# TOTAL O$_3$ COLUMNS FROM SCIAMACHY OL3.0 TO SCIAMACHY WEIGHTING FUNCTION DOAS (WFDOAS), OMI-TOMS AND GOME WFDOAS

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## ABSTRACT

Global stratospheric ozone columns from satellite instrument SCIAMACHY (SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY) on ENVISAT derived from the newest operational data product OL3.0 are compared to data products of the SCIAMACHY Weighting Function DOAS Algorithm (WFD), GOME WFD and OMI TOMS algorithm. The comparisons are also analysed for dependencies to total ozone, solar zenith angle and latitude. Due to the limited data set of SCIAMACHY OL3.0 with only 5 nearly complete days and 4 days with 4 orbits each the validation results are quite preliminary. There is an indication that OL3.0 data products show a major improvement compared to previous operational data versions with an agreement within 1% (RMS < 2.5%) to GOME WFD and OMI TOMS. No clear dependencies to total ozone and latitude are observed. In two cases there might be a dependency to SZA, which should be investigated further with a larger data set. The comparisons to SCIA WFD V2 showed the negative bias of 1-2% with SCIA OL3.0, which has been previously described in comparisons to GOME WFD and OMI TOMS and has been interpreted as a calibration error in SCIA lv-1, which has been accounted for in the OL3.0 processing. Despite this offset, SCIA WFD shows no dependencies to SZA, latitude and total ozone. Results help to understand how these different global total ozone data sets can be linked together for ozone trend studies.

## 1 INTRODUCTION

The stratospheric ozone layer protects the biosphere from harmful ultraviolet radiation. The discovery of the Antarctic ozone hole in the early 1980s [1], but also changes in the Arctic and lower latitudes, established the need for global measurements of ozone and other atmospheric trace gases [2]. To assess current and future changes long-term observations of ozone are urgently needed. Ground-based instruments can provide long and stable records for specified location, but satellite instruments are the most effective way to achieve a global view of the atmosphere. Currently there are three European satellite instruments successfully measuring ozone columns along with other atmospheric constituents in nadir viewing mode and contributing to the long-term ozone data record: the Global Ozone Monitoring Experiment (GOME) on ERS-2 [3] operating since April 1995, the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY) as part of the atmospheric chemistry payload of the third ESA Earth observation satellite platform called ENVISAT which was launched in March 2002 [4] and the Ozone Monitoring Instrument (OMI) onboard EOS-AURA [5] operating since July 2004. As satellite instruments age and unfortunately stop to measure, it is necessary to compare ozone measurements from older with those from newer instruments in order to ensure that long-term behaviour derived from a combination of ozone sensors will be useful (e. g. [6]). Furthermore, satellite instruments have to be validated during the complete lifetime to ensure ongoing quality of the measured data and to avoid long-term drifts due to instrumental aging. To link the total ozone data sets of SCIAMACHY, GOME and OMI cross comparisons between them are necessary. Recently a validation reference set of the new operational SCIAMACHY total ozone product version OL3.0 was released. In order to assess the quality of this data set and give recommendations for reprocessing, comparisons to another SCIAMACHY algorithm, Weighting Function DOAS (WFD V1 and V2) and two the total ozone product of the other satellite sensors OMI TOMS and GOME WFD have been performed.

## 2 DATA PRODUCTS USED IN COMPARISONS

### 2.1 SCIAMACHY operational products
The last operational SCIAMACHY data version, which reprocessed the entire data set, was NRT 5.01/5.04 released in March/August 2004. For this SCIAMACHY operational data version (based on GDP V2.7 algorithm) problems in dependencies to SZA, latitude, total ozone and season have been described in [7], [8] and [9]. Therefore, a new SCIAMACHY operational product, OL3.0 has been developed based on GOME GDP4.0 [described and validated in [10] and

[11], respectively) and first reprocessing for a limited data set, validation reference set, has been performed and has been released by DLR/ESA in August 2006 to the SCIAMACHY validation team. It has to be pointed out that in SCIA OL3.0 it has been accounted for in the processing that there is a calibration error in the SCIAMACHY level-1 product which causes a 2% negative offset in the total ozone product.

## 2.2 Weighting Function DOAS algorithm developed for GOME and SCIAMACHY data

The Function DOAS Algorithm (WFD) established for GOME has been described in detail in [12]. The main features can be summarized with the following: WFD fits vertically integrated ozone weighting functions rather than ozone cross-section to the sun-normalised radiances that enables a direct retrieval of vertical column amounts. The WFD algorithm also takes into account the slant column path length modulation as a function of wavelength that is usually neglected in standard DOAS when using single air mass factors to convert observed slant column into vertical column densities. Several auxiliary quantities directly derived from the GOME spectral range such as cloud-top-height and cloud fraction (O2-A band) and effective albedo using the Lambertian Equivalent Reflectivity (LER) near 377 nm are used in combination as input to the ozone retrieval. The most significant improvement over GOME V3.0 is the explicit treatment of the ozone dependent contribution in the Raman correction in scattered light known as Ring effect.

