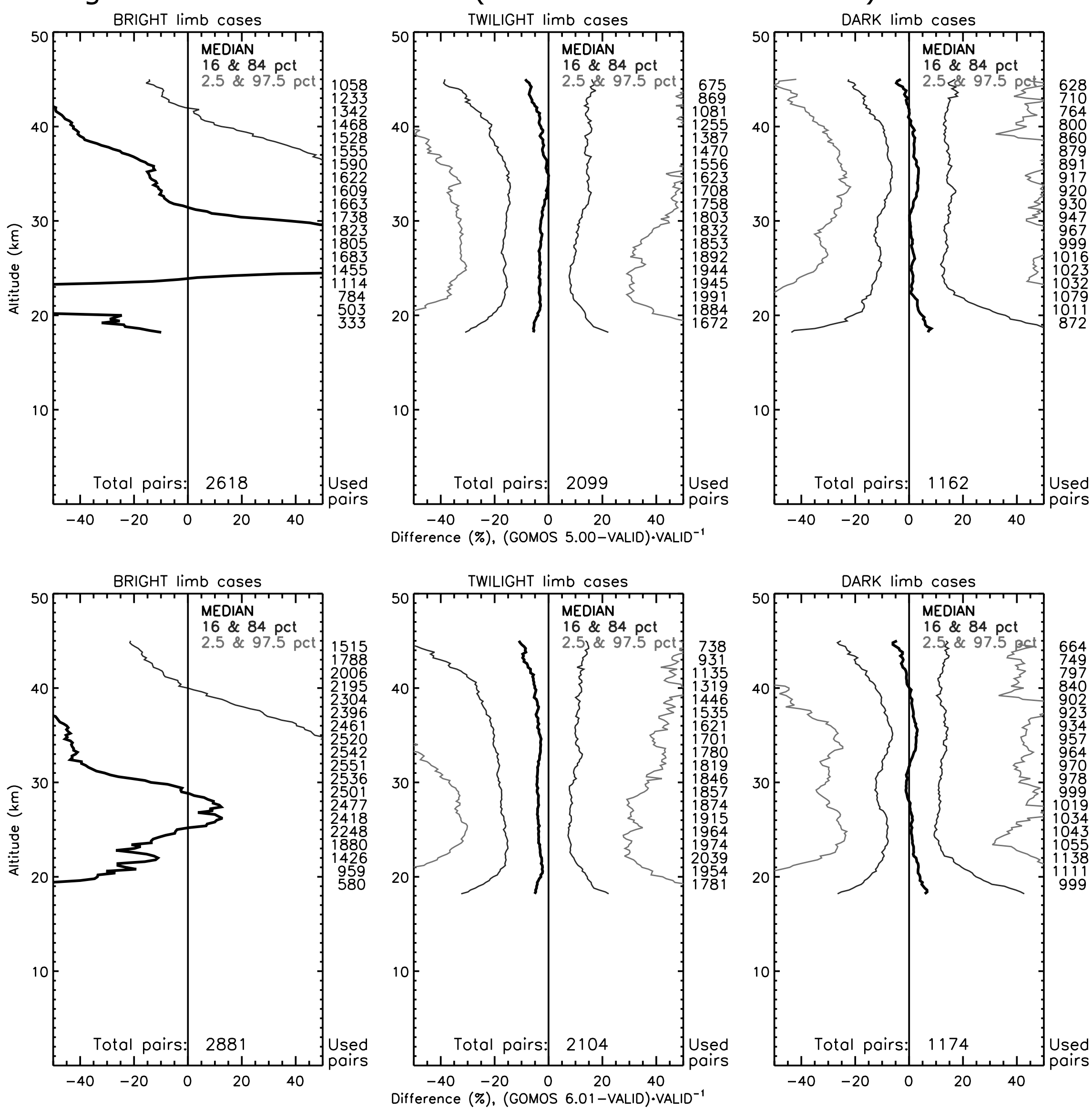

Figure 2. As Figure 1 but following the illumination condition flags inside the GOMOS products. Note that the twilight group also covers straylight contamination (flags 2-4).

Figure 2 shows the comparison with lidar following the grouping by these flags. We can see that more data are classified as having a bright limb and the group with dark limb conditions is more than halved, with most of those removed now falling into the group 'twilight'. As a consequence, the agreement with lidar shows an improvement with respect to Figure 1 for this group, but the underestimation by GOMOS is clear. The 'dark limb' flagged group has a relatively more positive bias for both versions than those data just selected to have a solar zenith angle greater than 108° (Figure 1 right panels). Again, version 6.01 data show a small negative shift of the median difference with lidar in comparison to version 5.00.

