VALIDATION OF GOMOS (GOPR 6.0A) AND SCIAMACHY (V5.1/2.1) O_3 AND NO_2 PRODUCTS WITH GOME (V3.0 AND IUP RETRIEVALS), HALOE (V19) AND SAGE II (6.2)

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ABSTRACT

The operational data products of O_3 and NO_2 from the two ENVISAT instruments GOMOS and SCIAMACHY are validated by comparison with other space borne instruments. Except for latitudes >40°S, SCIAMACHY operational O_3 columns (v5.1) show an agreement within 2% with GOME 3.0 and a negative bias of 0-5% with the scientific GOME-WFDOAS product [1]. Both SCIAMACHY NO_2 columns, the operational v5.1 compared to GOME 3.0 and the scientific SCIAMACHY_IUP compared to GOME_IUP [2], show an agreement within 15% at most latitudes. SCIAMACHY O_3 profiles (v2.1) are within –6 to 20% (RMS 20-25%) with HALOE and SAGE II. But, SCIAMACHY NO_2 profiles (v2.1) are showing a high positive bias of 50% (RMS 50%) to HALOE (including photochemical corrections for HALOE NO_2 data) and 10% of the profiles have unphysical values. The GOMOS O_3 profiles (v6.0a) are within 5% (RMS 5-15%) compared to SAGE II. GOMOS NO_2 profiles (v6.0a) are within -30 to +60% (RMS 10-30%) to SAGE II (including photochemical corrections).

1 INTRODUCTION

The SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography, see e.g. [3]) instrument, and the GOMOS (Global Ozone Monitoring by Occultation of Stars, see e.g. [4]) are part of the atmospheric instrumentation on the Environmental Satellite (ENVISAT) launched in March 2002. From both instruments the ozone and the NO_2 products were compared to the satellite measurements of the three instruments: the Global Ozone Montitoring Experiment (GOME, version 3.0 and for ozone columns from the WFDOAS by [1]), Halogen Occultation Experiment (HALOE, data version v19) and the Stratospheric Aerosol and Gas Experiment II (SAGE II, data version 6.2). The data products of all three are well validated and instruments are successfully operating since many years.

SCIAMACHY measures in nadir, limb and occultation geometry the UV-VIS-NIR range solar and backscattered radiation from Earth. From nadir measurements total columns of various trace gases, among them, ozone and NO_2, are derived with a spatial resolution of 30 km by 60 km. The SCIAMACHY ozone and NO_2 columns (version 5.1 and for NO_2 also the scientific IUP product by [2]) from the two calibration orbits from 2002/08/23 are compared to measurements from the nadir viewing instrument GOME, operational since 1996 on ERS-2. In addition, SCIAMACHY ozone and NO_2 profiles (version 2.1 from the validation master set) derived from limb measurements with a vertical resolution around 3 km are validated with measurements from the solar occultation instruments HALOE and SAGE II.

GOMOS measures ozone and NO_2 profiles with stellar occultation between 17-22 km up to 80-100 km with 1 km resolution, more details in [4]. GOMOS profiles version GOPR 6.0a from the ACRI processor were validated with collocated SAGE II measurements from 2002/09/01 to 2003/03/31. Results from these ENVISAT products validations are summarized in this paper.

2 SCIAMACHY O_3 COLUMNS WITH GOME

Since the validation reference set for the ACVE-2 workshop only contained incomplete orbits of SCIAMACHY data, we chose for this study to compare the SCIAMACHY O_3 total column data (version 5.1) of the two complete calibration orbits 2509 and 2510 from 2002/08/23 to GOME data, GDP 3.0 and from the scientific IUP-product using weighting function DOAS (WFDOAS) described in [2], from the same day.

Because GOME/ERS-2 and SCIAMACHY/ENVISAT are flying in the same orbit only 30 minutes apart, numerous collocated measurements can be detected (up to 28000 a day). In order to quickly compare collocations of a day up to a months period, and in addition to that, to overcome the difference in ground pixel size of 30 km x 60 km of SCIAMACHY and 40 km x 320 km for GOME, the following method was applied, already described in [5]: All O_3 total column data from SCIAMACHY calibration orbits and from GOME GDP 3.0 and WFDOAS from 2002/08/23 are spatially binned into regular 2.5° and 2.5° grids. Fig. 1 shows binned tO_3 for the three data sets. If both instruments have measurements in the same grid, then

