

# FIRST GROUND-BASED VALIDATION OF SCIAMACHY V5.01 OZONE COLUMN

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## ABSTRACT

In early 2004, the near real-time data processor of ENVISAT SCIAMACHY (SCI\_NL) was upgraded to version 5.01. Based on the correlative measurements acquired and collected during the commissioning phase of the satellite in 2002, a preliminary validation was organised to verify the improvement and assess the geophysical consistency of the new SCIAMACHY ozone vertical column data product. The present overview summarises the results obtained by a list of validation teams and involving ground-based data acquired from pole to pole by complementary ground-based sensors. The studies conclude to an improvement compared to previous versions 3.5x. They also confirm the presence of expected errors (e.g. dependence on solar elevation and on ozone column) inherited from the GOME Data Processor GDP 2.4, on which the SCIAMACHY processor SCI\_NL is based.

## 1. INTRODUCTION

On March 1, 2002, the third Earth observation satellite platform of ESA, ENVISAT, was launched onto a heliosynchronous polar orbit. As part of its atmospheric chemistry payload, the SCanning Imaging Absorption spectroMeter for Atmospheric CHartography (SCIAMACHY) is a joint project of Germany, The Netherlands and Belgium, aiming at the global measurement of key trace gases in the troposphere and

the stratosphere [1]. It is the successor of ERS-2 Global Ozone Monitoring Experiment (GOME), which operates since 1995 [2]. An extensive validation campaign of ENVISAT has been organised by ESA's Atmospheric Chemistry Validation Team (ACVT) [3] and by the SCIAMACHY Validation and Interpretation Group (SCIAVALIG) [4,5] through so-called Announcement of Opportunity (AO) projects. In this framework, correlative ground-based measurements have been acquired and collected into a centralised database.

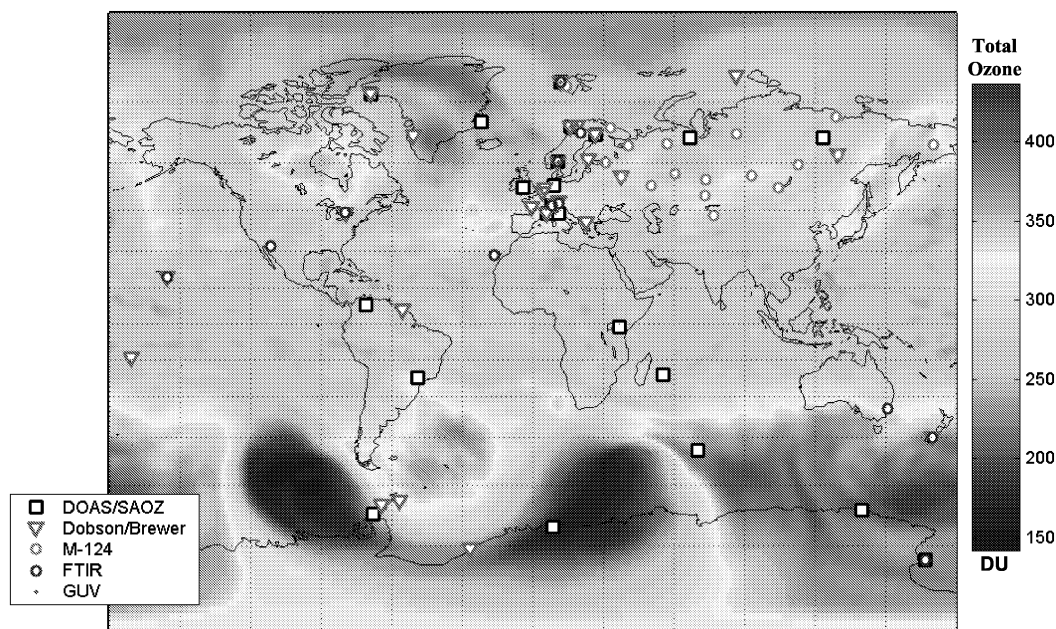
The vertical column of atmospheric ozone (O<sub>3</sub>) is derived from SCIAMACHY measurements of the solar irradiance and Earth nadir radiance spectra. In early 2004, the near real-time data processor of ENVISAT SCIAMACHY (SCI\_NL) was upgraded to version 5.01. Compared to previous version 3.53, the main changes are a new calibration of level-1 spectra, and the use of O<sub>3</sub> cross-sections measured with the SCIAMACHY flight model (FM). Based on limited data sets, a preliminary validation was organised in spring 2004 to verify the improvement and assess the geophysical consistency of the new SCIAMACHY O<sub>3</sub> columns. The present report summarises the outcome of the ground-based studies carried out during this campaign by a large number of validation teams and correlative data providers grouped in several AO projects, namely: AOID 126 (PI: M De Mazière), 158 (J.-C. Lambert), 174 (H. Kelder), 179 (R. McKenzie), 191 (T. Blumenstock), 300 (D. De Muer), 331 (J. P. Burrows), 427 (Yu. M. Timofeyev), and 429 (E. Kyrö). The results were exchanged and discussed

