DELTA-VALIDATION OF ENVISAT SCIAMACHY TOTAL OZONE AND NO_2 WITH THE DATA OF GROUND-BASED UV-VIS MEASUREMENTS (M-124 AND SAOZ)

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ABSTRACT

The present study is focused on validation of the recent SCIAMACHY nadir level 2 data by means of comparisons with correlative ground-based measurements over Russia and Western Europe in 2004. The newly available validation dataset, based on the SCIAMACHY level 2 off-line processor version 3.00 (OL 3.00), was compared with the measurements of 14 Russian UV filter ozonometers M-124 and 3 French SAOZ UV-visible zenith-sky spectrometers. According to the results, the new SCIAMACHY dataset, OL 3.00, demonstrate better agreement with ground-based M-124 ozone measurements. In addition, our ground-based validation datasets were compared with correlative measurements of ERS-2 GOME, AURA OMI and SCIAMACHY stratospheric NO_2 column (scientific product, University of Bremen).

1. INTRODUCTION

SCIAMACHY is a UV/visible/NIR grating spectrometer covering 220-2400 nm range with 0.2-1.5 nm spectral resolution depending on wavelength [1]. It was launched on ENVISAT on March 1st 2002 into a sun-synchronous orbit with a 10:00 equator crossing local time (descending node). The UV-visible nadir measurements of SCIAMACHY are very similar to those of ERS-2 GOME [2], but with better spatial resolution - 30×30 to 30×240 km^2. Global coverage at the equator is achieved in 6 days (due to alternative nadir and limb measurements along the orbit) and more frequently at higher latitudes.

The accurate retrieval of ozone and NO_2 vertical columns from SCIAMACHY UV-Visible nadir measurements present several difficulties and is still a matter of research. Therefore, before being used for scientific application, the relevance of level 2 data must be investigated carefully by means of geophysical validation studies. This paper focuses on comparisons of SCIAMACHY nadir level 2 data products, RT 5.04 and OL 3.00, with correlative ground-based vertical column observations made by Russian M-124 and French SAOZ networks.

Russia has a network of regular ground-based measurements of total ozone, which enumerates about 20 stations. The network is equipped with filter ozonometers M-124 [3] calibrated against Dobson spectrophotometer, which is regularly compared with WMO standard. The network covers a wide range of latitude – from 47 to 69 degrees north (Fig. 1), and the developed processing algorithm allows performing nearly all-weather observations of ozone vertical column.

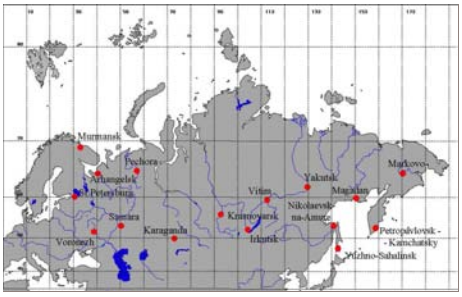

Fig. 1. Locations of M-124 Russian sites, contributing to validation of satellite total ozone observations in 1996-2006

The SAOZ spectrometer (Système d'Analyse par Observation Zénithale, [4]) has been developed in 1988 at Service d'Aéronomie/CNRS, to measure all year round, even when cloudy. SAOZ spectrometer allows measurements of total column of ozone and NO_2 from the ground by UV-visible spectrometry of the zenith sky at twilight. 20 SAOZ instruments have been installed around the globe creating the SAOZ network, with 10 of them being run by CNRS (Fig. 2). This network has been set up with international collaborations and following the recommendations for long-term monitoring and for data quality requirement of the Network for Detection of Stratospheric Changes (NDSC).

Proceedings of the Third Workshop on the Atmospheric Chemistry Validation of Envisat (ACVE-3)
4-7 December 2006, ESRIN, Frascati, Italy (ESA SP-642,February 2007)