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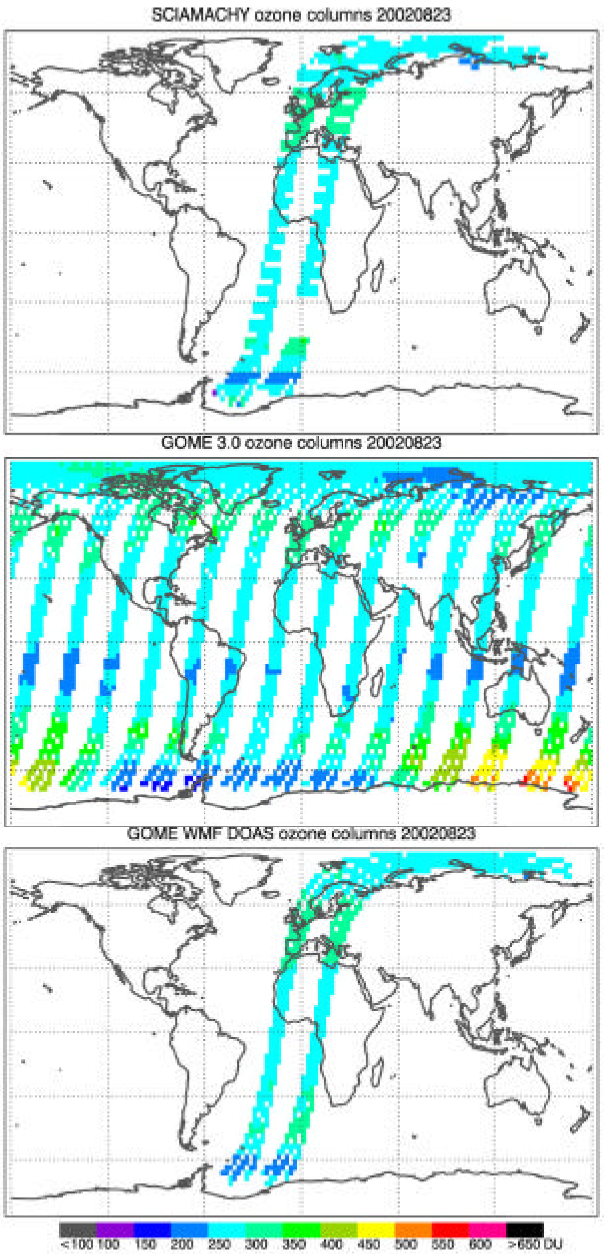

Fig. 1. Binned total O_3 from SCIAMACHY v5.1 (top), GOME 3.0 (middle), and GOME WFDOAS (bottom), from 2002/08/23.

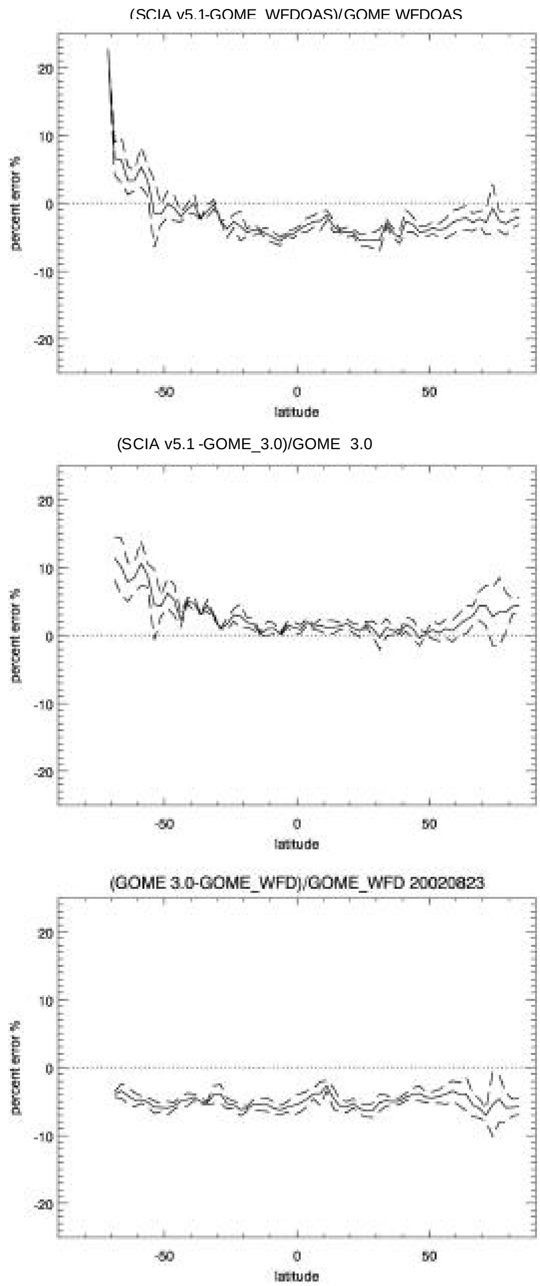

Fig. 2. Comparison of binned total O_3 from SCIAMACHY v5.1 with GOME WFDOAS (top), SCIAMACHY v5.1 with GOME 3.0 (middle), GOME 3.0 with GOME WFDOAS (bottom), from two orbits on 2002/08/23. The mean relative deviation (straight line) and the RMS of the mean relative deviation (dotted line) is shown as a function of latitude

the mean of the data of one instrument is compared to the mean of the data of the other instrument as follows:

$$(tO_3 \text{ of SCIA- } tO_3 \text{ of GOME})/\ tO_3 \text{ of GOME} \qquad (1)$$