among the SCIAMACHY validation community during two dedicated meetings: (i) the SCIAMACHY Validation Workshop organised by SCIAVALIG on April 5-6, 2004, at KNMI in De Bilt (The Netherlands); and (ii) the second workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2) held at ESA/ESRIN (Frascati, Italy) on May 3-7, 2004. Sections 2 and 3 describe the ozone column correlative ground-based database and the SCIAMACHY data set, respectively, which were available to the validation scientists in 2004. Sections 4 and 5 discuss preliminary ground-based comparison results. Section 4 summarises the overall agreement between SCIAMACHY and correlative ozone columns. Section 5 emphasises the detection of expected errors inherited from GOME Data Processor version 2 on which SCIAMACHY version 5.01 is based. More details and individual AO contributions are reported elsewhere in this issue, as well as the validation of SCIAMACHY ozone data generated by the TOSOMI data processor developed at KNMI. The paper concludes with perspectives for the consolidation of SCIAMACHY total ozone validation.

## 2. GROUND-BASED DATA SETS

O<sub>3</sub> column measurements have been collected from six types of sensors offering complementary capabilities. Dobson [6] and Brewer [7] ultraviolet spectrophotometers record daytime O<sub>3</sub> in the direct sun geometry (weather

permitting) or zenith-sky geometry (all weather conditions), till the solar zenith angle (SZA) reaches values of 70°-75°. Russian/NIS UV filter radiometers (M-124 model) use the same geometry as the Dobson [8,9]. DOAS/SAOZ UV-visible spectrometers measure O<sub>3</sub> column at sunrise and sunset from zenith-scattered sunlight measurements [10,11]. They allow year-round monitoring up to the polar circles. Fourier Transform infrared (FTIR) spectrometers measure daytime O<sub>3</sub> in the direct sun geometry [12], a few of them being also capable of moonlight observations [13]. Calibrated onto the Dobson but extending its capabilities towards lower solar elevation, multi-channel UV filter radiometers (GUV) deployed in Norway derive O<sub>3</sub> from total irradiance measurements [14]. Most of the contributing instruments participate to network programmes in the framework of WMO's Global Atmospheric Watch (GAW) and/or the Network for the Detection of Stratospheric Change (NDSC). During WMO- and NDSC-endorsed intercomparison campaigns [15,10,11], Dobson instruments can be adjusted to agree within 0.3-1%. The long-term agreement between the various instrument types generally falls within the 3% range at middle latitudes [16,17]. At higher latitudes, the enhanced amplitude of several sources of uncertainty (temperature dependence of the absorption cross-sections, profile shape effect, internal straylight at low sun elevation, sensitivity to stratospheric aerosols etc.) generates average differences of about ±3-7% varying with the season and other parameters [16-18].



**Figure 1** - Contributing ground-based total ozone instruments highlighted on top of the total ozone field measured on September 25, 2002, by ERS-2 GOME satellite. Symbols indicate the type of sensor: DOAS/SAOZ UV-visible spectrometers, Dobson and Brewer UV spectrophotometers, M-124 UV filter radiometers, Fourier Transform Infrared spectrometers, and Global UV radiometers.