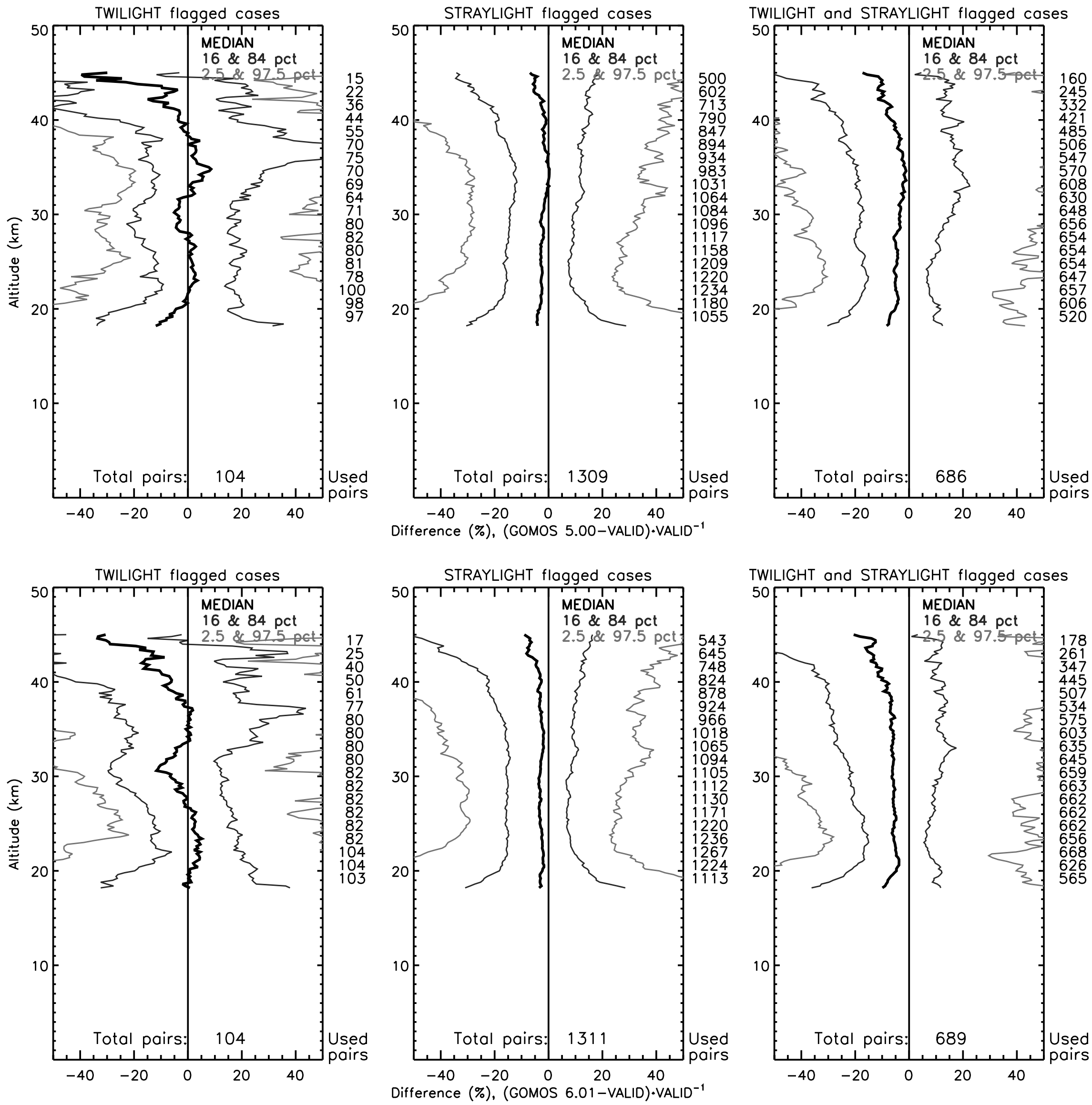

Figure 3. Validation results for version 5.00 (top) and version 6.01 (bottom) for twilight (left), straylight (middle) and twilight plus straylight (right) contaminated flagged GOMOS data.

Figure 3 shows that the greatest part of the twilight data is composed of data flagged straylight contaminated, followed by the data flagged twilight and straylight contaminated. Agreement with the lidar is best for both versions best for the straylight contaminated data, although there is a consistent underestimation of the ozone concentration, which is stronger for version 6.01.