Fig. 2 shows the results as a function of latitude of the comparison of binned SCIAMACHY (5.1) total ozone to binned GOME WFDOAS and GOME (3.0) ´data, and also the comparison of binned GOME (3.0) total ozone to GOME WFDOAS data from the two calibration orbits. At latitudes <55°S, SCIAMACHY is between 0% to 5% (±5%) lower than GOME WFDOAS, while at >55°S it between 0 and 20% higher. In comparison to GOME 3.0, SCIAMACHY is up to 2% (±5%) higher at 15°S to 65°N. Above 15°S SCIAMACHY reaches a positive bias up to 11% (±5%). GOME 3.0 shows a negative bias of 3 to 6% to GOME WFDOAS. GOME tO_3 data from both algorithms, GDP 3.0 and WFDOAS, still show a very good accuracy (around 3% [1] and [6]) despite aging of the instrument.

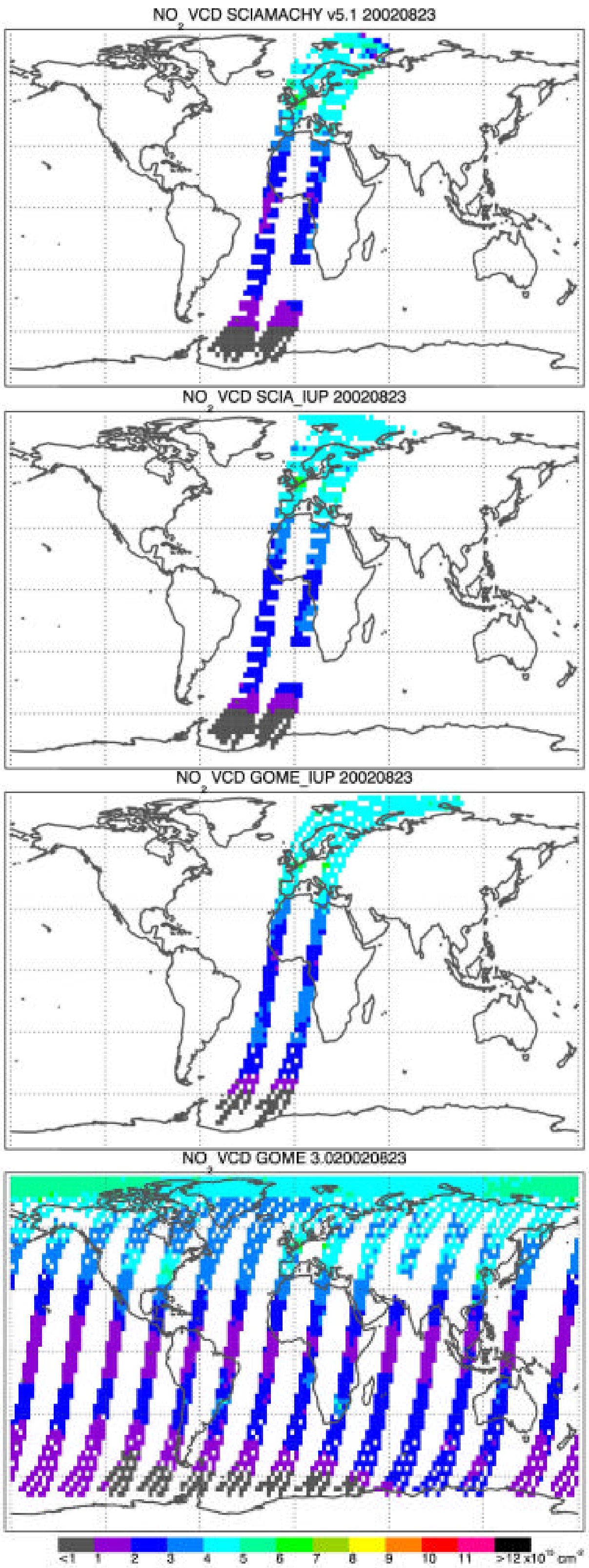

Fig. 3. Binned NO_2 vertical columns from SCIAMACHY v5.1, SCIAMACHY_IUP [2], GOME_IUP [2], and GOME 3.0 (from top until bottom) from 2002/08/23.

