# GLOBAL COMPARISONS OF TOTAL O<sub>3</sub> COLUMNS FROM SCIAMACHY WEIGHTING FUNCTION DOAS (WFDOAS) AND OL3.0 TO OMI-TOMS AND GOME WFD

A. Bracher, M. Weber, K. Bramstedt, J.P. Burrows

Institute of Environmental Physics, University of Bremen, NW1, Otto-Hahn-Allee 1, D-28359 Bremen, Germany, bracher at uni-bremen dot de

#### ABSTRACT

Global stratospheric ozone columns are currently derived from UV nadir spectra measured by the satellite instruments OMI (Ozone Monitoring Instrument) on AURA (since 2004), SCIAMACHY (SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY) on ENVISAT and GOME on ERS-2 (since 1995). The Weighting Function DOAS Algorithm (WFD) has been used to derive total ozone from SCIAMACHY and GOME (see [1]). Recently the new SCIAMACHY operational version OL3.0 of total ozone (based on GOME GDP 4.0) has been introduced and processed for a validation reference set. The paper presents global comparisons from the validation reference set of SCIAMACHY WFD and OL3.0 with GOME WFD and OMI TOMS algorithms. The comparisons were also analysed for dependencies to total ozone, solar zenith angle and latitude. Due to the limited data set of SCIAMACHY OL3.0 with only 4 nearly complete days and 4 days with 4 orbits each the validation results are quite preliminary. There is an indication that data products of both SCIAMACHY algorithms, WFD V2 and OL3.0, show a major improvement compared to previous versions with an agreement within 1% (RMS < 2.5%) to GOME WFD and OMI TOMS. After finishing the reprocessing of the entire SCIAMACHY level-1 data set with v6.03 and after that based on this with OL3.0 and WFD3.0 an extensive satellite validation of the entire data set is planned which will clarify if these results hold true or if still biases will be detected.

#### 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. 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 longterm 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 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-topheight 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.

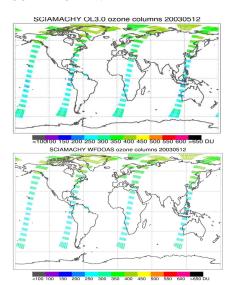
For the SCIA WFD V1 GOME cross section, TOMS V7 climatology and FRESCO cloud information has been used. V2 was developed in order to use the real SCIAMACHY information, regarding cross sections and cloud information. These changes are described in detail in [13]: Instead of GOME cross sections, we used SCIAMACHY FM O<sub>3</sub> cross-section from [14] scaled by 1.038 and wavelength shifted by +0.009 nm based on investigation carried out with FTS and Bass and Paur O3 cross-section, for details see [15]. Still TOMS V7 climatology has been used and implemented also in an appropriate Ring data bases. Instead of lookup tables online calculations using SCIATRAN V2.x included in retrieval were performed. We used FRESCO information, cloud but also SACURA/OCRA cloud information has been used and tested (see [1]). A difference of about 0.5% was found by choosing the different cloud information, although agreement with GOME WFD and OMI-TOMS was comparable. Still in this paper we only show comparisons processing SCIA WFD with FRESCO. 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 [16] showed a very good performance of this algorithm for GOME with no seasonal cycle and within 1 % of global Brewer measurements. A study by [17] showed for SCIA WFD a constant bias of -1% to -2% to GOME WFD, Brewer measurements and OMITOMS. 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 [18]). Global validation by [19] 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



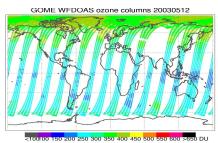
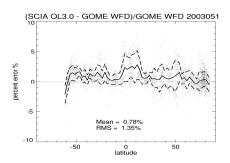
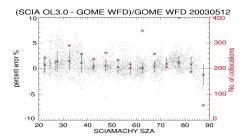


Fig. 1. Global total ozone distributions retrieved from SCIAMACHY OL3.0 (upper panel), WFD (middle panel) and GOME WFD (lower panel) on 12 May 2003.

complete orbits orbits 20020718,20021006, 20030302, 20030512) of level-2 Olv3.0 ozone columns have been compared to GOME-WFD and the data only from 20030512 and 20030302 to SCIA-WFD V2. 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 V2 (within 1%, RMS <1.5%). An example for the 12 May 2003 total ozone of SCIA OL3.0, SCIA WFD and GOME WFD and the comparisons of OL3.0, SCIA WFD and GOME WFD and 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 for comparisons to SCIA OL3.0. Overall the operational tO3 improved with OL3.0 compared to NRT5.01/5.04, see [9], because no dependencies to latitude, SZA and tO3 were found. Also SCIA WFD V2 improved because the negative offset seen in V1 see [17], disappeared.