Latitude

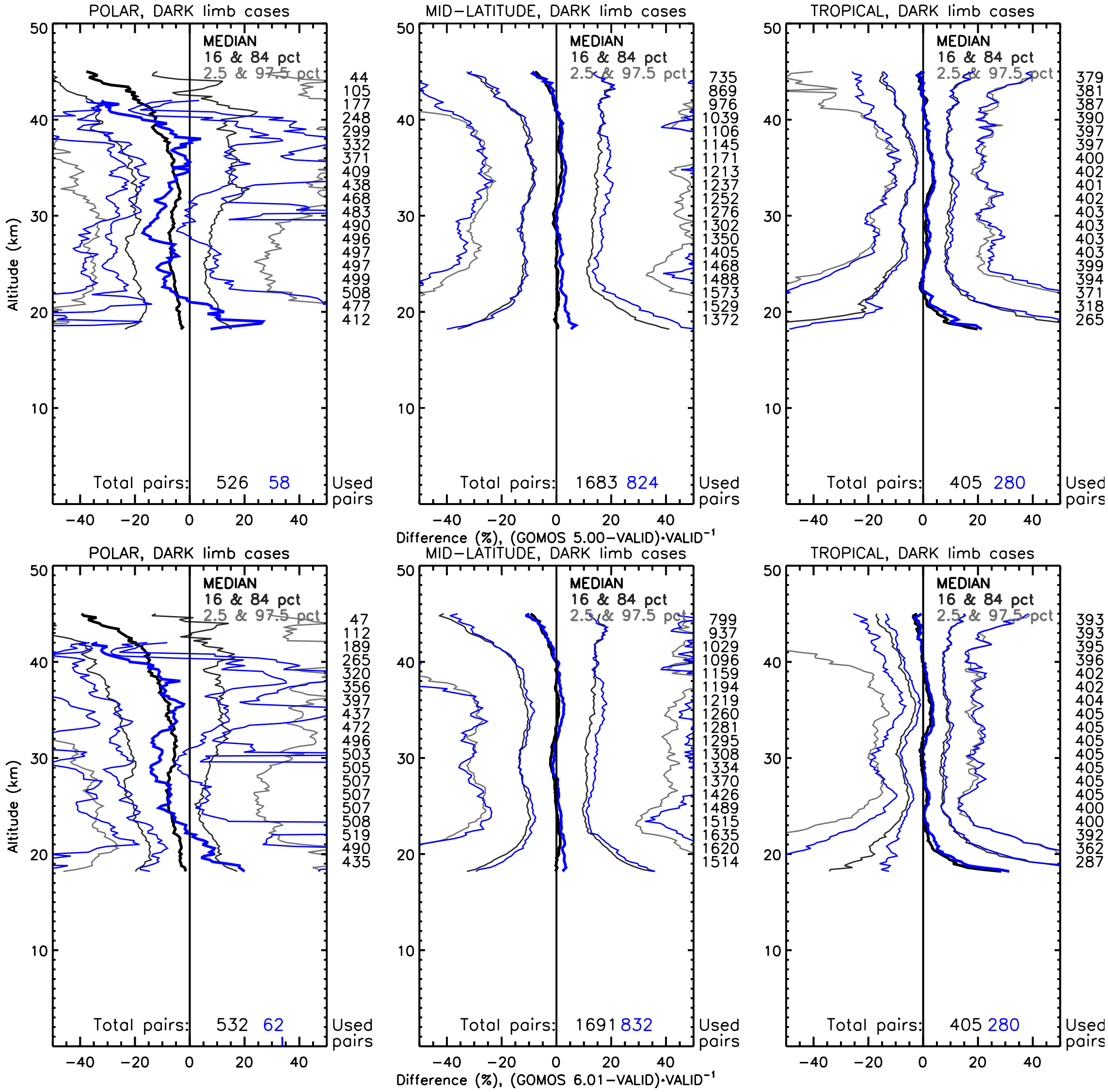

Figure 4. Validation results grouped by latitude class for version 5.00 (top) and version 6.01 (bottom) for data flagged dark (blue) and data with a solar zenith angle greater than or equal to 108° (black). Left panels: polar regions (|latitude| ≥ 66.5°); middle panels: mid-latitudes (23.5° ≤ |latitude| < 66.5°); right panels: tropics (|latitude| < 23.5°). Note that the number of collocative pairs per altitude is only given for the data with a sza ≥ 108°.

If we now split the datasets into three groups of latitude bins and overlay the two selections (solar zenith angle ≥ 108° and illum_cond flag = 0), we can see (Figure 4 bottom panel and Table 1) that largest differences occur in the polar regions and at low altitudes. Few collocations (at most 62 for a given altitude) are available in the polar regions that are flagged 'dark'. In the tropics and mid-latitudes differences are at most 1% except below 20 km, where the data flagged 'dark' have more positive median differences.

Comparing version 5.00 with version 6.01 median differences (Table 1 upper row with Table 2 and black lines in Figure 4 upper with lower panels) the largest differences (2 to 4%) between the two versions occur in the tropics below 25 km (version 6.01 larger), in the polar regions above 30 km and above 40 km for the mid-latitudes and tropics (version 6.01 lower). Outside these ranges (61%) differences between the versions are 0 or ±1%.