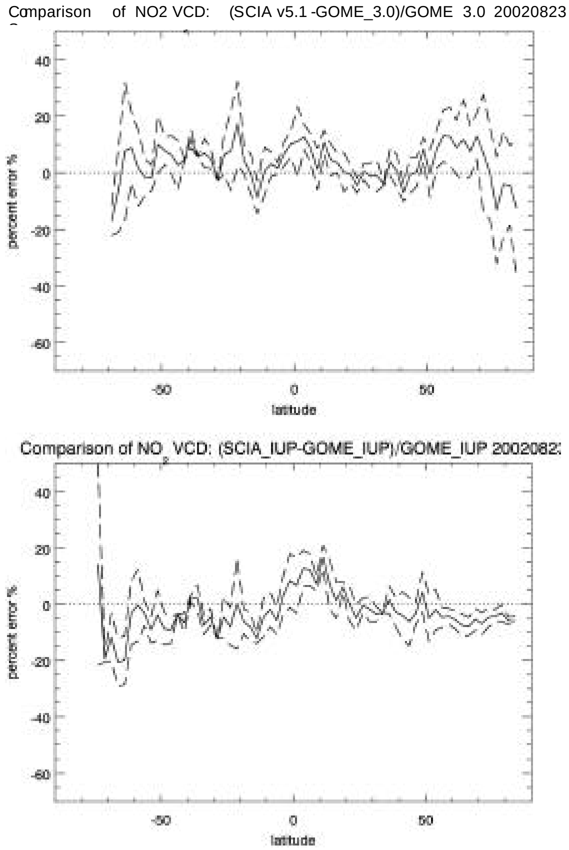

Fig. 4. Comparison of binned NO_2 vertical columns from SCIAMACHY v5.1 with GOME 3.0 (top) and SCIAMACHY_IUP with GOME_IUP [2] from two (calibration) orbits on 2002/08/23. The mean relative deviation (straight line) and the RMS of the mean relative deviation(dotted line) is shown as a function of latitude

The results of the comparison of SCIAMACHY 5.1 tO_3 with both GOME algorithms shows a big improvement to former versions and is recommended from this study to public release.

3 SCIAMACHY NO2 COLUMNS WITH GOME

SCIAMACHY NO_2 vertical column densities (VCD) of the operational product (5.1) and of the scientific product by IUP [2] were compared to GOME 3.0 and the GOME IUP product [2] using the same method as described in section 2. Fig. 3 shows binned NO_2 VCD for the four data sets. Fig. 4 shows the results as a function of latitude of the comparison of binned SCIAMACHY (5.1 and IUP) NO_2 VCD to binned GOME (3.0 and IUP). At all latitudes, SCIAMACHY 5.1 is within 15% (±5-20%) of GOME 3.0 and SCIAMACHY IUP is within –20 to +15% (±2-15%) of GOME IUP. The results of the comparison of

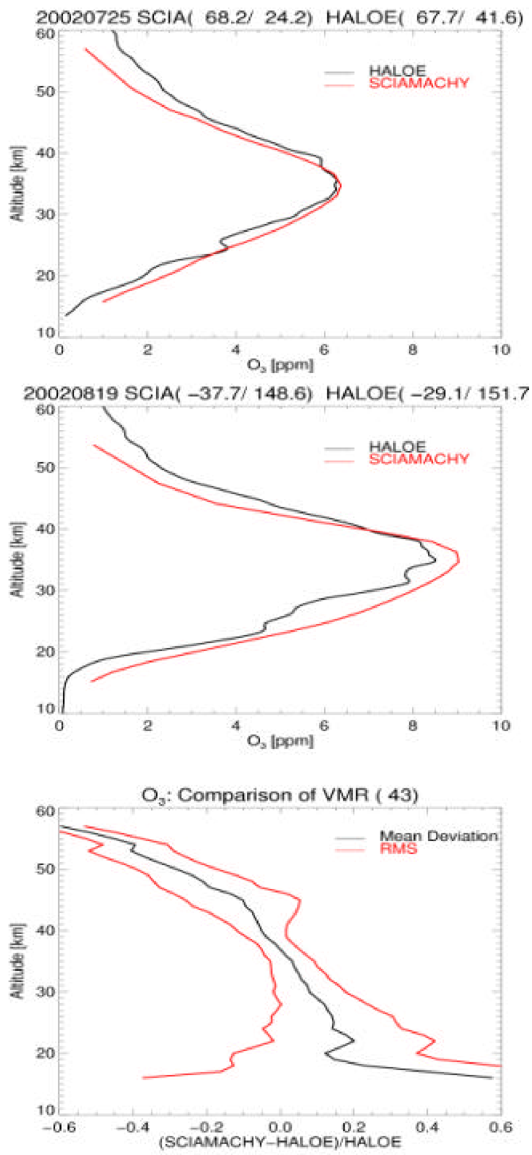

Fig. 5. Comparison of collocated SCIAMACHY O_3 profiles with HALOE profiles from validation reference set in 2002. Two Examples of a collocated measurement (two upper figures) from HALOE (black) and SCIAMACHY (red) in VMR (second lowermost figure) and mean relative deviation (black) and root mean square of mean relative deviation (red; bottom) of the comparison of all collocations (n=43)