### 3. SCIAMACHY DATA SETS

During the commissioning phase (CP) of ENVISAT (2002), SCIAMACHY O<sub>3</sub> column data generated by four versions of the near real time processors (SCI\_NL) were distributed to validation scientists. Each of those data sets sampled a different time period in 2002: (i) a few orbits in August with v3.51; (ii) a few orbits in early September with v3.52; (iii) v3.53 data starting from October; and (iv) one orbit on August 23 processed with v4.0. This composite, sparse data set was used for preliminary quality checks as reported in [19], which pointed out major problems and led to the improvement of the SCI\_NL processor studied hereafter. After CP, in order to test quickly the improvement of the data products after any future SCIAMACHY processor change, a validation reference data set of 3026 SCIAMACHY states – the so-called Master Set (MS) – was selected to provide sufficient and suitable coincidences with the CP ground-based measurements, as well as appropriate sampling of the time period from July 2002 to mid 2003.

In early 2004, the SCI\_NL processor was upgraded to the newly operational version 5.01, including new calibration of level-1 data and the use of SCIAMACHY FM O<sub>3</sub> cross-sections. Unfortunately, only 1927 states of MS were processed and delivered to the validation teams in March 2004 for the studies reported here. Limited to the period from July to November 2002, this subset is by far not sufficient for a complete validation of all major geophysical features, but it should at least yield indication of the improvement with respect to the previous SCI\_NL processor versions.

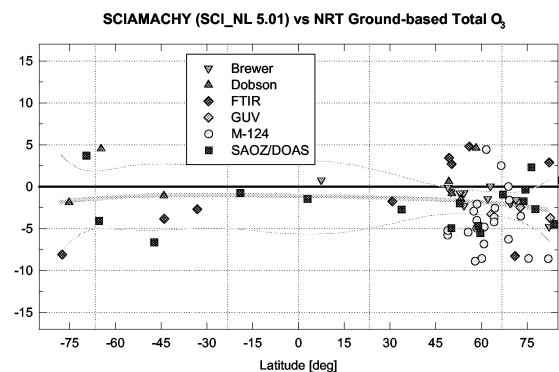
The operational delivery of the Meteo product (SCI\_RV) started in summer 2002. Nevertheless, the time-series available for validation are a composite of successive versions. Some of them are of questionable quality and therefore useless for accurate validation. Moreover, only basic information is available in the Meteo data files (i.e. primarily the ozone column value and its geolocation), which limits the field of investigation. Detailed studies as reported in Section 5 require additional parameters (e.g. solar zenith angle) detailed in the SCI\_NL product. Therefore only SCIAMACHY SCI\_NL results will be reported. At the time of this report, too few orbits have been processed with the off-line data processor (SCI\_OL) developed at DLR-Oberpfaffenhofen (Germany). Moreover, those orbits have been selected for verification of the level-1-to-2 retrieval processing chain rather than for validation. Therefore no SCI\_OL results are reported here. Finally, a few scientific institutes have developed independent retrieval algorithms and generate their own SCIAMACHY ozone column data product. Some of them are described elsewhere in this issue, together with preliminary validation results.

### 4. COMPARISON RESULTS

#### 4.1 Overall Agreement

SCIAMACHY (SCI\_NL 5.01) total ozone data sets delivered for validation purposes and the ground-based data records have been compared qualitatively and, data sets permitting, quantitatively. Qualitatively, short- and medium-term fluctuations captured by ground-based sensors are reproduced similarly by SCIAMACHY. Other scales of geophysical variability such as the seasonal cycles cannot be studied satisfactorily with the current data set, which is too sparse and furthermore limited to the 2002 Northern summer-fall/Southern winter-spring.

On an average, most of the stations conclude to a slight underestimation of the ground-based values by SCIAMACHY. The average underestimation is about 1%. Comparisons based on the Russian/NIS network of M-124 radiometers conclude however to an average 4% underestimation. Figure 2 displays the average relative difference obtained at each station, plotted all together as a function of latitude. For the July–November 2002 time period, no marked meridian structure is to note. The relative difference at a single station can increase or decrease slightly with time, by a few percent. This suggests that seasonally varying differences are to be expected once complete time-series will be available.



**Figure 2** - Mean percentage relative difference between SCIAMACHY SCIA\_NL 5.01 and ground-based total ozone at all stations ( (SCIA-ground)/ground ), from August through November 2002, as a function of latitude.