Table 1. Percentile differences between GOMOS version 6.01 ozone profiles and lidar data for different latitude zones. Given are the median difference and the 68% interquantile spread at a representative altitude (e.g. 22.5 km for the class 20 to 25 km). Top part corresponds to GOMOS data with a solar zenith angle ≥ 108° (black lines in Figure 4), bottom part to validation for GOMOS data flagged dark (illum_cond=0, blue lines in Figure 4).

Sza ≥ 108°	Polar		Mid-latitudes		Tropics	
Altitude	median	68-iq spread	median	68-iq spread	median	68-iq spread
<20 km	-3	29	0	51	+11	72
20-25 km	-5	24	+1	23	+1	23
25-30 km	-8	30	-1	23	0	14
30-35 km	-6	36	0	24	+1	15
35-40 km	-11	41	0	27	+1	12
40-45 km	-21	51	-3	44	-2	20
Flag = dark						
<20 km	14	71	+3	51	+15	61
20-25 km	-2	120	+2	22	+2	21
25-30 km	-9	30	0	26	+1	14
30-35 km	-12	31	+1	25	+2	15
35-40 km	-10	56	+1	29	+2	11
40-45 km	n/a	n/a	-3	43	-2	19

Table 2. As Table 1 (upper half) but for GOMOS version 5.00 ozone profiles.

Sza ≥ 108°	Polar		Mid-latitudes		Tropics	
Altitude	median	68-iq spread	median	68-iq spread	median	68-iq spread
<20 km	-3	29	0	59	+7	95
20-25 km	-6	24	0	26	-1	28
25-30 km	-7	30	0	25	+1	16
30-35 km	-3	38	+1	25	+2	16
35-40 km	-8	40	+1	26	+2	13
40-45 km	-19	46	-1	42	0	21

In the following part we will show comparisons with the GOMOS data having a solar zenith angle greater than 108°. This will include data flagged to have straylight and/or twilight contamination, but increases the size of the dataset.

Equivalent latitude filtering

A further filtering using the calculated difference between the ground-based and satellite data in equivalent latitude at 475K from the ERA-interim data was carried out in order to see if differences are introduced by comparing two distinct air masses. This would be expected to occur especially in the polar regions where large dynamics are seen in Spring.

Figure 5 shows that such filtering reduces the available data by more than two. The spread is well reduced and the mean better follows the median difference below 30 km. Above differences between the mean and median difference have increased. The median difference is nearly the same before and after filtering though (before filtering it is smoother due to the larger dataset), except below 21 km where filtering makes the negative bias larger. Note that a large part (~3/4) of these equivalent latitude-filtered measurements are flagged in the product as being straylight contaminated.