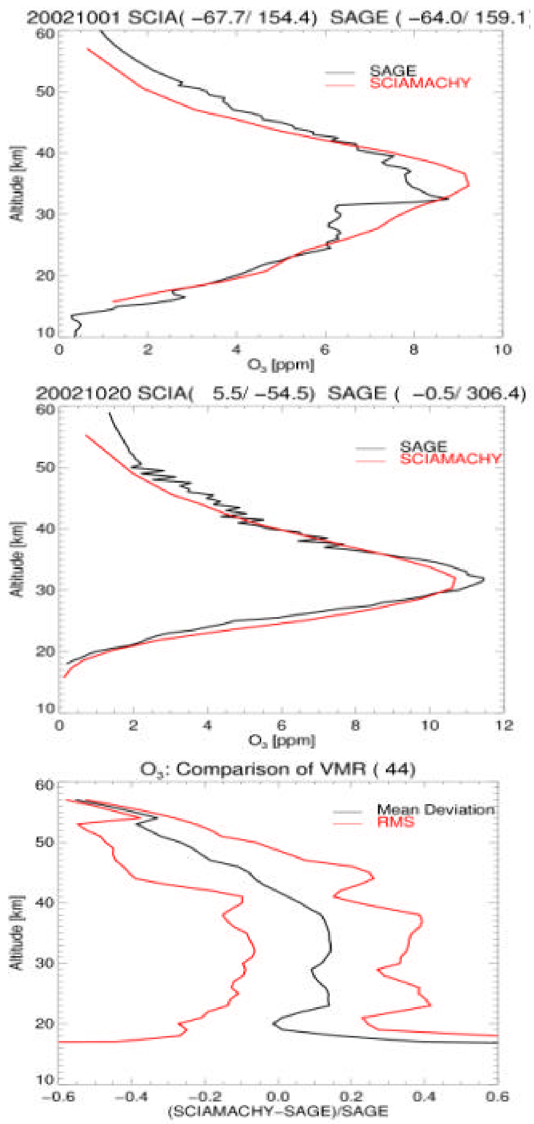

Fig. 6. Comparison of collocated SCIAMACHY O_3 profiles with SAGE II profiles from validation reference set in 2002. Two Examples of a collocated measurement (two upper figures) from SAGE II (black) and SCIAMACHY (red) in VMR (second lowermost figure) and mean relative deviation (black) and root mean square of mean relative deviation (red; bottom) of the comparison of all collocations (n=44)

SCIAMACHY 5.1 with GOME 3.0 shows a big improvement to former versions. After reprocessing all SCIAMACHY data with this version, an extended validation can be done once again to prove if these data can be released to public soon.

4 SCIAMACHY O_3 PROFILES WITH HALOE AND SAGE

The complete SCIAMACHY O_3 profiles from the validation reference set (data from 2002/07/18–12/16) are searched for coincident measurements with HALOE and SAGE II with the coincidence criteria, that the tangent point of the HALOE or SAGE II is within 1000 km of SCIAMACHY and measurements were performed within 12 hours. The relative deviation for each collocated match pair is determined as in Eq. 1:

Relative deviation = $(SP_{SCIAMACHY} - SP_{SAT})/ SP_{SA}$ (1),

where SP is the concentration of the trace gas species and SAT is the correlative measurement, either of HALOE or SAGE II. During the time period of the validation reference data set altitude errors up to 3 km due to an ENVISAT pointing problem have been observed in SCIAMACHY, but also in MIPAS data [7,8].

For the O_3 profile comparisons with HALOE, 51 collocations are found. Eight collocations are excluded from further analysis, because UKMO PV data at 475 K and used to calculate the tropopause height indicated that the SCIAMACHY and the HALOE profile are coming from different air masses (method described in more detail in [9]). The collocation distribution is highly biased towards the northern latitudes, with 24 at 60°N to 90°N, 12 at 30°N to 60°N, one in the tropics, and only 5 in the mid and high southern latitudes. Fig. 5 shows two examples in the high northern latitudes and the subtropics and the statistical results of collocated O_3 profiles from SCIAMACHY and HALOE in volume mixing ratios (VMR). In both examples, there is a fair agreement between the two measurements at 20 to 42 km, but especially at high altitudes the pointing problem becomes obvious. The statistical results show between 22 and 57 km an agreement of SCIAMACHY O_3 VMR from -6 to 20% (±20%) to HALOE.