#### 4.2 Split of the Antarctic Ozone Hole in 2002

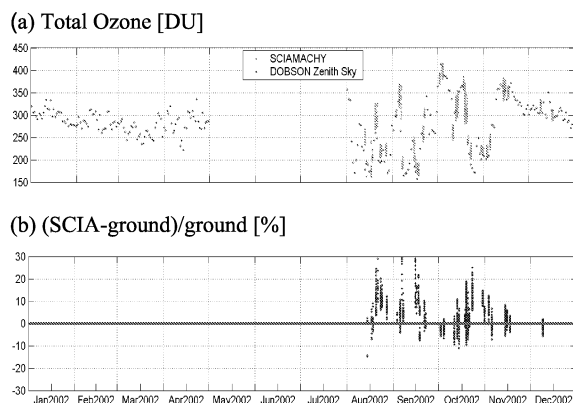
During late September and early October 2002, unusual patterns in the atmospheric circulation surrounding the Antarctic polar vortex distorted it and made it split. This event gave an exceptional morphology to the springtime ozone hole (see e.g. ozone field map on September 25,

displayed in Figure 1), and decreased the level of ozone depletion by raising stratospheric temperatures to sufficiently high to hamper the formation of polar stratospheric clouds. Based on several Dobson and SAOZ UV-visible instruments operating in Antarctica and surroundings, first ground-based comparisons reported in [19] demonstrated how well SCIAMACHY v3.53 reproduced this unexpected behaviour. Studies summarised here confirm that the new version 5.01 of SCIAMACHY SCI\_NL data yields the same level of agreement. Figure 3 and Figure 4 show the comparison at two opposite places on the Antarctic Polar Circle, where it is striking that SCIAMACHY values follow closely the short-term fluctuations recorded from the ground, of which the amplitude sometimes reaches 250 DU in a few days. SCIAMACHY and the BAS/KTSU Dobson at Vernadsky (65°S, 64°W) report mutually consistent observations of the distortion of the polar vortex at the end of September. The agreement even reaches a few percent when exceptionally high values of about 400 DU are recorded for the first time in this season. SCIAMACHY and the CNRS/SA SAOZ at the station of Dumont d'Urville (67°S, 140°E), a station usually alternating between in-vortex and out-of-vortex conditions during spring, report again mutually consistent observations of the high ozone column values over 400 DU characteristics of the mid-latitude circumpolar belt. Figure 4 also illustrates the importance of the SCIAMACHY/SAOZ coincidence criteria in such variable conditions: part (b) includes all SCIAMACHY pixels within a radius of 300 km around the station, which is a criterion widely used; part (c) includes only SCIAMACHY pixels matching the actual geolocation of the air mass probed by a zenith-sky sensor [20]. The drastic reduction in the general scatter and the disappearance of a few biases observed during short periods of a few days illustrate the benefits of using physically based coincidence criteria instead of arbitrary distance criteria. From a more global point of view, SCIAMACHY and ground-based sensors give a view of dynamical features consistent with those described in the WMO Antarctic Bulletins [21] and in [22].

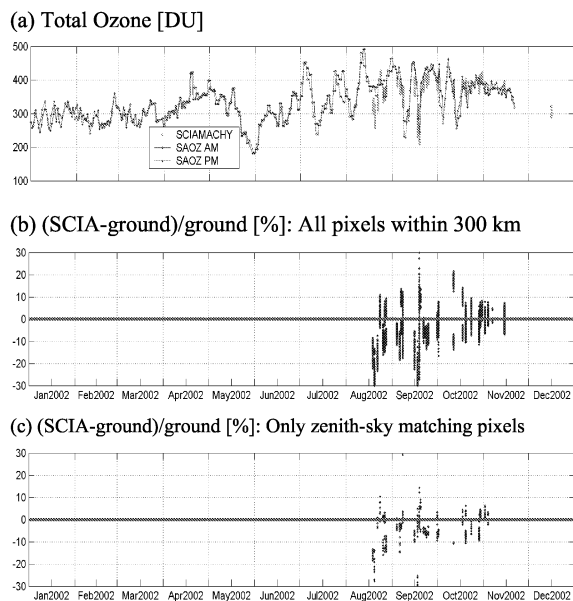
#### 4.3 Comparison with GOME GDP 3

The ground-based correlative database has also been used to carry out a similar investigation of GOME O<sub>3</sub> column data generated by GDP 3. Figure 5 displays the meridian variation of the average relative difference between GOME and ground-based data for the period July–November 2002. The meridian structure of 4% from peak to peak had already been reported in previous validation studies [23]. A new generation of GOME algorithms is on the way to reduce significantly such dependences on the latitude and the season. A priori, the apparent absence of meridian structure between SCIAMACHY and ground-based total ozone (Figure 2)