For the SCIA WFD V1 GOME cross section, TOMS V7 climatology and FRESCO cloud information has been used. This version is used in comparisons described in chapter 3 in the year 2003. V2 was developed in order to use the real SCIAMACHY information, regarding cross sections and cloud information. These changes are described in detail in [13]: Instead of GOME cross sections, we used SCIAMACHY FM $O_3$ cross-section from [14] scaled by 1.037 and wavelength shifted by +0.016 nm based on investigation carried out with FTS and Bass and Paur $O_3$ cross-section, for details see [15]. An improved climatology described in [16] has been used and implemented also in an appropriate Ring data bases. Instead of look-up tables online calculations using SCIATRAN V2.x included in retrieval were performed. We used the SACURA/OCRA cloud information has been used and because of the higher spatial resolution of SCIAMACHY compared to GOME an improved topographic data base (15 km x 15 km). Retrievals of SCIAMACHY WFD shown in this study are based on Level-1 data v5.04 and ESM solar data.

GOME WFD has been used to retrieve total ozone for the entire GOME data set and an extensive validation study by [17] showed a very good performance of this algorithm for GOME with no seasonal cycle and within 1 % of global Brewer measurements. A study by [18] showed for SCIA WFD a constant bias of –1% to –2% to GOME WFD, Brewer measurements and OMI-TOMS. This constant negative offset was explained by a calibration error in the SCIAMACHY level-1 product, which has been not accounted for as it has been done for OL3.0. Despite this bias, the WFD algorithm had been successfully adapted to SCIAMACHY and showed negligible dependencies to seasons, latitudes, SZA, cloud fraction and total ozone.

## 2.3 OMI TOMS algorithm

For OMI data we used the level-3 product from the public website http://toms.gsfc.nasa.gov/pub/omi/data/ozone which is based on TOMS v8 algorithm (OMI TOMS; see [19]). Global validation by [20] of a one year OMI TOMS data set showed an agreement remarkably stable around 0% to ground based Brewer measurements with RMS less than 2%.

## 3 COMPARISONS OF SCIAMACHY NRT 5.01/5.04 AND OL 3.0 WITH GOME WFD AND SCIAMACHY WFD

16 complete orbits (4 orbits each on 20020718,20021006, 20030302, 20030512) of level-2 Olv3.0 ozone columns have been compared to GOME-WFD and the data only from 20030512 to SCIA-WFD V1. Direct comparisons were made for the same pixels in the comparisons of the two SCIAMACHY algorithms and for the mean of all SCIAMACHY pixels from OL3.0 or WFD V1 within one GOME ground pixel. Preliminary validation of 16 orbits shows new operational SCIAMACHY total ozone (OL3.0) around +1% (RMS <2%) of GOME WFD and are comparable to SCIA WFD V1. An example for the 12 May 2003 total ozone of SCIA OL3.0, NRT5.04, WFD and GOME WFD and the comparisons of OL3.0 to SCIA WFD and GOME WFD are shown in Fig. 1 and 2, respectively. These results are consistent with the comparisons for the three other compared days. The scatter is a bit larger in tropics. Overall the operational tO3 improved with OL3.0 compared to NRT5.01/5.04 (shown in Fig. 3 for the same day), because no dependencies to latitude, SZA and tO3 were found. These dependencies have been found in NRT5.01/5.04 comparing half a year data set in 2003 [see 9]. For the