For the O_3 profile comparisons with SAGE II, 56 collocations are found. 12 collocations were excluded from further analysis, because as indicated by UKMO data the SCIAMACHY and the SAGE II profile are coming from different air masses. As in the other comparison, the collocation distribution is highly biased towards the northern latitudes, with 26 at 60°N to 90°N, 11 at 30°N to 60°N, one in the tropics, and only 5 in the mid and high southern latitudes. Fig. 6 shows two examples in the high southern latitudes and the tropics and the statistical results of collocated O_3 profiles from SCIAMACHY and SAGE II in VMR. In both examples, there is a fair agreement between the two measurements at 20 to 42 km, but also here at high altitudes the pointing problem becomes obvious. Also the O_3 maximum of SCIAMACHY in the high latitudes is significantly higher and in the tropics is lower than the SAGE II data. The statistical results show between 22 and 57 km a positive bias of SCIAMACHY O_3 VMR from 0 to 15% (± 20 to 25%) to SAGE II.

The accuracy of HALOE O_3 profiles is given with about 6% between 30 and 60 km and 20% between 15 to 30 km [10] and of SAGE II with 10% between 10 and 50 km [11]. Taking these accuracies and the generally observed 10% bias between HALOE and SAGE II O_3 values, results show that between 21 and 50 km reasonable SCIAMACHY O_3 VMR (v2.1) are retrieved. But, still the tangent height offset resulting from the pointing problem problem, affects tremendously the results.

5 SCIAMACHY NO2 PROFILE WITH HALOE

The complete SCIAMACHY NO_2 profiles from the validation reference set (data from 2002/07/18–12/16) are searched for coincident measurements with HALOE with the same coincidence criteria, as described in section 4. For the NO_2 profile comparison with HALOE, 26 collocations are found. The collocation distribution is as for the other trace gas validations highly biased towards the northern latitudes, with 17 at 60°N to 90°N, 4 at 30°N to 60°N, 1 in the tropics, and only 4 in the mid and high southern latitudes. Since NO_2 by HALOE is measured during local sunrise or sunset, and by SCIAMACHY at different solar zenith angles (SZA) during the day (~10 LT), the HALOE measurements are scaled to the SCIAMACHY SZA using a 1-dim version of a chemistry and photolysis model with reaction and photolysis rates from the JPL 2000 [12] (method described in [13]).

Fig. 7 presents four examples of the comparison of HALOE and SCIAMACHY NO_2 profiles including the results from scaling the HALOE measurement with the photochemical model. SCIAMACHY measurements shown in the examples are taken during daytime at 27°, 30°, 50° and 69° SZA. Two kind of modelled NO_2 profiles are shown: The model at 90° signifies where the model is scaled in such a way that NO_2 values correspond to the HALOE NO_2 measurement at the HALOE SZA of 90° in dependence to the type of twilight (sunrise or sunset) during the measurement. Taking this model at 90° NO_2 value and running it to the individual SZA of the SCIAMACHY measurement, gives the modelled NO_2 profile at SCIAMACHY SZA (HALOE_Model at SCIAMACHY SZA). Comparing the model results at 90° to the HALOE measurement illustrates the possibility of the model to be applied for scaling NO_2 in dependence to SZA variations at a certain latitude and a certain time. Like in 10% of all cases, Fig. 7 (top) shows an example of SCIAMACHY NO_2 profile with exhibiting unphysical behaviour. The next two example (Fig. 7, middle) only show reasonable values down to 30 km which is also the case in about 40% of all investigated profiles. The last example shows the typical case for the last 50% of investigated profiles, with SCIAMACHY NO_2 concentrations being systematically to high as compared to HALOE_Model at SCIAMACHY SZA. Fig. 8 shows the mean profiles and the relative differences of all profiles from these comparisons of SCIAMACHY to HALOE_Model at SCIAMACHY SZA. SCIAMACHY NO_2 profile (v2.1) are about 50% (± 50%) higher at 25 to 40 km to HALOE_Model. The accuracy of HALOE NO_2 profiles is given with about 15% between 25 and 45 km [14] and the total error of the model between 20 and 40 km was calculated to be ~5% for daytime (SZA <94°) measurements [13]. The significant high bias of SCIAMACHY NO_2 profiles require further work.