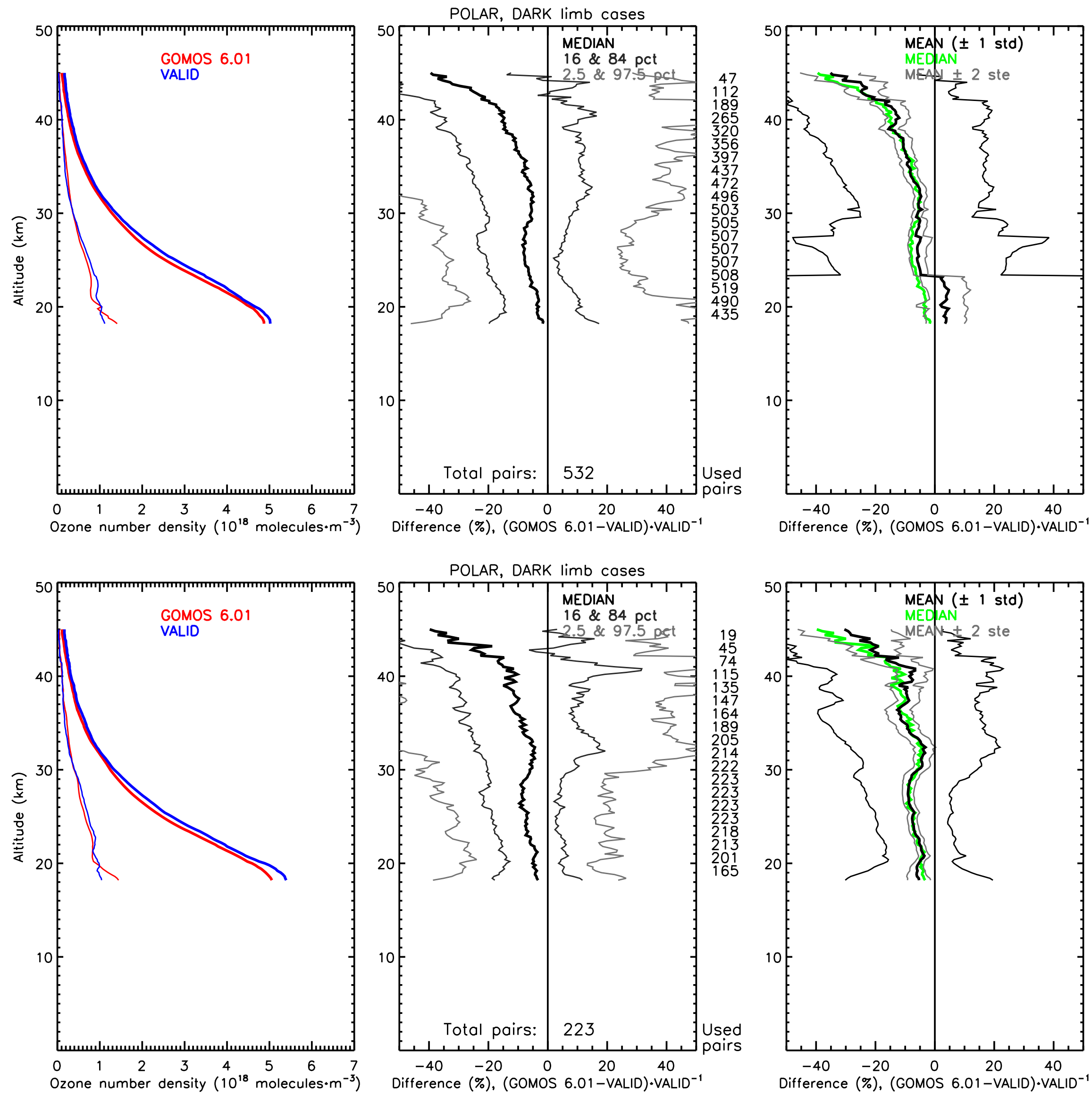

Figure 5. Comparison of GOMOS ozone profiles with lidar in the polar regions. Top: all data with solar zenith angle ≥108°; bottom: further filtering with a maximum difference in equivalent latitude of 5°. Left panels show the mean ozone profiles for GOMOS (red) and lidar (blue) as a function of altitude together with their respective standard deviation as thin lines. Middle panels show the relative differences in percentiles as in previous figures. Right panels show the median (green), mean (thick black line) ± 1 standard deviation (thin black lines) and mean ± 2 standard error (gray).

Observation geometry

The GOMOS data have also been grouped by the azimuth angle of the observation. Three classes were defined: slant view: 10° to 45°, back line of sight: -10° to 10°, and side-way looking line of sight: 45° to 90°.

Figure 6 shows the validation results for three classes for version 5.00 in pink and version 6.01 in black. Best agreement between the two versions is reached for the side line of sight (max. 285 cases), whereas discrepancies between the two versions appear to be largest for the slant line of sight (max. 1583/1593 cases). Also in the back line of sight (max. 746/745 cases) we see a small shift for version 6.01 in all percentiles to a more negative difference.

Note that the window of allowed azimuth angles has changed various times during the course of the GOMOS mission. See the last GOMOS monthly report for an overview table of the changes in these windows.