comparisons to SCIA NRT 5.04 the data have been also compared after gridding the SCIA and GOME data in 2.5° x 2.5° latitudinal/longitudinal boxes. Results are very similar for both methods and therefore in comparisons were no corners coordinates are know (as described in chapter 4) the gridding method is used in the comparisons.
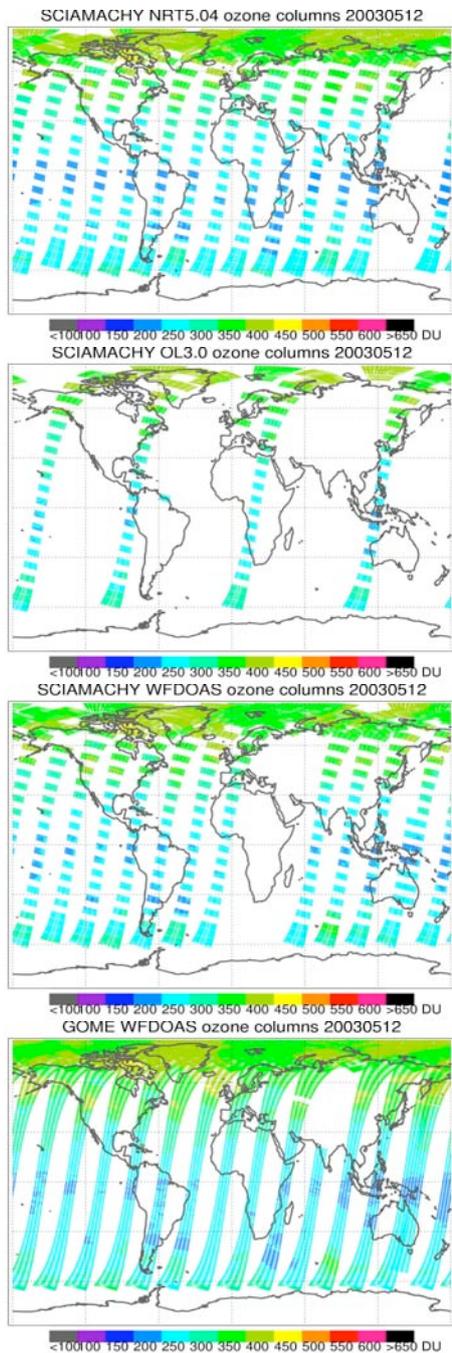


*Fig. 1. Global total ozone distributions retrieved from SCIAMACHY NRT 5.04 (upper panel), OL3.0 (second upper panel), WFD (second lower panel) and GOME WFD (lower panel) on 12 May 2003.*
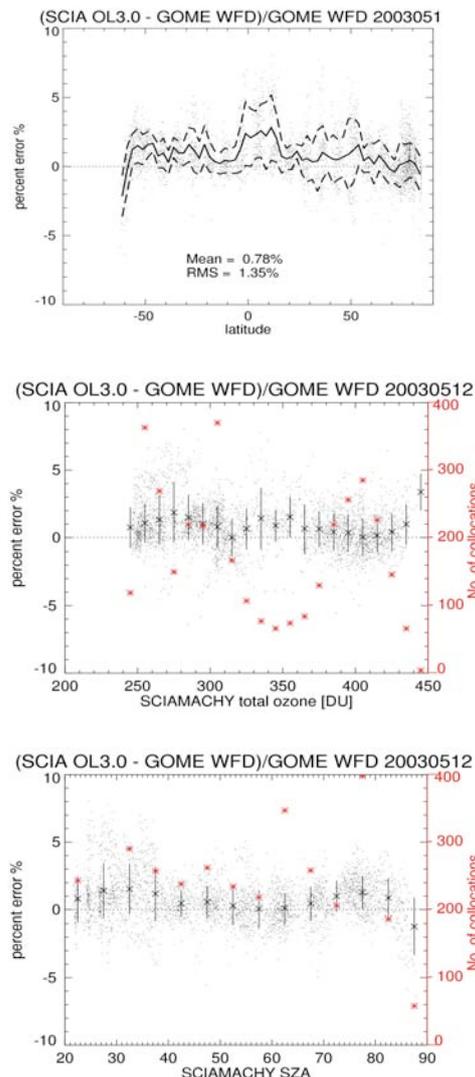