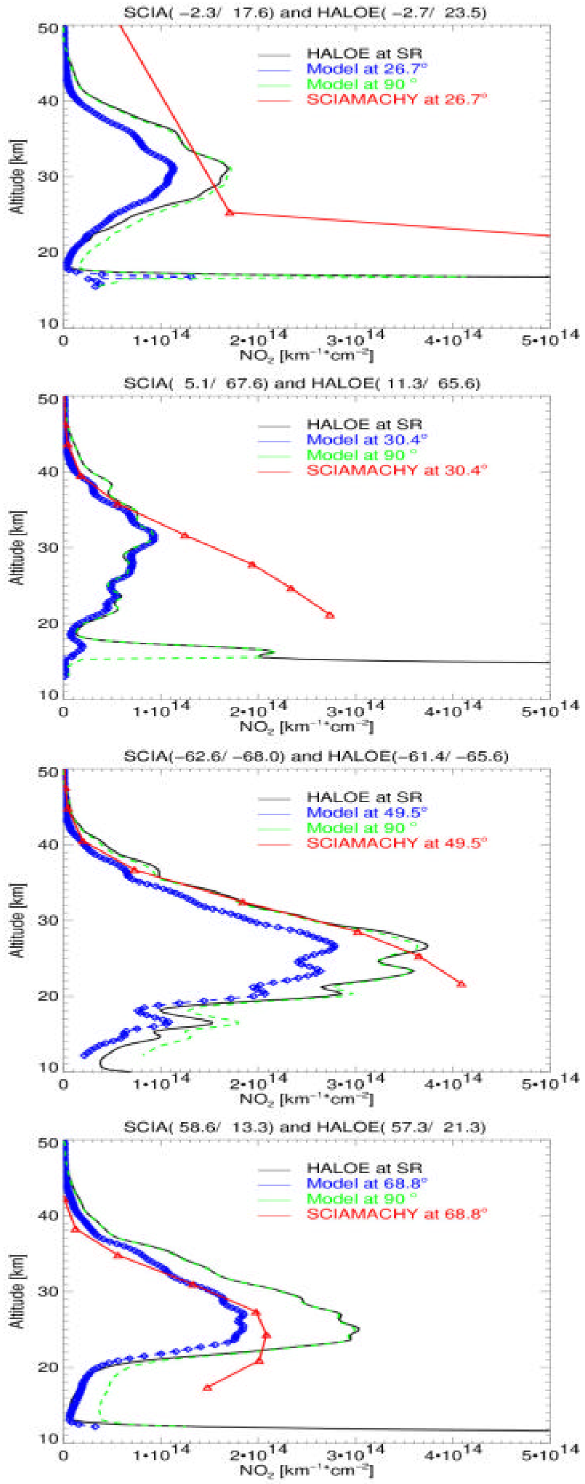

Fig. 7. Comparisons of NO_2 profiles from HALOE (black) and SCIAMACHY (red) from the validation reference set in 2002 with results from model runs described in [6]: Model at 90° (green) signifies where model NO_2 values are scaled to correspond to HALOE NO_2 at HALOE SZA of 90°. Then Model at 90° NO_2 values are scaled to the certain SZA of the SCIAMACHY measurement which gives the modelled NO_2 values at SCIAMACHY SZA (Model at SCIAMACHY SZA, blue). Examples (from top to bottom) at 27°, 30°, 50° and 69° SZA

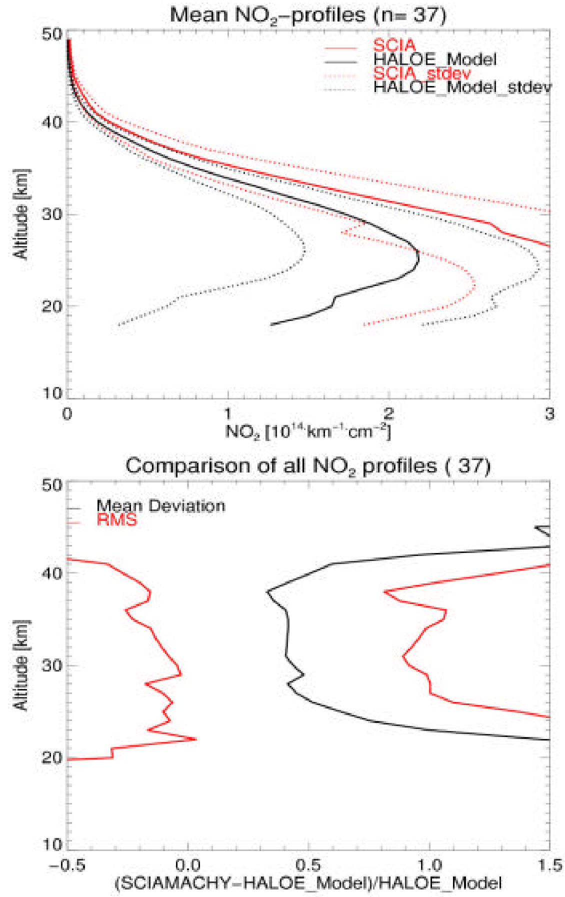

Fig. 8. Statistical results of the comparisons of NO_2 profiles from all collocated HALOE and SCIAMACHY measurements from the validation reference set in 2002. Top: Mean profiles (straight line) with standard deviation (dotted line) of HALOE_Model (black) and SCIAMACHY (red). Bottom: Mean relative deviation (black) and RMS of mean relative deviation (red) of all comparisons of NO_2 values from SCIAMACHY to HALOE_Model.