is surprising. However, it must be kept in mind that in the SCI\_NL v5.01 algorithm, several errors are known to compensate, which vary with time and latitude – e.g. errors associated with the Ring effect and with the absorption cross-sections and their temperature dependence. It is thus likely by chance that no meridian structure has been observed with SCIAMACHY.



**Figure 3** – Comparison of total ozone recorded in 2002 by SCIAMACHY v5.01 and by BAS/KTSU Dobson at the NDSC/Antarctic station of Vernadsky (formerly Faraday): (a) total ozone values within 300 km; and (b) percent relative difference.



**Figure 4** - Comparison of total ozone recorded in 2002 by SCIAMACHY v5.01 and by CNRS/SA SAOZ at the NDSC/Antarctic station of Dumont d'Urville: (a) total ozone values; (b) percent relative difference for all pixels within 300 km; and (c) percent relative difference only for pixels matching the ground-based zenith-sky air-mass.

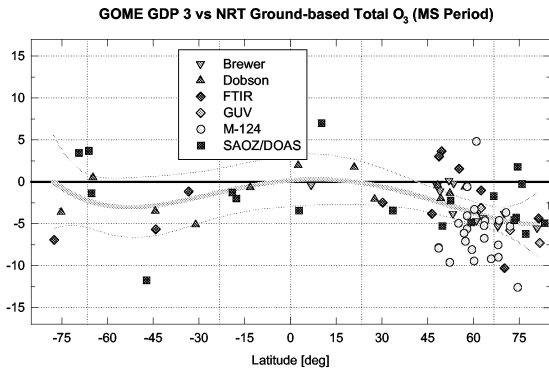


Figure 5 – Same as Figure 2, but SCIAMACHY SCI\_NL 5.01 is replaced by GOME GDP 3.

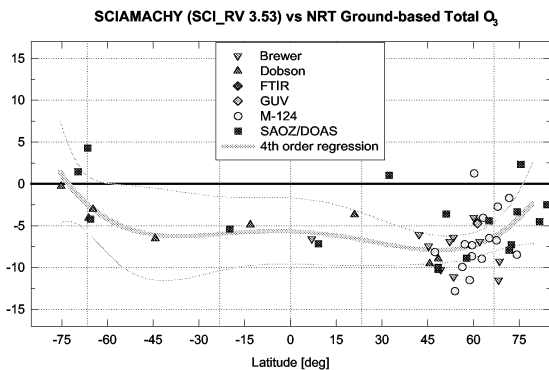
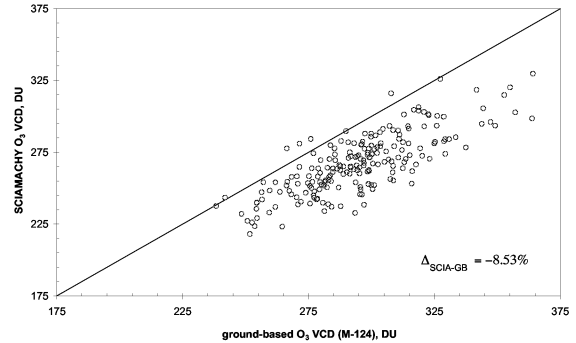


Figure 6 – Same as Figure 2, but SCIAMACHY v5.01 is replaced by SCIAMACHY v3.53.