*Fig. 2 a. Comparison of total $O_3$ from SCIAMACHY OL3.0 and GOME WFD from 12 May 2003. Upper panel: mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as a function of latitude. Mean relative deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as a function of SCIAMACHY SZA (middle panel) and total ozone (lower panel).*
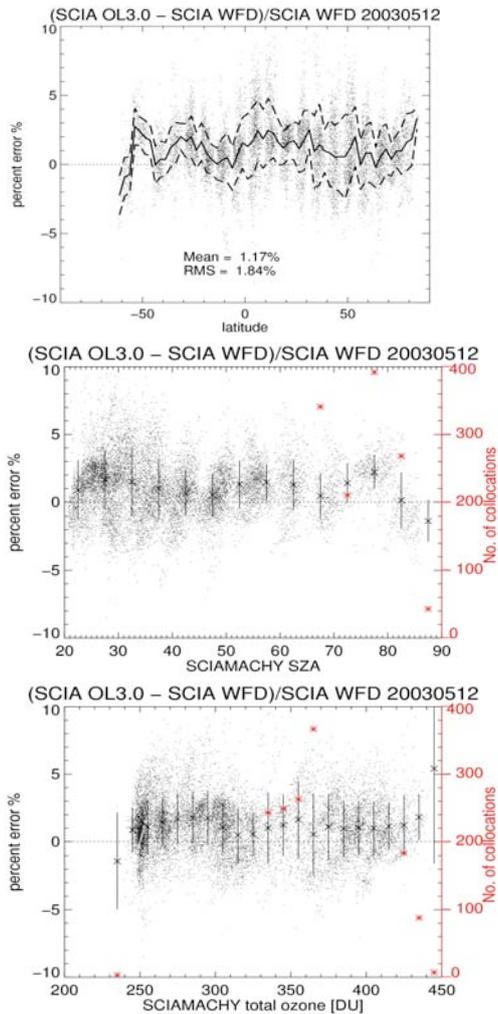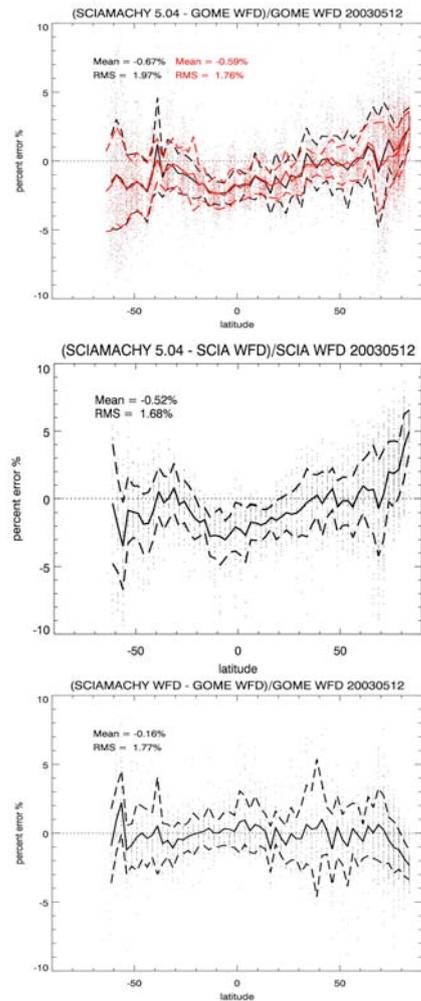
*Fig. 2 b. Comparison of total O₃ from SCIAMACHY OL3.0 and SCIAMACHY WFD from 12 May 2003. Upper panel: mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted l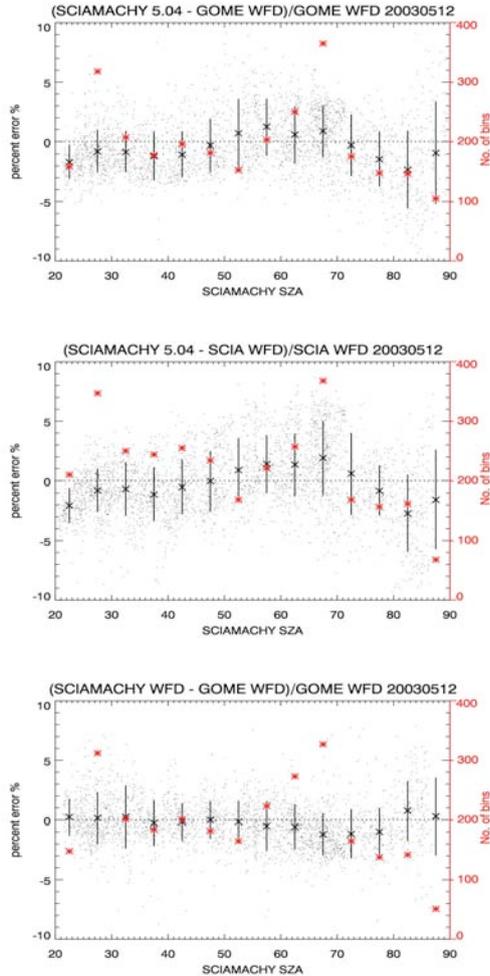ine) as a function of latitude. Mean relative deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as a function of SCIAMACHY SZA (middle panel) and total ozone (lower panel).*



*Fig. 3 a. Comparison of total O₃ on 12 May 2003 from SCIAMACHY NRT 5.04 with GOME WFD (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and GOME WFD (lower panel): Mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as a function of latitude.*

*Fig. 3 b. Comparison of total O₃ on 12 May 2003 from SCIAMACHY NRT 5.04 with GOME WFD (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and GOME WFD (lower panel): mean relative deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function of SCIAMACHY SZA.*



*Fig. 4 a. Comparison of total O₃ on 15 May 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as a function of latitude.*