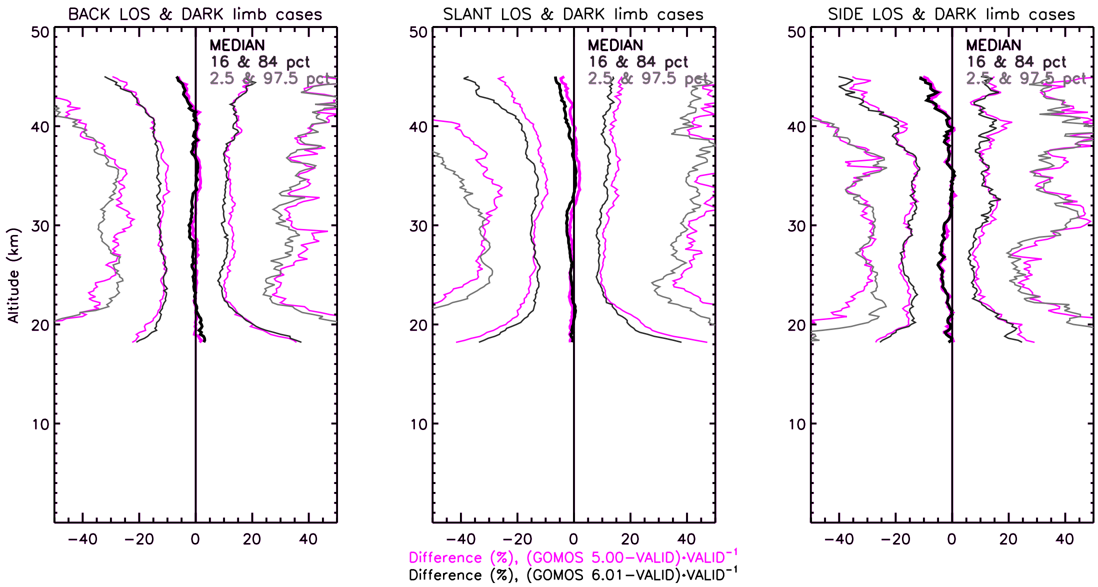

Figure 6. Comparison of version 5.00 (pink) and version 6.01 GOMOS ozone profiles with lidar grouped by azimuth angles. Left: back line of sight, middle: slant line of sight, right: side line of sight.

Stellar properties

Figure 7 presents the mean ozone profiles for GOMOS and lidar together with the standard deviation of the data (left panels) as well as the relative differences (right panels) for version 5.00 and version 6.01 splitting the data into cool and hot stars used in the GOMOS retrieval. We can see differences between the average GOMOS profiles and standard deviations below ~25 km for the two versions and for both cold and hot stars. In comparison to the lidar, the relative differences show a change for cool stars between version 5.00 and 6.01 (with 6.01 underestimating the ozone concentrations), whereas for hot stars relative differences are very similar for the two versions. The total number of pairs used is similar for the two versions, but for cool stars, the number of pairs used at a given altitude is often higher in version 6.01. This is likely due to the filtering on maximum error allowed and the difference in computation of the GOMOS error. Best agreement with lidar is thus achieved for hot stars, whereas version 6.01 data show a negative bias for cold stars. However, the presence of strong outliers - as e.g. visualised by the peaks in standard deviation of the GOMOS profiles for version 5.00 (pink thin lines in left panels) - has been reduced substantially in version 6.01.

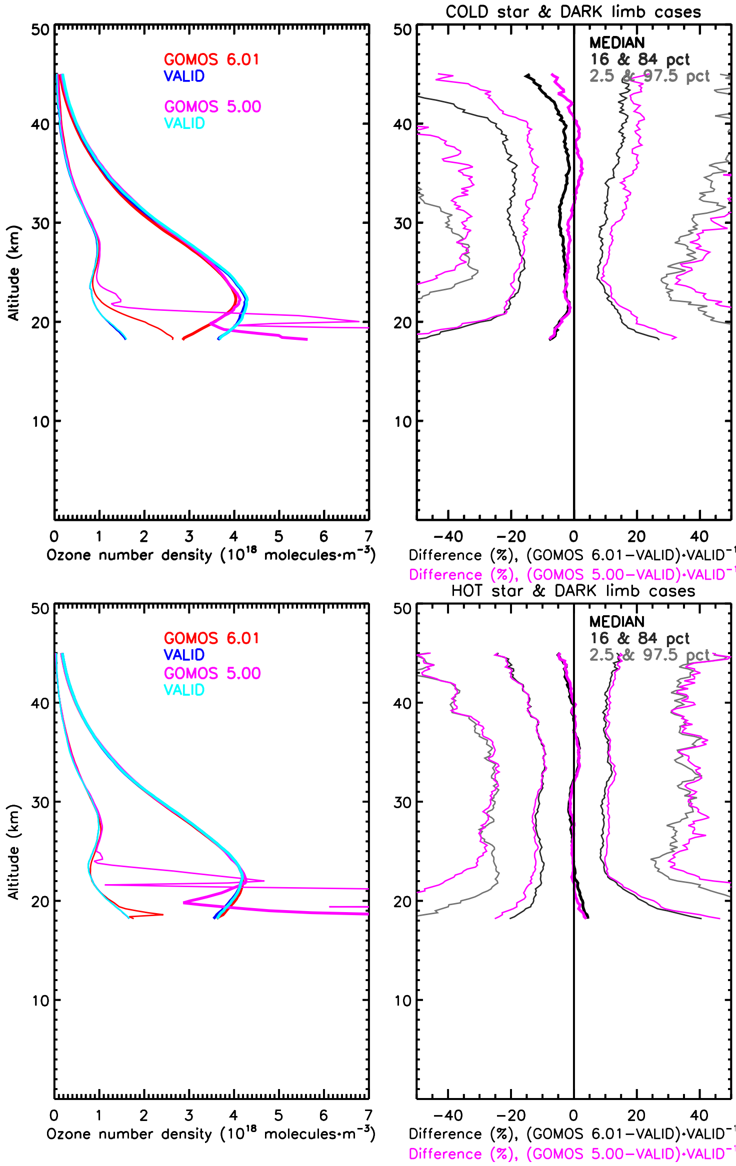

Figure 7. Validation results grouped by stellar temperature. Top: cool stars; bottom: hot stars. Version 5.00 results are shown in pink (with corresponding collocated lidar data in light blue). Red (dark blue for the collocated lidar) and black are used for version 6.01.