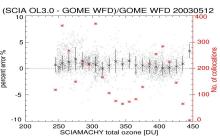
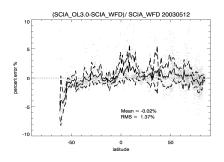


Fig. 2 a. Comparison of total  $O_3$  from SCIAMACHY OL3.0 and GOME WFD from 12 May 2003. Upper panel: mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as a function of latitude. Mean relative 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).



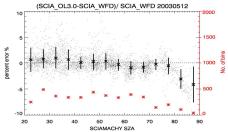
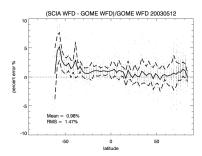


Fig. 2 b. Comparison of total  $O_3$  from SCIAMACHY OL3.0 and SCIAMACHY WFD V2 from 12 May 2003. Mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as a function of latitude (upper panel) and as a function of SCIAMACHY SZA (lower panel).



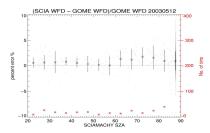


Fig. 2 c. Comparison of total  $O_3$  on 12 May 2003 from SCIAMACHY WFD V2 with GOME WFD: mean relative deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function of latitude (upper panel) and SCIAMACHY SZA (lower panel).

## 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 where 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.

Results for the comparisons on 15 May 2005 (Fig. 3) 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 between 2.5 and 3% 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. 4 and 5) 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 (Fig 4b and 5b). In line are the comparisons of SCIA WFD with SCIA OL3.0 and OMI TOMS, which show are within 0.5% with a lower RMS of 1.5 to 2% (compared to SCIA OL3.0). SCIA OL3.0 to SCIA WFD are as for the days in 2003 within 0.5% and RMS <1.5%. At SZA >80° there is a dependence in the comparison to SCIA WFD which is not unusual for such high SZA.

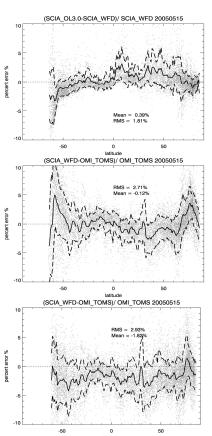
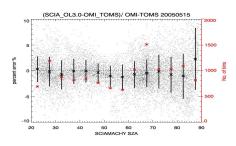
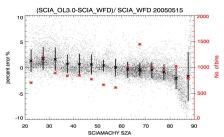


Fig. 3 a. Comparison of total  $O_3$  on 15 May 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as a function of latitude.





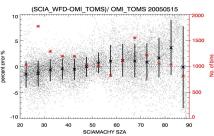
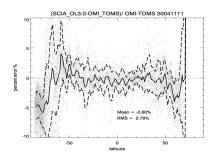


Fig. 3b. Comparison of total  $O_3$  on 15 May 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean rel. deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function SCIAMACHY SZA.



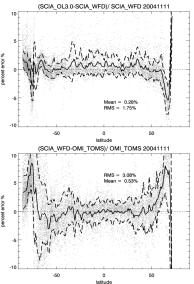
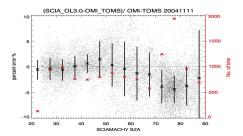
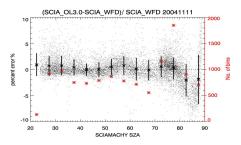


Fig. 4a. Comparison of total  $O_3$  on 11 Nov 2004 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean relative deviation (black dots), mean values of mean relative deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as a function of latitude.





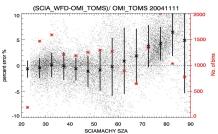


Fig. 4b. Comparison of total O<sub>3</sub> on 11 Nov 2004 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and

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.