## 4 COMPARISONS OF SCIAMACHY OL 3.0 WITH OMI TOMS AND SCIAMACHY WFD

SCIAMACHY OL3.0 total ozone data of 5 nearly complete days (9 to 12 orbits) from 2004/2005 (20040916, 20041111, 20050210, 20050515, 20050814) were compared by gridding into 0.5°x0.5° lat/lon to OMI TOMS data and to SCIA WFD (only available for 20041111, 20050210, 20050515). We show only the results for the three days whe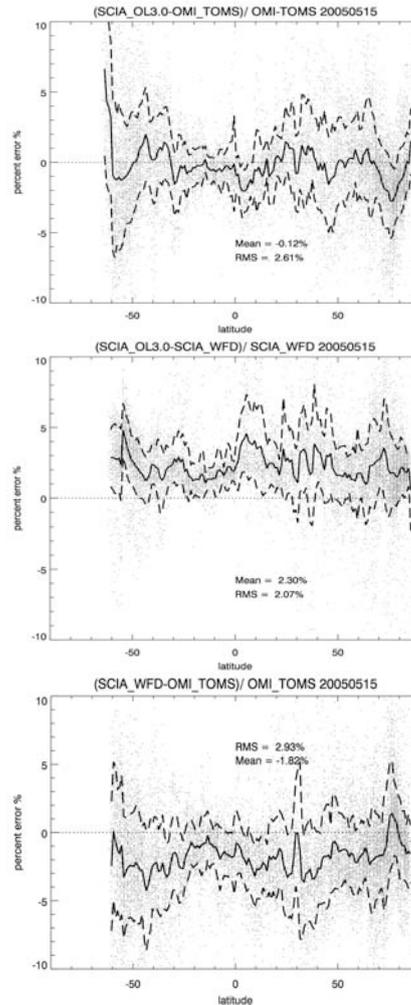re SCIA WFD are available and interpret them because for the other two days the comparisons of SCIA OL3.0 to OMI TOMS are biased by an incomplete OMI TOMS data set (only less than 50% data are available). In order to quickly compare collocations and to overcome the difference in ground pixel sizes (SCIAMACHY 60 km x 30 km, OMI 24 km x 18 km), a method using binning data as described in [9] was applied: OMI-TOMS level-3 products are produced anyway by binning daily level-2 products; therefore the same was done for the SCIAMACHY WFD data.
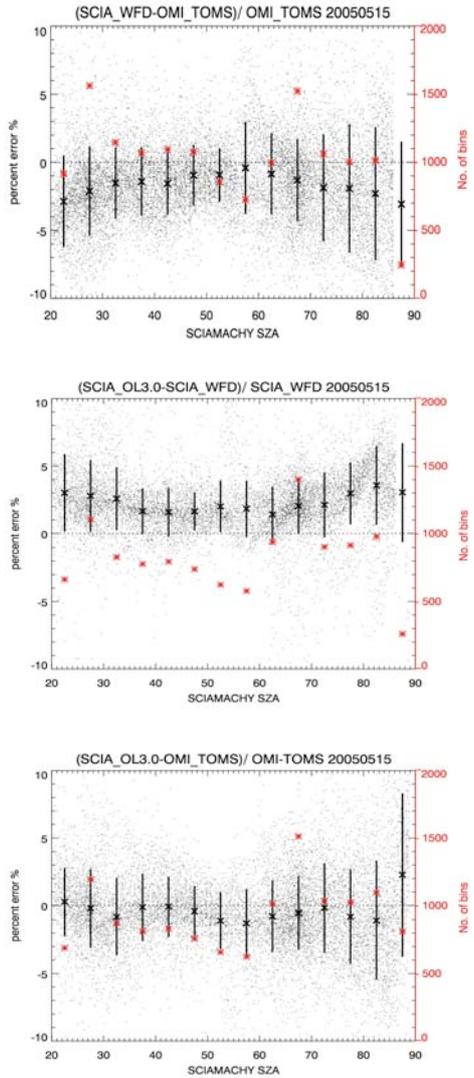
*Fig. 4 b. Comparison of total $O_3$ on 15 May 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean rel. deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function SCIAMACHY SZA.*
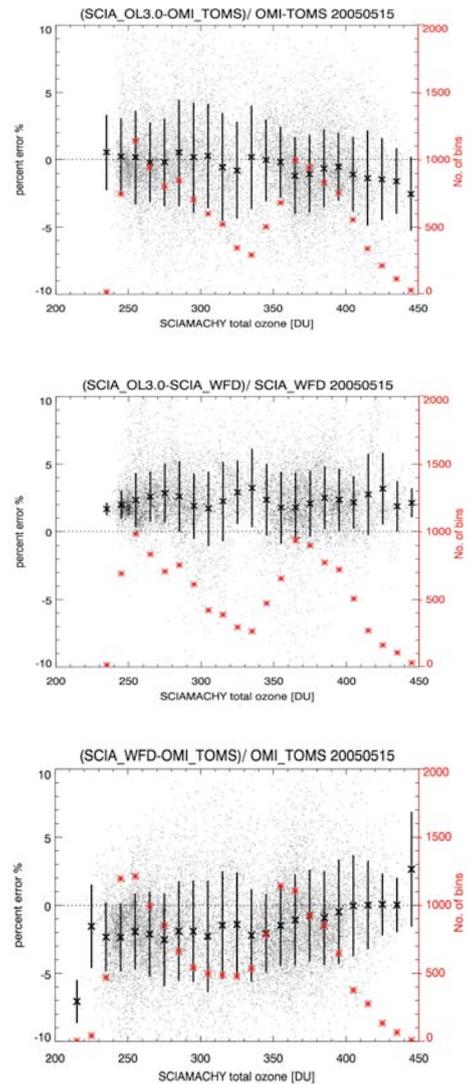
*Fig. 4 c. Comparison of total $O_3$ on 15 May 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean relative deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function of SCIAMACHY total ozone.*