In Figure 8 the same data are now grouped by visual magnitude of the stars. Here version 5.00 and version 6.01 show some differences in the relative differences with lidar, but less pronounced than for the cool stars (Figure 7 top). Again version 6.01 shows somewhat lower ozone concentrations. The large standard variation peaks seen around 22 km in version 5.00 for weak stars and below 21 km for strong stars has been removed in version 6.01. For strong stars, the numbers are similar over all altitudes. For weak stars, the total number of used collocated pairs is also similar for the two versions, but for individual altitudes the numbers differ between versions. This is again probably attributable to the new error computation.

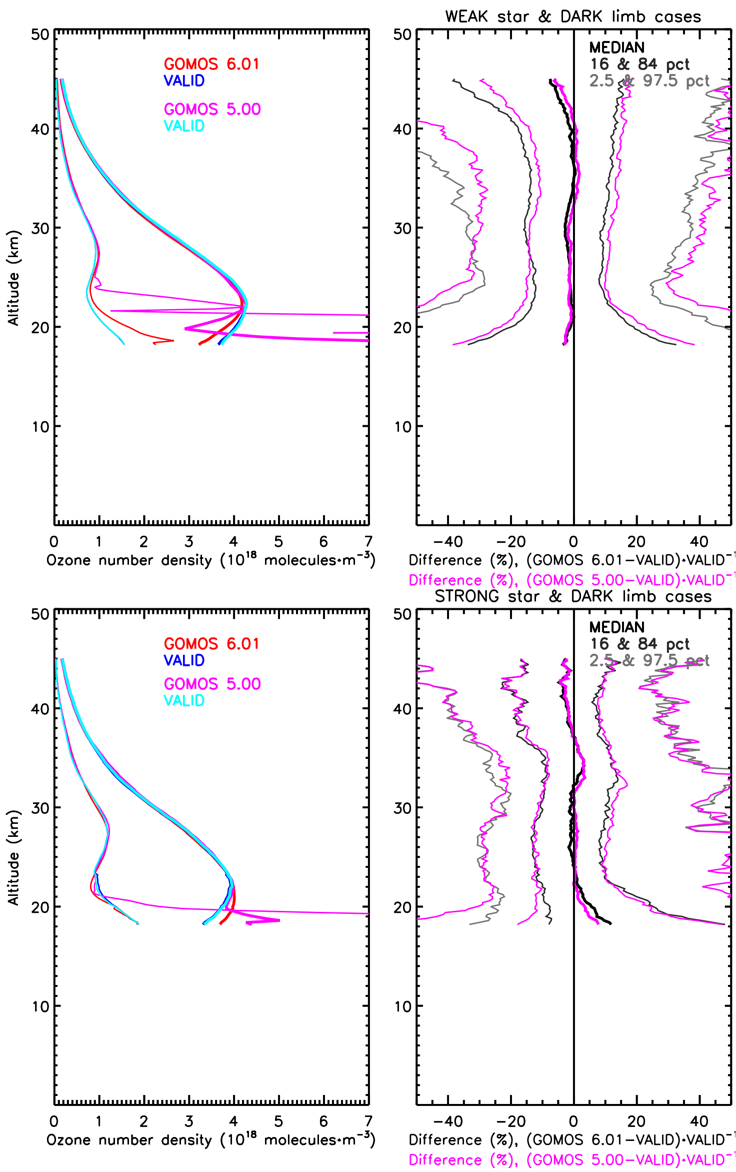

Figure 8. Validation results grouped by stellar magnitude. Top: weak stars; bottom: strong stars. Version 5.00 results are shown in pink (with corresponding collocated lidar data in light blue). Red (dark blue for the collocated lidar) and black are used for version 6.01.

As shown in the document "The influence of (not) using cool and weak stars in GOMOS ozone retrieval on comparison with lidar data." in figures 4-7 where the version 6.01 data were subjected to additional filtering based on difference in equivalent latitude and the same criteria as here (solar zenith angle ≥ 108°, maximum difference with the lidar of 800 km and 20 hours, maximum reported error of 30%), an increased presence of outliers below 25 km was found for weak and cold stars.