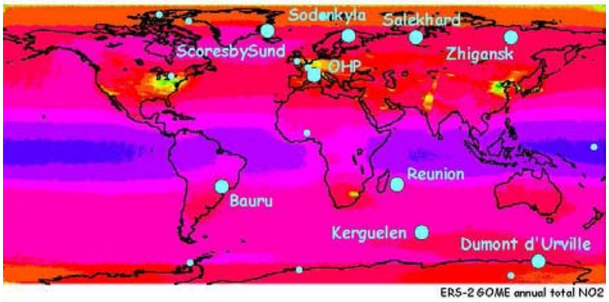

Fig. 2. Locations of ground-based SAOZ instruments

2. GROUND-BASED UV-VIS MEASUREMENTS

2.1 Russian ozonometer M-124

Russian network of total ozone (TO) observations is equipped with filter ozonometers M-124 measuring the direct sun or scattered zenith radiation. Two spectral intervals with 302 and 326 nm maxima and half-width of about 20 nm are used for the observations. TO is retrieved from direct sun measurements at zenith angles 20-70° and zenith scattered (both clear-sky and cloudy) radiation measurements at zenith angles 20-85°. The method provides measurements at high latitude stations and practically all-weather conditions. All the M-124 ozonometers are calibrated against the standard (for Russian network) measurement instrument - the Dobson spectrophotometer No.108, which is regularly compared with the WMO standard. Intercomparisons in Boulder (1988), Hradec Králové (1993), Kalavrita (1997) and Hohenpaissenberg (2001 and 2005) showed that the measurement-scale drift of the Dobson No.108 did not exceed 1.0%. A permanent control of M-124 measurement scale is the obligatory part of instrument verification and provides TO measurements with errors less than 4%. In general, the measurements of TO with M-124 ozonometer apply Dobson-like technique, based on the registration of the ratio of solar radiation fluxes within and outside the ozone absorption band. For zenith sky measurements, an empirical coefficient is used to transfer this ratio from zenith sky measurements to corresponding direct Sun intensities. Within a fixed TO and air mass, this ratio is changing negligibly and depends only on cloud optical density at the sky zenith. Thus, another empirical coefficient, which characterizes this dependence, is determined by the visual estimation of cloud optical density through the color scale and homogeneity of clouds at the sky zenith.

2.2 SAOZ spectrometer

The SAOZ instrument is recording zenith-sky spectra using a wide spectral range (300 - 600 nm) in the UV-visible with a resolution of about 1 nm. Measurements are made at twilight, morning and evening year round even during bad weather conditions. The instrument is composed of a flat field spectrometer with a concave holographic grating and by a photodiode array of 1024 pixels. The field of view of the instrument is about 10° toward the vertical. The O_3 and NO_2 vertical columns are retrieved using the DOAS (Differential Optical Absorption Spectroscopy, [5]) technique applied to zenith-sky measurements in the visible range, 410-618 nm for O_3 and 410-530 nm for NO_2, at twilight. The measurements are averaged in the range of 86-91° sun zenith angle, providing an accurate estimate of O_3 and NO_2 vertical column at sunrise and sunset. This method allows measurements even in cloudy conditions because multiple scattering in clouds affects measurements only slightly. The spectral analysis is conducted in real-time by the instrument, retrieving target species interatively, step by step for each absorbent. It takes the ratio of the observed spectrum to the reference one, which is assumed to be less affected by molecular absorption. This ratio, proportional to the optical thickness, is then analysed using a least-squared fit with absorption cross sections for each constituent determined from laboratory measurements. Resulting line-of-sight amounts (or slant columns) are further converted to corresponding vertical columns, with an enhancement or air-mass factor (AMF), calculated using a radiative transfer model for each constituent at each SZA [6]. The SAOZ instrument has been qualified for ozone and NO_2 measurements in the framework of the NDSC during several international intercomparison campaigns [7-10]. SAOZ measurement errors are estimated to be ~3% for ozone and ~5% for NO_2.

2.3 Comparisons of M-124/SAOZ total ozone with satellite data

Both SAOZ and M-124 network measurements have been intensively used for satellite validation, including comparisons with Nimbus 7, Meteor 3, and EarthProbe TOMS, ERS-2 GOME, ENVISAT SCIAMACHY, and recently AURA OMI data. Thus, Fig. 3 presents comparison of EarthProbe TOMS (version 7 and 8) and ERS-2 GOME (GDP 2.7, 3.0 and 4.0) total ozone data with correlative ground-based measurements at 17 sites of Russian M-124 network in 1996-2001. According to these results, an average difference between TOMS V7 and M-124 total ozone data is only –0.3%, with r.m.s. of 5.6%. Continuous re-processing of GOME measurements demonstrates clear improvements in agreement with M-124: starting from a difference of -3.0% for GDP 2.7, reducing then to -2.5% for GDP 3.0 and finally -1.3% for GDP 4.0. The seasonal dependence of relative “satellite – ground-based” total ozone difference is also considerably reduced in GDP 4.0, compared to 2.7 and 3.0. As for the TOMS V8 re-processed dataset, it was found to be ~2% lower than V7 total ozone data, thus increasing the difference with M-124 from -0.3% to -2.3%.