#### 4.4 Improvement Since v3.53 (2002 Processing)

From the previous subsections we may conclude that SCI\_NL 5.01 has improved compared to versions 3.5x. Ground-based validation studies carried out in 2002 [19] indicated that, from version 3.51 to 3.53, the best results were obtained with version 3.53. The most striking feature of the latter was a general underestimation of ground-based  $O_3$  column values attributed to the inappropriate use of GOME FM  $O_3$  cross-sections, as reminded in Figure 6. This underestimation vanished near the poles. With the new version 5.01 (see Figure 2) using  $O_3$  cross-sections measured by Bogumil et al. with the SCIAMACHY flight model, the underestimation and the meridian distortion have nearly disappeared. Figure 7 shows the improvement over Eurasia, by comparison to correlative data from the Russian/NIS M-124 network: the average difference of  $-8.5\%$  decreases with version 5.01 to an average difference of  $-4\%$ , with no apparent dependence on the  $O_3$  column. This value of  $4.5\%$  is consistent with the improvement noted at other stations of the low and middle latitudes.

(a) SCIAMACHY v3.53 vs. M-124 Network



(b) SCIAMACHY v5.01 vs. M-124 Network

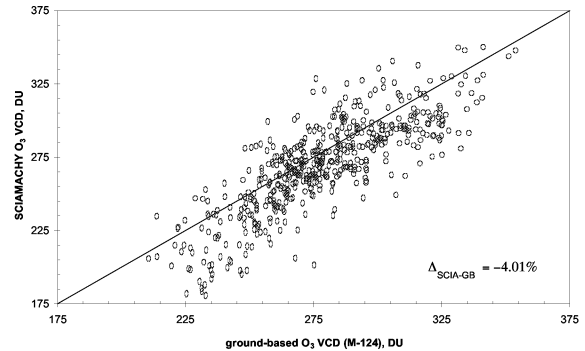


Figure 7 – Regression between SCIAMACHY and ground-based total ozone data acquired at Russian/NIS M-124 stations ( $43^{\circ}$ - $78^{\circ}$ N /  $14^{\circ}$ - $170^{\circ}$ E) from August through November 2002: (a) SCIAMACHY v3.53, and (b) SCIAMACHY v5.01.

## 5. ERRORS INHERITED FROM GOME GDP

All versions of the SCI\_NL processor delivered so far are an adaptation of version 2.4 of the GOME Data Processor, which was operational till 1999. As such, they are expected to produce SCIAMACHY ozone column data that are affected by a variety of known errors resulting in dependences on the SZA of the measurement, the ozone column, the temperature etc. We have already noted in Section 4 that no meridian dependence seems to appear with SCI\_NL 5.01, a fact probably due to compensating errors. Here, we will try to detect in SCIAMACHY data other known dependences of GDP.

### 5.1 Solar Zenith Angle Dependence

The first periodic error detected with GOME GDP appeared as a SZA dependence of the relative difference between GOME and ground-based total ozone values [24-26]. This dependence interferes with and must be decoupled from seasonally varying errors of SCIAMACHY not linked directly with the SZA (e.g. AMF- and temperature-related errors), and with seasonally