Collocation criteria

In this study we have used a maximum difference between the GOMOS observation and the lidar measurement of 20 hours in time and 800 km in space. Figure 9 shows the effect of making these criteria more strict. In general, the patterns are very similar for the three sets, but with stricter criteria, the number of available pairs naturally reduces and the percentile difference figures are less smooth. The 16-84 interpercentile spread does reduce with more strict collocation requirements. The lower ozone concentrations seen in version 6.01 with respect to version 5.00 persist under the stricter collocation conditions.

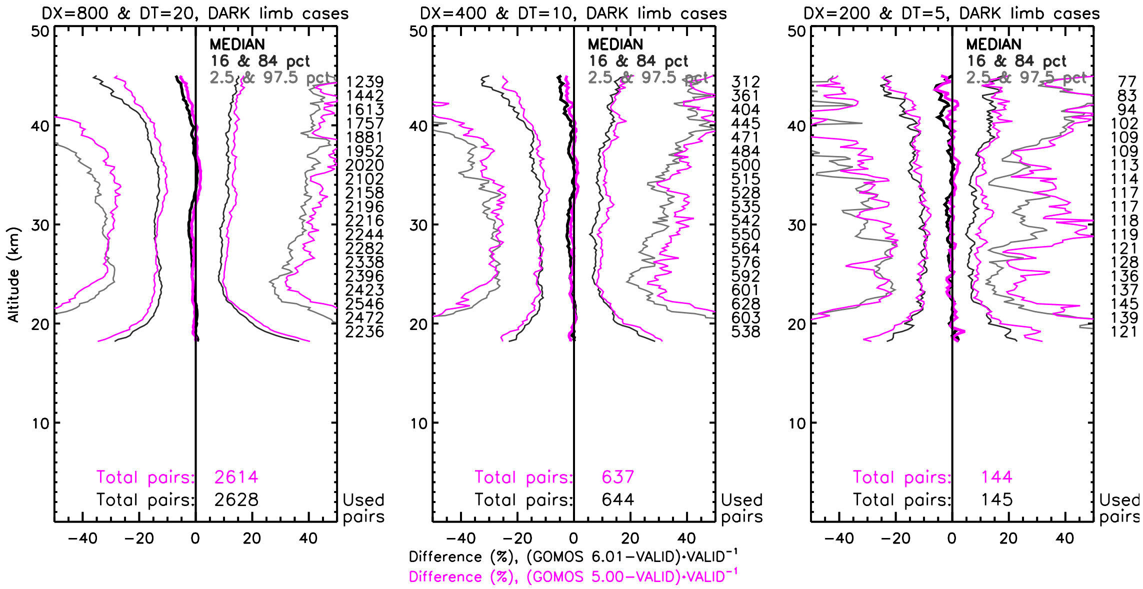

Figure 9. Validation results for GOMOS version 5.00 (pink) and version 6.01 (black) ozone profiles for different collocation criteria. Left panel: maximum difference of 800 km and 20 hours; middle panel: 400 km and 10 hours; right panel: 200 km and 5 hours. The number of collocated pairs at a given altitude is only given for version 6.01 data.

Conclusions

GOMOS ozone profiles acquired between the years 2002 and 2011 have been validated using collocated lidar data where both versions 5.00 and 6.01 GOMOS data were available. Collocations were restricted to data with a maximum reported error of 30% and maximum spatiotemporal difference between the GOMOS and lidar observations of 800 km and 20 hours.

Ozone concentrations tend to be somewhat lower in GOMOS version 6.01 data compared to 5.00. This behaviour is present in the validation results above 25 km for bright and twilight observations and to a smaller extent in the dark limb observations. The presence of outliers in the GOMOS data seems to have reduced, notably under dark limb conditions and below 25 km, but outliers continue to exist.

Data with a straylight plus twilight contamination flag show a stronger deviation from the lidar data (GOMOS being too low) than data with a straylight contamination flag only, which also underestimate the ozone concentrations in comparison to lidar. Data flagged dark in contrast show a small overestimation for most of the altitudes below 40 km.

Differences in validation results between GOMOS data flagged data dark and GOMOS data with a solar zenith angle ≥108° (this includes data flagged dark, but also straylight and/or twilight contaminated data) are most clear in the polar regions, but the number of collocated pairs is very limited for dark flagged data. Differences between the solar zenith angle ≥108° and dark flag selections are within 1% for the mid-latitudes and tropics (except below 20 km) whereas the contribution of non-dark-flagged data is substantial.

Differences with respect to the lidar data were seen between version 5.00 and version 6.01 retrievals for cool stars (< 7000K), to a lesser extent for weak stars, and even less for strong stars, whereas agreement with lidar for the two versions is very similar for retrievals using hot stars.

Best agreement with lidar is obtained over large altitude ranges using weak, hot stars and in the mid-latitudes up to 40 km and in the tropics above the ozone maximum.