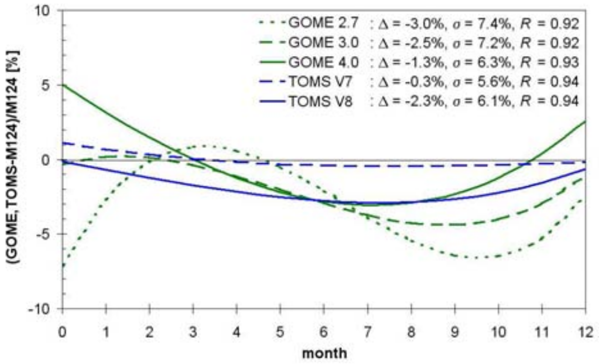

Fig. 3. Relative difference between satellite TO data (TOMS V7 and 8, GOME V2.7, 3.0 and 4.0) and ground-based measurements (M-124) over Russia in 1996-2001 (Δ, σ and *R* correspond to the average, r.m.s. deviation in % and correlation coefficient, respectively)

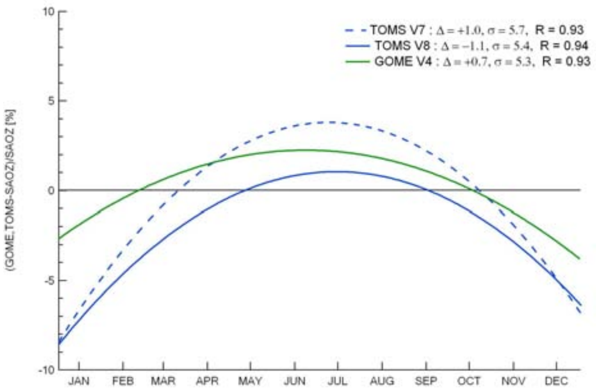

Fig. 4. Relative difference between satellite TO data (TOMS V7 and 8, GOME V4.0) and ground-based measurements (SAOZ) over Scoresby Sund, Sodankyla and OHP in 2004-2006 (Δ and σ correspond to the average and r.m.s. deviation in %, R – correlation coefficient)

Similar comparison of satellite (ERS-2 GOME GDP4, EP TOMS V7 and 8) total ozone data with correlative ground-based SAOZ measurements at 3 northern mid-latitude and arctic stations (OHP, Sodankyla and Scoresby Sund) in 1996-1999 is presented in Fig. 4. A seasonal dependence of difference between SAOZ and satellite data is found for both versions of TOMS, and GOME GPD4, as well. On the average, TOMS V8 data is about ~2% lower, than V7 – which is in agreement with what we have found in comparison with M-124 (see Fig. 3). The seasonal amplitude of relative difference is less for GOME (~4%), compared to TOMS V8 (~8%) and TOMS V7 (~12%).

Finally, Fig. 5 presents comparison of AURA OMI TOMS-like total ozone data (OMTO3) with correlative ground-based measurements by M-124 and SAOZ instruments in 2004-2006. Both ground-based systems demonstrate similar agreement with satellites, to what was found before in comparison with TOMS V8. For SAOZ, the seasonal amplitude of relative difference is reduced with OMI (~6%), compared to ~8% with TOMS V8.

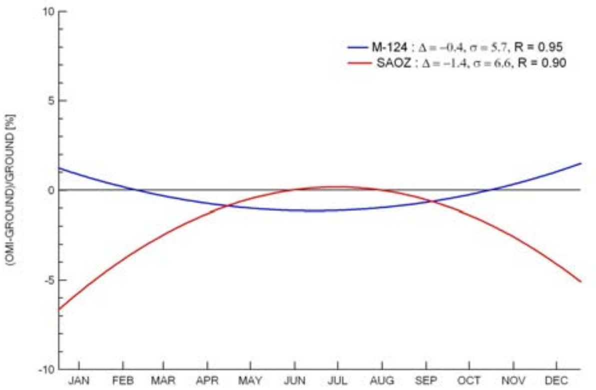

Fig. 5. Relative difference between satellite TO data (OMI TOMS-like), and ground-based measurements – M-124 (over Russia) and SAOZ (over Scoresby Sund, Sodankyla and OHP) in 1996-1999 (Δ and σ correspond to the average and r.m.s. deviation in %, R – correlation coefficient)

2.4 Comparisons of SAOZ total NO_2 with satellite data

Usually, daytime satellite NO_2 data is found closer to ground-based SAOZ measurements at sunrise, rather than sunset value (especially in the tropics and mid-latitudes). At high latitudes – e.g. Scoresby Sund, Dumont d'Urville, Salekhard, during summer, satellites show less NO_2 compared to SAOZ, due to the strong NO_2 diurnal variation along the polar day. Therefore there is a need to correct for the NO_2 photochemical change between sunrise and the satellite overpass.