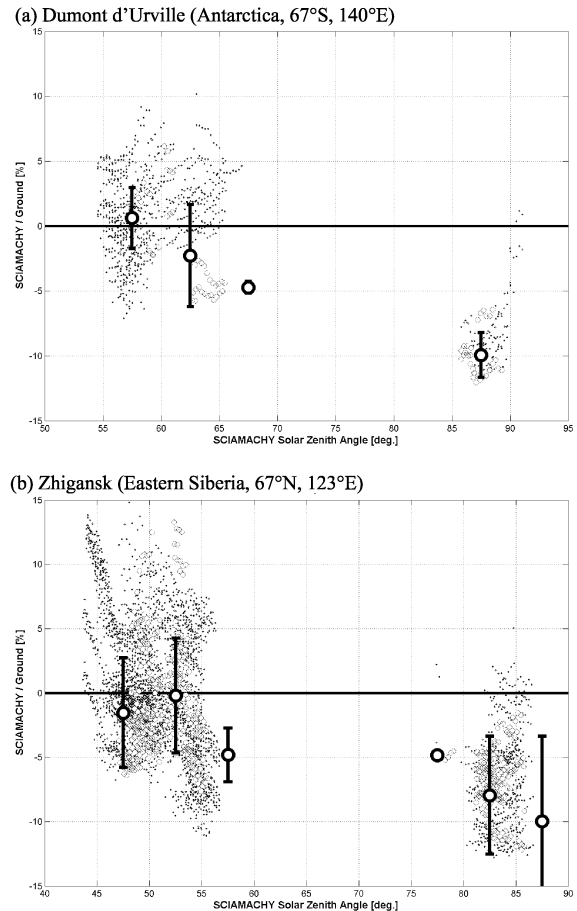
varying errors affecting ground-based data (see e.g. [16]). The available SCIAMACHY states are not sufficient to separate clearly SZA and other seasonal dependences. However, during polar day, thanks to the 960 km swath width of the instrument and the 98.5° inclination of the ENVISAT orbit, SCIAMACHY overpasses polar sites several times a day at different solar local time, that is, under different SZA. Concentrating on the polar day time period when multiple overpasses occur, it is thus possible to detect a SZA dependence between SCIAMACHY data acquired at moderate SZA (mid-morning and noon overpasses) and at high SZA (midnight sun overpass). Using this method, SCIAMACHY data acquired at large SZA (beyond 75°) are found to underestimate by 8% to 10% nearly collocated SCIAMACHY data acquired at moderate SZA. The latter are found in much better agreement with the ground-based SAOZ data (acquired at 86°-91° SZA), as illustrated in Figure 8 where SCIAMACHY O<sub>3</sub> is confronted to the CNRS/CAO SAOZ measurements at the NDSC/Arctic station of Zhigansk in Eastern Siberia and to the CNRS SAOZ measurements at the NDSC/Antarctic station of Dumont d'Urville in Terre Adélie. The 8%-10% SZA dependence of SCIAMACHY SCI\_NL 5.01 is exactly that detected previously in versions 2.0 to 2.7 of GOME GDP.

## 5.2 Ozone Column Dependence

Another significant feature of GOME GDP 2.4 ozone column data is the dependence on the ozone column value [25]. Very low ozone columns observed during springtime ozone depletion at Antarctic stations and, to a less extent, at Arctic stations, are overestimated by GOME by up to 30%, while moderate ozone columns are in much better agreement with correlative ground-based observations. The limitations of the available data sets make it difficult to detect such an ozone column dependence of SCIAMACHY via classical correlation plots. Looking carefully at the fine, short-frequency structures visible in Figure 3 and Figure 4, we can nevertheless note that the difference between SCIAMACHY and ground-based total ozone (parts (a)) is found to correlate with the ozone column variations (parts (b) and (c)). The column dependence known between nearly collocated SAOZ data at Rothera and Dobson data at Vernadsky, can certainly not account for the strong correlation reported here: the SAOZ/Dobson deviation can be significant on the lowest values but is limited to a few percent at 200 DU.

## 5.3 Other Known GDP Errors

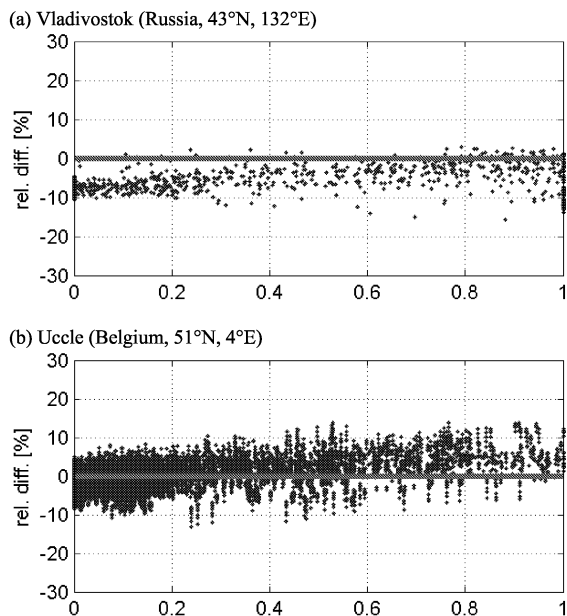
Dependences on other parameters had been identified with versions 2.0 to 2.7 of GOME GDP. Those dependences are caused by errors varying with vertical distributions of pressure, temperature and ozone, with surface albedo, and with the presence of tropospheric and



**Figure 8** – Solar zenith angle dependence of the percentage relative difference between SCIAMACHY O<sub>3</sub> columns and ground-based SAOZ measurements in Antarctica (a) and in Arctic Siberia (b), during polar day 2002. Blue dots include all SCIAMACHY pixels within 300 km around the station; red dots show only pixels matching the zenith-sky air mass, and black dots stand for the average of 10°SZA-binned red dots.