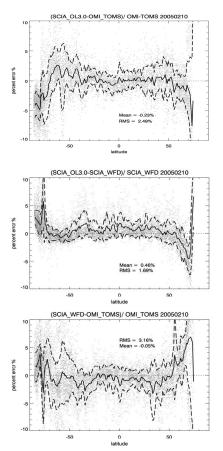
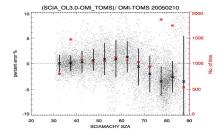
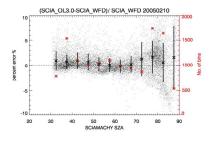


Fig. 6 a. Comparison of total  $O_3$  on 10 Feb 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean re. deviation (black dots), mean values of mean rel. deviations (straight line) and root mean squares of the mean relative deviation (dotted line) as function of latitude.





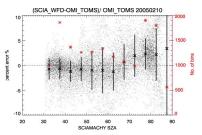


Fig. 6 b. Comparison of total  $O_3$  on 10 Feb 2005 from SCIAMACHY OL3.0 with OMI TOMS (upper panel) and SCIAMACHY WFD (middle panel) and SCIAMACHY WFD and OMI TOMS (lower panel): mean rel. deviation (black cross), root mean square of daily mean relative deviation (black line) and number of data bins (red stars) of all comparisons as function SCIAMACHY SZA.

#### 5 CONCLUSIONS AND OUTLOOK

The newest operational data version of SCIAMACHY OL3.0 and WFD V2 show an improvement to the previous data versions. SCIA OL3.0 deviates within +1% (RMS ~1-2%) and 0 and -0.6 (RMS ~2.5-3%) from GOME WFD and OMI TOMS, respectively, and SCIA V2 within 0 to +1% (RMS ~1.5-2%) and 0 to -0.5 (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 V2 show no indications of dependencies to SZA, latitude and total ozone results. 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 comparable to SCIAMACHY OL3.0 with those results and the two algorithms are on average within 0.5% and an RMS of ~1.5%. The constant negative offset observed in SCIAMACHY WFD V1 in comparisons to GOME WFD, OMI-TOMS and groundbased [17] disappeared, probably due to a more appropriate shifting and scaling of the SCIAMACHY cross sections.

It seems like that the SCIA OL3.0 and the WFD V2 algorithm have been successfully adapted to SCIAMACHY and show large improvements compared to the previous versions. But a larger (global, longterm) satellite validation effort after finishing the reprocessing of the entire SCIAMACHY level-1 data set with v6.03 and after that the based on this level-1 data set the reprocessing with OL3.0 and WFD3.0 covering the entire SCIAMACHY data is planned and will clarify that.

#### 6 ACKNOWLEDGEMENTS

We thank DLR and ESA/ESRIN for providing GOME and SCIAMACHY calibrated level 1 spectral and OL3.0 data, and NASA and the OMI/AURA team for OMI level 3 data. This work is funded by ESA-ESRIN (project SciLoV). The SCIAMACHY and GOME WFDOAS data shown here were calculated on the HLRN (High-Performance Computer Center North) and NIC/JUMP (Juelich Multiprocessor System). Services and support are gratefully acknowledged.

#### 7 REFERENCES

- 1. Weber M., Lamsal L.N., Burrows J. P. (2007) Improved SCIAMACHY WFDOAS total ozone retrieval: steps towards homogenising long-term total ozone datasets from GOME and SCIAMACHY. ENVISAT Symposium 2007. 3P4.27
- 2. Farman J. C., Peters D. and Greisinger, K. M., Large losses of total ozone in Antarctica reveal seasonal ClOX / NO interaction, Nature, 315, 207 210, 1985.
- 3. Burrows J. P., Weber M., Buchwitz M., Rozanov V. V., Ladstädter-Weissenmayer A., Richter A., de Beek R., Hoogen R., Bramstedt K., Eichmann K.-U., Eisinger M. and Perner D., The Global Ozone Monitoring Experiment (GOME): Mission Concept and First Scientific Results, J. Atmos Sci., 56, 151-175, 1999.
- 4. Bovensmann H., Burrows J. P., Buchwitz M., Frerick J., Noël S., Rozanov V. V., Chance K. V. and Goede A. H. P., SCIAMACHY Mission Objectives and Measurement Modes, J. Atmos Sci., 56, 125-150, 1999.
- 5. Veefkind J.P. and J.F. de Haan, OMI Algorithm Theoretical Basis Document, Barthia, P.K (ed), Volume II 620 19 Chapter 3, DOAS Total Ozone Algorithm, ATBD-OMI-02, Version 2.0, http://www.knmi.nl/omi/documents/ data/OMI ATBD Volume 2 V2.pdf, August 2002.
- 6. Cunnold D. M., Wang H., Chu W. P. and Froidevaux L., Comparisons between Stratospheric