Atmospheric NO_2 is known to exhibit a strong photochemical cycle throughout the day due to its daytime photolysis into NO and nighttime conversion into N_2O_5. The NO_2 daily cycle starts with a fast drop a little after sunrise followed by a quasi-linear slow increase during the day, a fast increase at sunset, and finally a slow decrease during night. The diurnal cycle has been simulated with a box photochemical model derived from the SLIMCAT 3D chemical-transport model [11]. It includes 98 chemical and 39 photochemical reactions, including heterogeneous chemistry on liquid and solid particles. Calculations are made at 17 altitude levels with a time step of 1 minute. The NO_2 total column is obtained by integrating the profile assuming a constant density in each layer.

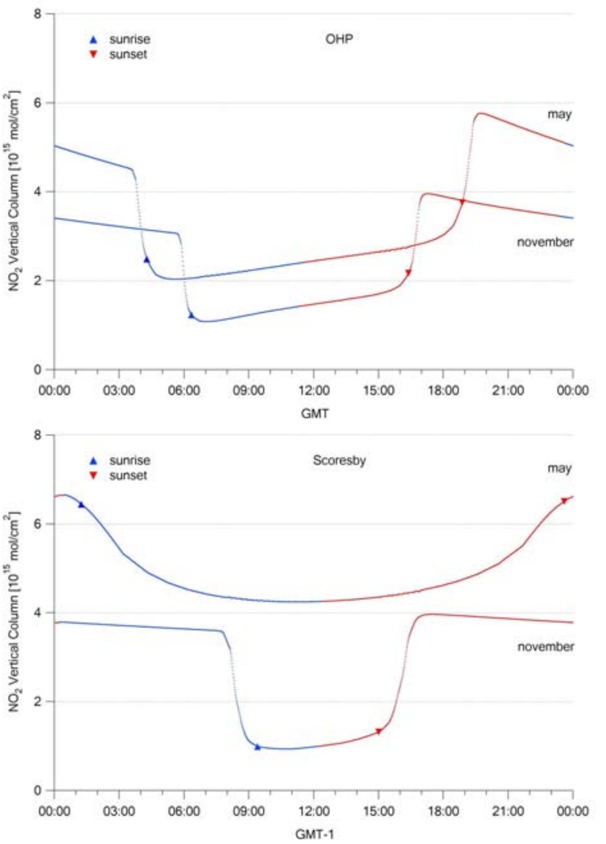

Fig. 6. Diurnal cycle of NO_2 total column at OHP, 44° N (top) and Scoresby Sund, 70° N (bottom), simulated for May and November. The time of 90° SZA is shown by markers.

Fig. 6 shows the results of simulations at two SAOZ stations, OHP at mid-latitude and Scoresby Sund in the Arctic for summer and winter. The noontime column is found close to its sunrise value most time of the year, as expected. However, the ratio between these two changes with the season. The noontime column is larger than that of sunrise in the winter and smaller in the summer, especially during polar day. In addition, a difference also appears between satellites measurements at 10:00 (SCIAMACHY), 10:30 (GOME) and 13:45 (OMI), which needs to be taken into account particularly at low- and mid-latitudes, when the daytime NO_2 is changing faster. For doing this, the daily variation of the ratio NO_2(sunrise)/ NO_2 as been calculated for each of the 12 months at each SAOZ location. As SAOZ is an average of measurements between 86 and 91 SZA the NO_2 column at 88.5° SZA is considered as sunrise reference. All satellite measurements have been normalized to sunrise values using these ratios. This approach proved to be useful for the comparison of satellite NO_2 data with ground-based SAOZ [12]. An example of this correction applied to the measurements over the Arctic Scoresby Sund SAOZ station is displayed in Fig. 7. After correction for the photochemical change the agreement between satellite and SAOZ sunrise measurements improves showing also less scatter during summertime.