polar stratospheric clouds, thus, errors varying with the latitude, season and meteorological state. They are generated by uncertainties in the determination of the temperature of the absorption cross-sections, in the treatment of the Ring effect, in the treatment of the clouds and the determination of the ghost column hidden by the clouds, and in the calculation of the air mass factor used to convert slant column amounts retrieved from the spectra into vertical column amounts. The detection of such features is difficult with the available SCIAMACHY data sets. We have nevertheless noticed that, at about one third of the involved stations, the relative difference between SCI\_NL 5.01 and the correlative O<sub>3</sub> data depends unexpectedly on the fractional cloud cover. Figure 9 illustrates this cloud dependence with the M-124 ozone columns at Vladivostok and the KMI Brewer data at Uccle in Belgium: using ground-based values as

a standard transfer, SCIAMACHY O<sub>3</sub> column is found to increase linearly with the cloud fraction derived with Optical Cloud Recognition Algorithm (OCRA), by about 5%-10% from cloud-free to fully cloudy pixels. Such a large cloud dependence was not observed with GDP 2.x, which used cloud fraction values retrieved from the O<sub>2</sub> A absorption band (around 760 nm) with Initial Cloud Fitting Algorithm (ICFA). As OCRA is expected to work efficiently with to the good statistics offered by the numerous, small SCIAMACHY pixels, the linear cloud dependence could originate from the O<sub>3</sub> profile climatology used to estimate the ghost column.



**Figure 9** – Percent relative difference between SCIAMACHY 5.01 and ground-based total ozone [ (SCIA-ground)/ground ] as a function of the fractional cloud cover: comparison with (a) M-124 data at Vladivostok, and (b) Brewer data at Uccle.

## 6. CONCLUSION AND PERSPECTIVES

Following the recommendations drawn at the end of the ENVISAT CP in 2002, the SCIAMACHY near real-time data processor SCI\_NL has been upgraded to version 5.01. Based on the correlative measurements acquired and collected during CP, a preliminary validation was organised in March and April 2004 to verify the improvement and assess the geophysical consistency of the new SCIAMACHY ozone vertical column data product. The present overview summarises the outcome of ozone validation results obtained by a list of validation teams, through comparisons with ground-based measurements acquired from pole to pole by networks of complementary sensors (Brewer, DOAS/SAOZ, Dobson, FTIR, GUV and M-124).

The late delivery of ENVISAT data products, furthermore limited to a part of the 2002 Northern summer-fall/Southern winter-spring season, hampered the output of the planned validation effort. Nevertheless, the amount of available collocations with ground-based data was sufficient to demonstrate that SCIAMACHY ozone column data product v 5.01 contains consistent geophysical information. It may be used for quantitative studies of the Southern Hemisphere polar vortex split of September 2002, provided that end-of-orbit and aberrant data are properly filtered out and that errors inherited from GDP 2.4 are taken into account. The studies also conclude to an improvement compared to previous versions 3.5x of the SCI\_NL processor. The overall agreement of about 1% seems excellent, however, this result must be considered with circumspection, as it is known that major errors in the current retrieval algorithms compensate. The poor space/time sampling of the SCIAMACHY data available for the reported studies might also bias the results. Comparisons confirm the presence of expected errors inherited from version 2.4 of the GOME Data Processor, on which the SCIAMACHY processor is based: SZA dependence of 8%-10% a high latitudes in summertime; overestimation of lowest O<sub>3</sub> columns recorded during springtime O<sub>3</sub> depletion events; fractional cloud cover dependence at one third of the stations. Other known errors are difficult to assess but they cannot be ruled out.

The aforementioned errors, and other limitations in the current processing, require urgently an upgrade of the SCI\_NL processor to state-of-the-art ozone column processing. Provided that the operational delivery of ENVISAT gets on and that at least one entire year of SCIAMACHY data is reprocessed with future upgrades of the level-1-to-2 processor, consolidated geophysical validation results, that is, firm conclusions on the quality and geophysical usability of SCIAMACHY O<sub>3</sub> column data, could be drawn in the second half of 2004.

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