- Aerosol and Gas Experiment II and microwave limb sounder ozone measurements and liasing SAGE II ozone trends in the lower stratosphere, J. Geophys. Res., 101, 10,061–10,075, 1996.
- 7. Lambert J.-C., Granville J., Blumenstock T., Boersma F. Bracher A., et al., Geophysical validation of SCIAMACHY NO<sub>2</sub> vertical columns: overview of early 2004 results, In: Danesy D. (ed.), Proceedings of the Second Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2), 3-7 May 2004, ESA ESRIN, Frascati, Italy, ESA Publications Division, Nordwijk, The Netherlands, SP-562, 59-71, 2004
- 8. Hilsenrath E., Bojkov B., Labow G. and Bracher, A., SCIAMACHY Column Ozone Validation, In: Danesy D. (ed.), Proceedings of the Second Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2), 3-7 May 2004, ESA ESRIN, Frascati, Italy, ESA Publications Division, Nordwijk, The Netherlands, SP-562, 47-50, 2004.
- 9. Bracher A., Lamsal L. N., Weber M., Bramstedt K., Coldewey-Egbers M. and Burrows J. P., Global satellite validation of SCIAMACHY ozone columns with GOME WFDOAS, Atmos. Chem. Phys., 5, 2357-2368, 2005
- 10. Van Roozendael M., et al., Reprocessing the 10-year GOME/ERS-2 total ozone record for trend analysis: the new GOME Data Processor Version 4.0, Algorithm Description, J. Geophys. Res. 111, D14311, 2006.
- 11. Balis D., et al., Reprocessing the 10-year GOME/ERS-2 total ozone record for trend analysis: the new GOME Data Processor Version 4.0, Validation, J. Geophys. Res. 111, D14311, 2006.
- 12. Coldewey-Egbers M., Weber M., Lamsal L.N., de Beek R., Buchwitz M., and Burrows J.P., Total ozone retrieval from GOME UV spectral data using the weighting function DOAS approach, Atmos. Chem. Phys., 5, 1015-1025, 2005.
- 13. Weber M., Lamsal L. N., Coldewey-Egbers M., Dhomse S., Bracher A., and Burrows J. P., Weighting Function DOAS total ozone from GOME and SCIAMACHY during the last decade, Poster at ESA Atmospheric Science Conference 8-12 May 2006, ESA-ESRIN, Frascati, Italy, 2006.
- 14. Bogumil K., Orphal J. and Burrows J. P., Temperature dependent absorption cross sections of O3, NO2, and other atmospheric trace gases measured with the SCIAMACHY spectrometer, Proceedings of the ERS Envisat Symposium, Goteborg, Sweden, 2000.
- 15. Weber M. and Lamsal L. N., Recommendations of ozone-cross-sections for SCIAMACHY ozone retrieval in the 325-335 nm spectral window. Technical Note, IUP/IFE, University of Bremen, Bremen, Germany, 2005.

- 16. Weber M., Lamsal L. N., Coldewey-Egbers M., Bramstedt K., and Burrows J. P., Pole-to-pole validation of GOME WFDOAS total ozone with groundbased data, Atmos. Chem. Phys., 5, 1341-1355, 2005.
- 17. Bracher A., Lamsal L. N., Weber M., Burrows J. P. (2006) Global comparisons of total O3 columns from SCIAMACHY weighting function DOAS (WFD) algorithm to OMI-TOMS, GOME WFD and groundbased measurements. In: Proceedings of the 2006 ESA Atmospheric Science Conference, 8-11 May 2006, Frascati, Italy. ESA Publications Division, Nordwijk, The Netherlands, SP-628: p2\_3\_bra.pdf 18. Bhartia P. K. and Wellemeyer, C. W., TOMS v8 Algorithm Theoretical Basis Document, http:
- Algorithm Theoretical Basis Document, http://toms.gsfc.nasa.gov/version8/v8toms atbd.pdf, NASA, 2004.
- 19. Balis D., Brinksma E., Kroon M., et al., Validation of OMI total ozone using ground-based brewer observations. In: Proceedings of the 2006 ESA Atmospheric Science Conference, 8-11 May 2006, Frascati, Italy. ESA Publications Division, Nordwijk, The Netherlands, SP-628: p2\_2\_bal.pdf.