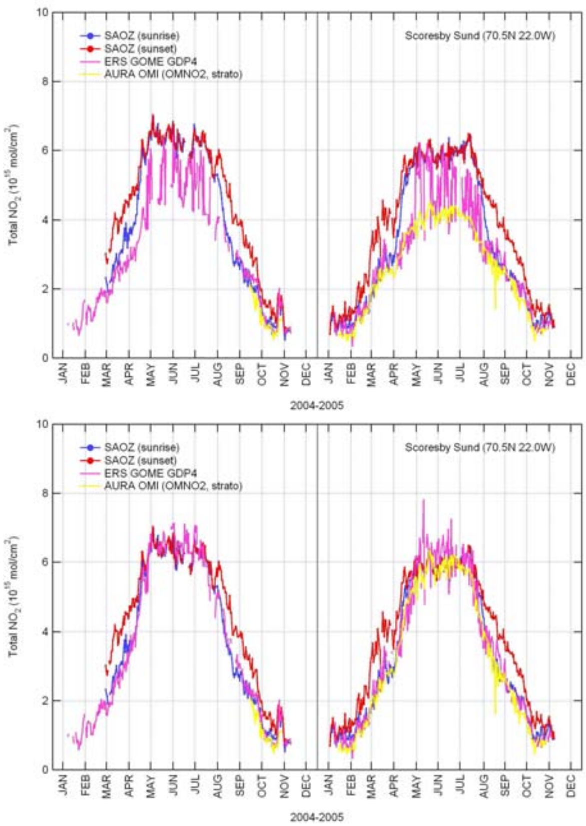

Fig. 7. Comparison of ground-based SAOZ at Scoresby Sund with GOME and OMI NO_2 columns before (top) and after (bottom) photochemical adjustment to sunrise.

3. SCIAMACHY LEVEL 2 DATASETS

Here we are using two SCIAMACHY level 2 datasets to compare with ground-based measurements - real-time processor version 5.04 (RT 5.04) and off-line processor version 3.00 (OL 3.00). We focus on the year 2004 only, when we have most of correlative measurements with both datasets. However, the number of co-locations is rather limited, especially for the recent dataset OL 3.00, and does not cover all of the year (January-April and July-November). SCIAMACHY nadir measurements co-located with the location of ground-based station within a range of 500 km were extracted from the level 2 data and the nearest pixel was selected for the comparison. Overall, more than 9000 M-124 total ozone daily measurements were available for validation, and finally 1772 of them were found to correlate with the data of SCIAMACHY RT 5.04, but only 720 - with OL 3.00. As for the NO_2 data, we have limited our study to comparison over 3 SAOZ ground-based stations, providing most part of correlative measurements with SCIAMACHY in 2004 –

Sodankyla, OHP and Salekhard. From those 10000 daily SAOZ measurements (sunrise, sunset) available for validation, 549 were found to correlate with SCIAMACHY RT 5.04, and only 180 – with OL 3.00.

4. COMPARISON RESULTS

4.1 Ozone vertical column

Both SCIAMACHY datasets – previous RT 5.04 and recent OL 3.00, compared to ground-based M-124 daily total ozone observations, are presented in Fig. 8. It shows regression plots, considering either all correlative data (top) or only those measurements available in both SCIAMACHY datasets (bottom). The numbers on the plots provide relative mean and r.m.s. deviations, and correlation coefficient.

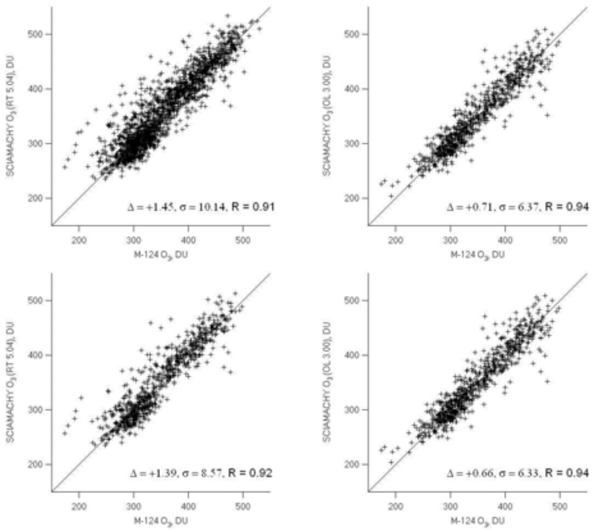

Fig. 8. Comparison of SCIAMACHY total ozone validation datasets with correlative ground-based measurements over Russia (M-124) in 2004: all states SCIAMACHY RT5.04/OL3.00 (top, left/right), and concurrent RT5.04/OL3.00 states only - (bottom, left/right); Δ and σ correspond to the average and r.m.s. deviations in %, R – correlation coefficients

According to these results, the new off-line processor provides better agreement with ground-based M-124 measurements. Thus, the average deviation has changed from 1.4%, found with RT 5.04, to 0.7%, found now with OL 3.00. The r.m.s. deviation has also reduced from 8.6% (RT5.04) to 6.3% (OL3.00).