Results for the comparisons on 15 May 2005 (Fig, 4) are quite consistent with the findings in the comparisons of SCIA OL3.0 with GOME WFD, despite that SCIA OL3.0 are on average only slightly lower (on average –0.12%) and has no positive bias as compared to GOME WFD. The RMS is a bit higher with average values around 2.5% as compared to 1.5% in the comparisons to GOME WFD. No dependencies to latitude, SZA and total ozone are observed. Results for the comparisons on the two other days (Figs.5 and 6)

show similar deviations on average and for the RMS of SCIA OL3.0 to OMI-TOMS, but it is not clear that there is no dependency to SZA (Figs 5b and 6b). In line are the comparisons of SCIA WFD with SCIA OL3.0 and OMI TOMS, which show a general negative offset around 2% of SCIA WFD and no dependencies of latitude, SZA and total ozone to OMI TOMS. SCIA OL3.0 to SCIA WFD also shows a dependence to SZA at 20041111 and 20050210, but not for 20050515 as observed for SCIA OL3.o to OMI TOMS.
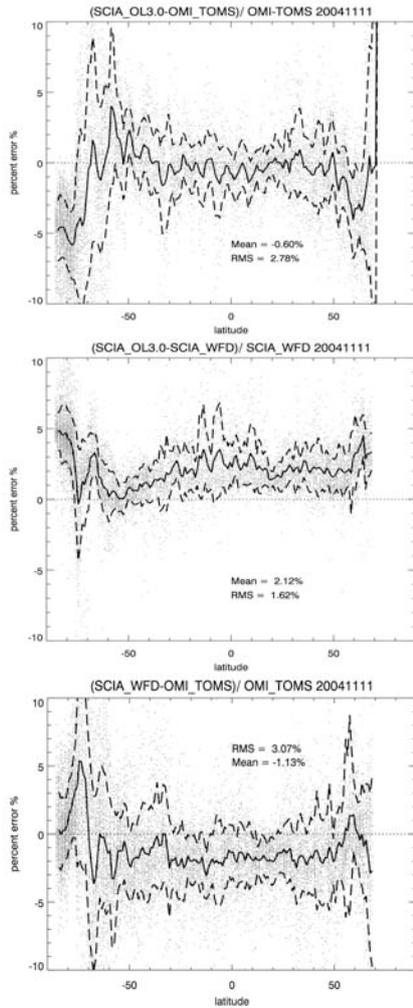
Fig. 5 a. Comparison of total $O_3$ on 11 Nov 2004 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as a function of latitude.
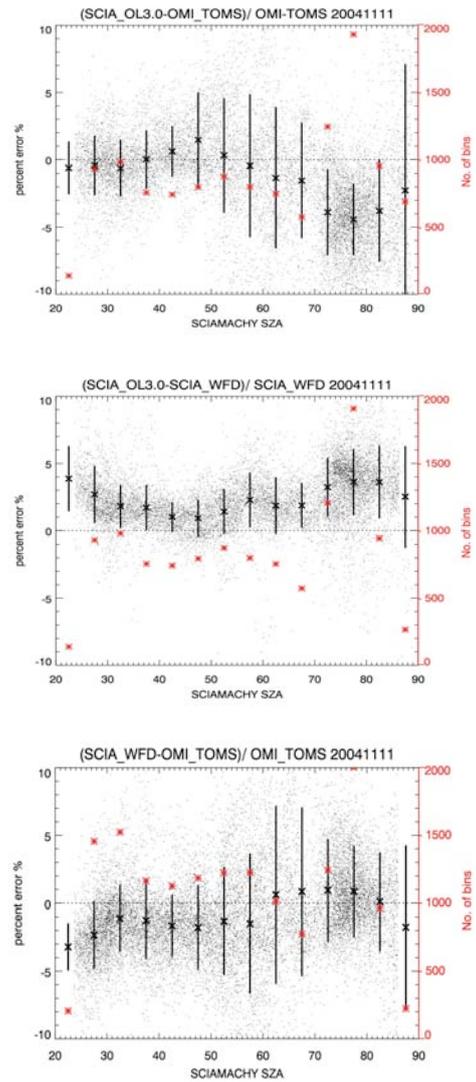
Fig. 5 b. Comparison of total $O_3$ on 11 Nov 2004 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean rel. deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function SCIAMACHY SZA.
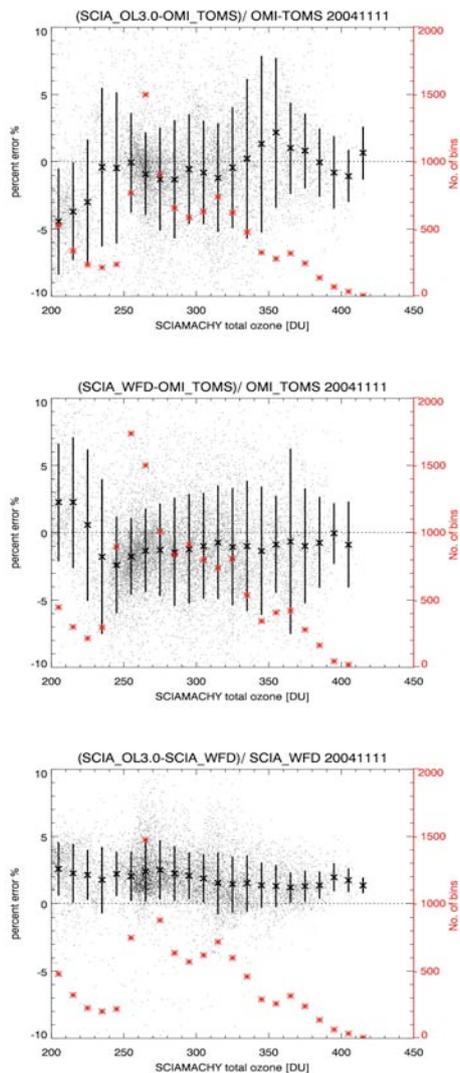
*Fig. 5 c. Comparison of total $O_3$ on 11 Nov 2004 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean rel. deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function SCIAMACHY total $O_3$.*
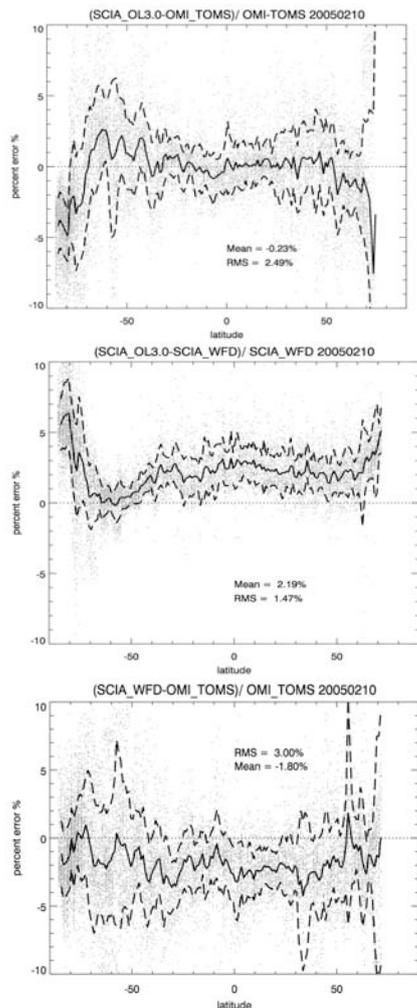