It is also interesting to investigate if the agreement between satellite and ground-based total ozone measurements depends on cloudiness conditions, as it is an important part of satellite retrieval processor – clouds detection with further correction of ghost (below cloud) ozone column. This algorithm is different for GOME processor, which uses OCRA (Optical Cloud Recognition Algorithm), and SCIAMACHY, using SACURA (SemiAnalytical CloUd Retrieval Algorithm). Fig. 9 presents relative difference [(satellite-ground)/ground] between SCIAMACHY RT5.04/OL3.00, GOME V4.0 and M-124 over Russia in 2004.

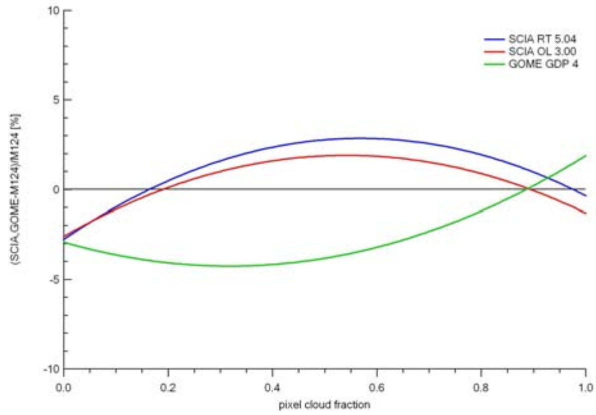

Fig. 9. Relative difference between satellite (SCIAMCHY RT5.04/OL3.00, GOME V4.0) and ground-based (M-124 over Russia) total ozone measurements in 2004, as a function of cloud fraction

According to Fig. 9, there is ~5% dependence of [SCIA,GOME-M124] relative difference, which is similar for both RT 5.04 and OL 3.00 SCIAMACHY, but differs from GOME dataset. However, GOME and SCIAMACHY datasets provide similar results for cloud-free (cloud fraction = 0) or full-cloud (cloud fraction = 1), suggesting an impact of different cloud detection algorithms in case of partial cloud coverage.

4.2 NO_2 vertical column

SCIAMACHY RT 5.04 and OL 3.00 datasets, compared to ground-based SAOZ total NO_2 sunrise observations, are presented in Fig. 10. To compare daytime satellite data with SAOZ measurements in the morning, all SCIAMACHY data were normalized to sunrise NO_2 vertical column, based on its time, day of the year and location (as explained here in 2.3). The figure shows regression plots, considering either all correlative data (top) or only those measurements available in both SCIAMACHY datasets (bottom). The numbers on the plots provide absolute mean and r.m.s. deviations, and correlation coefficient.

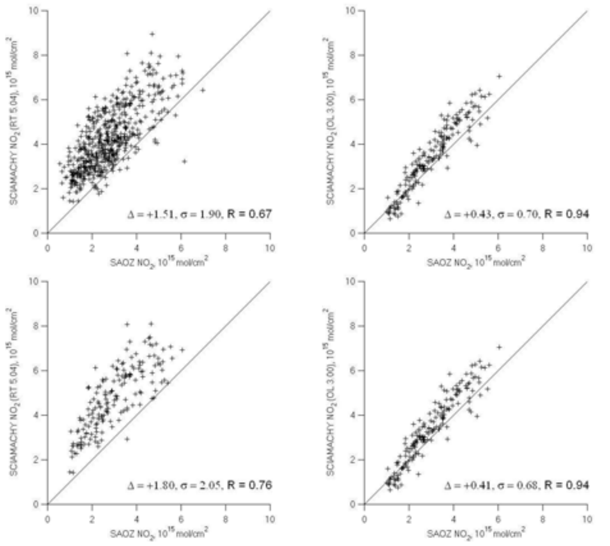

Fig. 10. Comparison of SCIAMACHY total NO_2 validation datasets with correlative ground-based measurements by SAOZ (Sodankyla, OHP and Salekhard) in 2004: all states SCIAMACHY RT5.04/OL3.00 (top, left/right), and concurrent RT5.04/OL3.00 states only - (bottom, left/right); Δ and σ correspond to the average and r.m.s. deviations in 10^{15} mol/cm^2, R – correlation coefficients

As follows from the plots, SCIAMACHY OL 3.00 dataset demonstrate considerably better agreement with ground-based SAOZ measurements. Thus, the average difference has changed from 1.8 (RT 5.04), to $0.4 \cdot 10^{15}$ mol/cm^2, (OL 3.00); the scatter and r.m.s. deviation are less – 0.7 for OL3.00 instead of $2.0 \cdot 10^{15}$ mol/cm^2 for RT5.04; the correlation coefficient is now much closer to 1 – 0.94 instead of 0.76.

4.3 NO_2 stratospheric column (scientific product)

Along with operational SCIAMACHY processing, a number of independent retrieval algorithms were developed for research purposes by different scientific institutes. Compared to operational, such algorithms are usually more flexible and allow detailed investigation of specific retrieval issues. Here we present preliminary comparison of SCIAMACHY NO_2 product, provided by the Environmental Physics Institute of the Bremen University, Germany (hereafter IUPB) with correlative ground-based measurements by SAOZ at 3 sites - Sodankyla, OHP and Salekhard. To compare with SAOZ we used IUPB NO_2 stratospheric columns within a 200 km radius over ground-based station, for the period 08.2002-10.2006 (IUPB data release version 2.0 on 20.11.06). IUPB retrieval uses all operational level 0 and uncalibrated level 1 SCIAMACHY spectra available. Data analysis is based on DOAS technique; in analogy to the GOME retrieval, the wavelength window 425-450 nm in channel 3 was chosen for the fit [13]. Conversion of slant to vertical column amount involves the use of stratospheric AMF calculated by SCIATRAN [14] (full multiple scattering) with the following settings: US Standard profiles of the AFGL reference atmosphere, but without tropospheric content; and a constant surface albedo of 5%. IUPB stratospheric NO_2 columns in 2002-2006, normalized to sunrise, are presented together with SAOZ correlative measurements in Fig. 11.

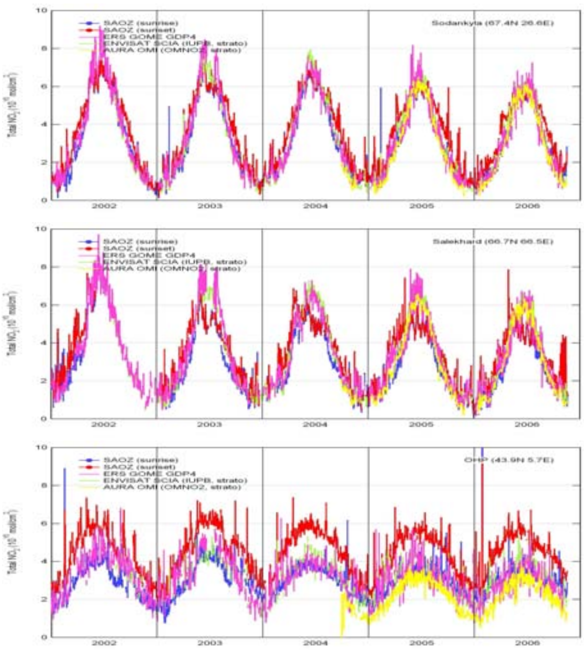

Fig. 11. Comparison of ground-based SAOZ at Sodankyla, OHP and Salekhard with GOME, OMI (stratospheric) and SCIAMACHY (IUPB, stratospheric) NO_2 columns in 2002-2006, photochemically adjusted to sunrise.

On the average, IUPB SCIAMACHY stratospheric columns agree with selected SAOZ measurements in 2002-2006 within $\pm 0.66 \cdot 10^{15}$ mol/cm^2 (r.m.s.), but the estimate of agreement vary from station to station. The best agreement is observed at Sodankyla – mean and r.m.s. differences [SCIA-SAOZ] are +0.03 and $0.50 \cdot 10^{15}$ mol/cm^2, respectively. At OHP IUPB retrievals produce somewhat more NO_2, even compared to SAOZ total column – the average difference is $+0.21 \cdot 10^{15}$ mol/cm^2. This is probably due to frequent tropospheric pollution in that region, which is likely to happen during daytime (thus seen by SCIAMACHY), rather than in the morning and evening (SAOZ twilight observations). Agreement with SAOZ at Salekhard is somewhat worse – mean difference [SCIA-SAOZ] is $+0.51 \cdot 10^{15}$ mol/cm^2; but this is due to systematic underestimation in SAOZ summertime NO_2, compared to all other satellite datasets – GOME, SCIAMACHY and OMI, which is currently investigated. One may also notice a clear systematic bias in the data of OMI stratospheric NO_2 at OHP (OMNO2 overpass data, [NO2-NO2Trop]) – OMI provides 0.8-1.0 [10^{15} mol/cm^2] less NO_2, compared to SAOZ, SCIAMACHY and GOME.