*Fig. 6 a. Comparison of total $O_3$ on 10 Feb 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean re. deviation (black dots), mean values of mean rel. deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as function of latitude.*
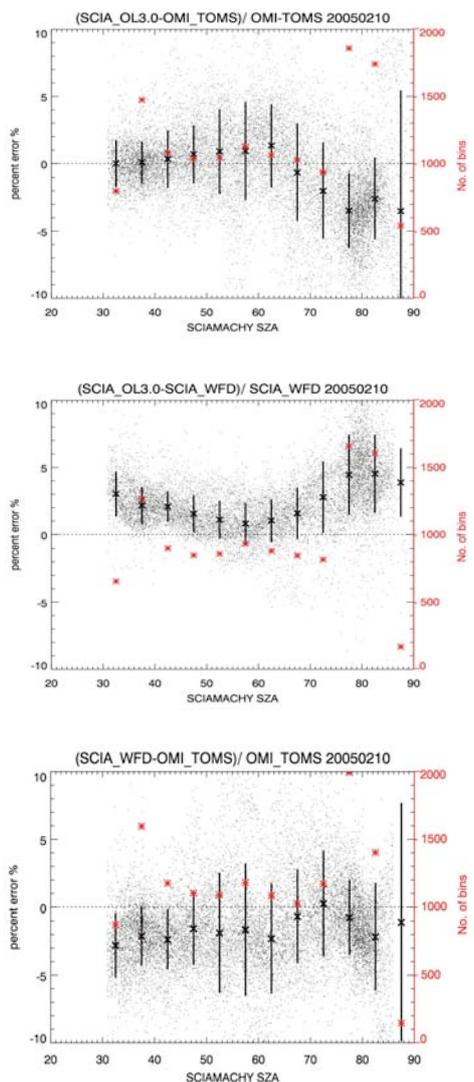
*Fig. 6 b. Comparison of total O₃ on 10 Feb 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean rel. deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function SCIAMACHY SZA.*
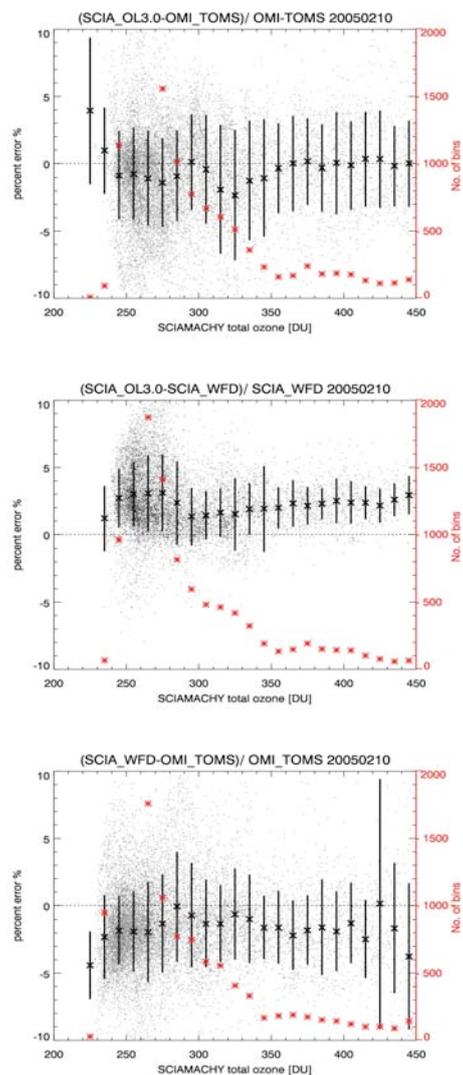
*Fig. 6 c. Comparison of total O₃ on 10 Feb 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean rel. deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function SCIAMACHY total O₃.*

## 6 CONCLUSIONS AND OUTLOOK

The newest operational data version of SCIAMACHY OL3.0 show an improvement to the previous data versions. SCIA OL3.0 deviates within +1% (RMS ~1.5%) and –0.3 (RMS ~2.5%) from GOME WFD and OMI TOMS, respectively. Still these conclusions are preliminary because the validation of the validation reference set with GOME WFD and OMI TOMS and the comparisons with SCIAMACHY WFD V1 and V2 show that in respect to investigate dependencies to SZA, latitude and total ozone results are not clear.

While for most of the compared days 6 out 8 no dependences are found. A larger data set of SCIA OL3.0 data with a minimum of 12 complete days with evenly distributed 1 day per month is necessary to clarify this issue.

The newest version of SCIA WFD V2 is 2% low compared to OMI TOMS and SCIA OL3.0, which has also previously observed in broader comparisons to GOME WFD, OMI TOMS and Brewer ground based measurements. As an explanation for this offset the calibration error in the SCIA lv-1 product has been

given and the SCIA OL3.0 retrieval accounted for this offset (Van Roozendael, pers. comm.. 2006). Probably by luck the previous SCIA WFD V1 did not have this offset which might have been cancelled out by using GOME cross section and different climatology and cloud correction. The upcoming SCIAMACHY WFD version will account for the calibration error. Despite this bias, the WFD algorithm has been successfully adapted to SCIAMACHY and shows large improvements compared to the recent operational SCIAMACHY v5.04 and negligible dependencies to seasons, latitudes, SZA, cloud fraction and total ozone.

# 7 ACKNOWLEDGEMENTS

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