To compare results for IUPB SCIAMACHY NO_2 in 2002-2006 with our studies of operational NO_2 product in 2004, we have extracted SCIAMACHY states, which correspond to RT 5.04 and OL 3.00 2004 validation datasets only. Resulting subsets of IUPB stratospheric NO_2 versus ground-based SAOZ measurements are presented in Fig. 12, for RT 5.04 (left) and OL 3.00 (right), respectively.

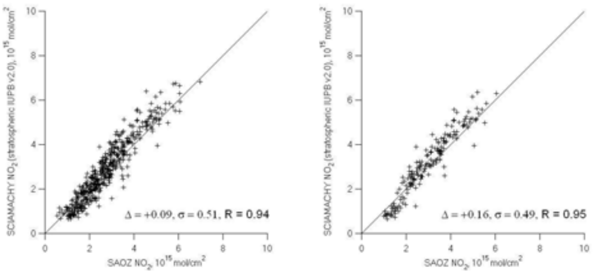

Fig. 12. Comparison of SCIAMACHY stratospheric NO_2 (IUPB) with correlative ground-based measurements by SAOZ (Sodankyla, OHP and Salekhard) in 2004: SCIAMACHY states RT5.04 (left), and SCIAMACHY states OL3.00 (right); Δ and σ correspond to the average and r.m.s. deviations in 10^{15} mol/cm^2, R – correlation coefficients

According to Fig. 12, IUPB SCIAMACHY retrievals provide better agreement with SAOZ, compared to operational RT 5.04 and OL 3.00 – within $\pm 0.5 \cdot 10^{15}$ mol/cm^2 (r.m.s.), which is less than relevant estimates presented in Fig. 10 (bottom): ± 2.0 and $\pm 0.7 \cdot 10^{15}$ mol/cm^2, respectively.

5. SUMMARY

SCIAMACHY nadir level 2 datasets, RT 5.04 and OL 3.00, have been compared with correlative ground-based UV-Vis measurements of total ozone over Russia (M-124) and NO_2 measurements over arctic and mid-latitudes (SAOZ). Both O_3 and NO_2 SCIAMACHY products demonstrate improved agreement with ground-based data, for the recent OL 3.00 dataset, compared to RT 5.04. Thus, the average difference between SCIAMACHY and M-124 ozone column measurements in 2004 was reduced from ~1.4±8.5% (RT 5.04) to ~0.7±6.3% (OL 3.00); the average difference between SCIAMACHY and SAOZ NO_2 column measurements in 2004 was reduced from $\sim 1.8 \pm 1.0 \cdot 10^{15}$ mol/cm^2 (RT 5.04) to $\sim 0.4 \pm 0.6 \cdot 10^{15}$ mol/cm^2 (OL 3.00). Compared to operational, scientific stratospheric NO_2 columns (IUPB) provide slightly better agreement with SAOZ – the average difference is $0.16 \cdot 10^{15}$ mol/cm^2 for the year 2004 SCIAMACHY reference set (OL 3.00), and $0.22 \cdot 10^{15}$ mol/cm^2 for all available SCIAMACHY states in the period 2002-2006.

6. ACKNOWLEDGEMENTS

The authors thank the SAOZ stations operators. Operational GOME data (GDP4) was provided by ESA. GOME data extraction was carried out with a software tool developed by K. Bramstedt (University of Bremen). Non-operational (scientific) data of SCIAMACHY stratospheric NO_2 column were provided by A. Richter (University of Bremen). We gratefully acknowledge H. Roscoe (British Antarctic Survey) for providing an operational software suite (developed in the frame of QUILT EC project) for the retrieval of NO_2 vertical profile, including a photochemical box model developed by M.P. Chipperfield (University of Leeds). In this study data from the Ozone Monitoring Instrument aboard the NASA EOS-Aura satellite has been explored. These data resulted from cooperative research between the Netherlands (NIVR/KNMI), Finland (FMI) and the United States of America (NASA) in the Earth Observing System (EOS) Aura mission. This work was partly supported by ESA (TASTE project), the President of Russia grant (MK-5390.2006.5), and the Government of St.Petersburg (PD06-1.5-5).

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