6 GOMOS O3 PROFILES WITH SAGE II

The complete GOMOS O_3 profiles from 2002/09/01–2003/03/31 are searched for coincident measurements with SAGE II with the coincidence criteria, that the tangent point of the SAGE II is within 250 km of GOMOS and measurements are taken at the same day. The relative deviation between the collocated measurement pairs is calculated as described in section 4. 367 collocations are found with SAGE II with 157 at 30°N to 60°N, 96 at 30°N to 30°S, 58 at 30°S to 60°S, and 56 at 60°S to 90°S. 177 GOMOS measurements were dark observations, 7 taken during daylight, 30 under twilight, 97 under straylight, and 56 under twilight and straylight conditions. Fig. 9 and 10 show examples and the statistical results from GOMOS O_3 profiles taken under the five different light conditions with SAGE II. In all examples, the GOMOS profile agrees very well with the SAGE II profile between 17 to

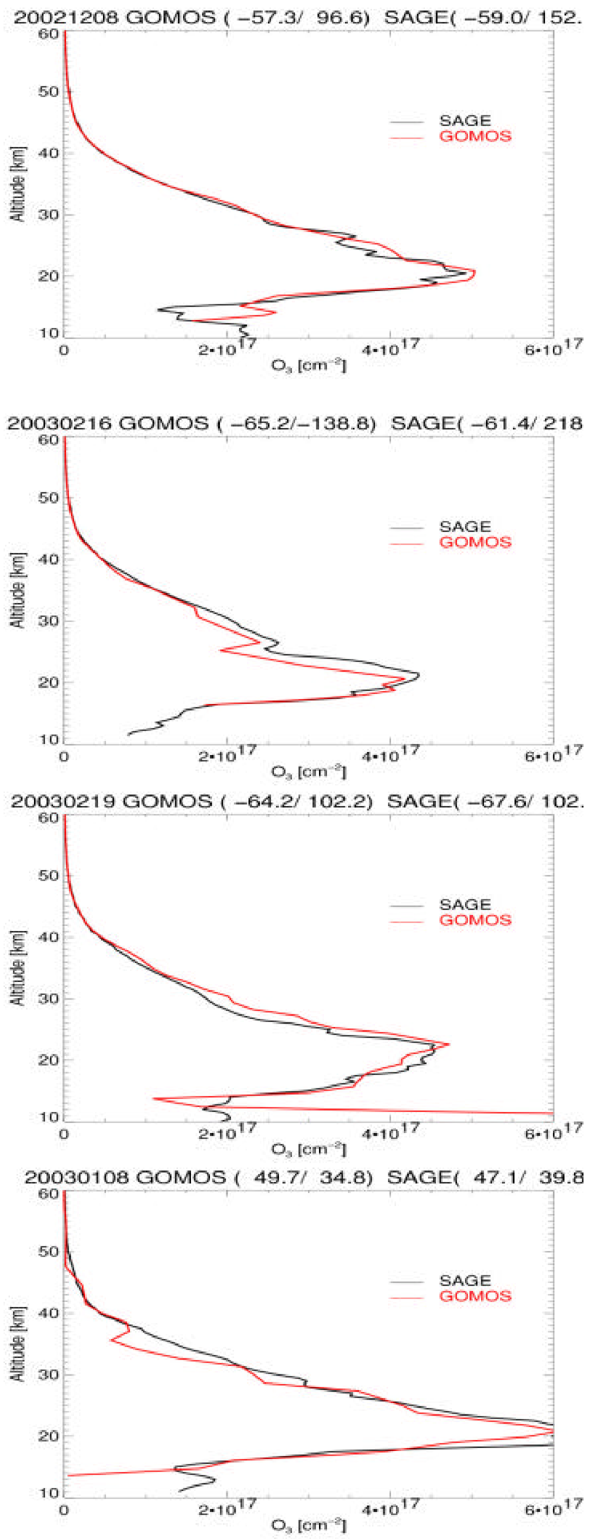

Fig. 9. Comparison of collocated GOMOS (red) O_3 profiles with SAGE II (black) from 20020901 to 20030331: Examples of matches where GOMOS measurement was taken under twi- and straylight, twilight only, daylight and straylight only (from top until bottom)

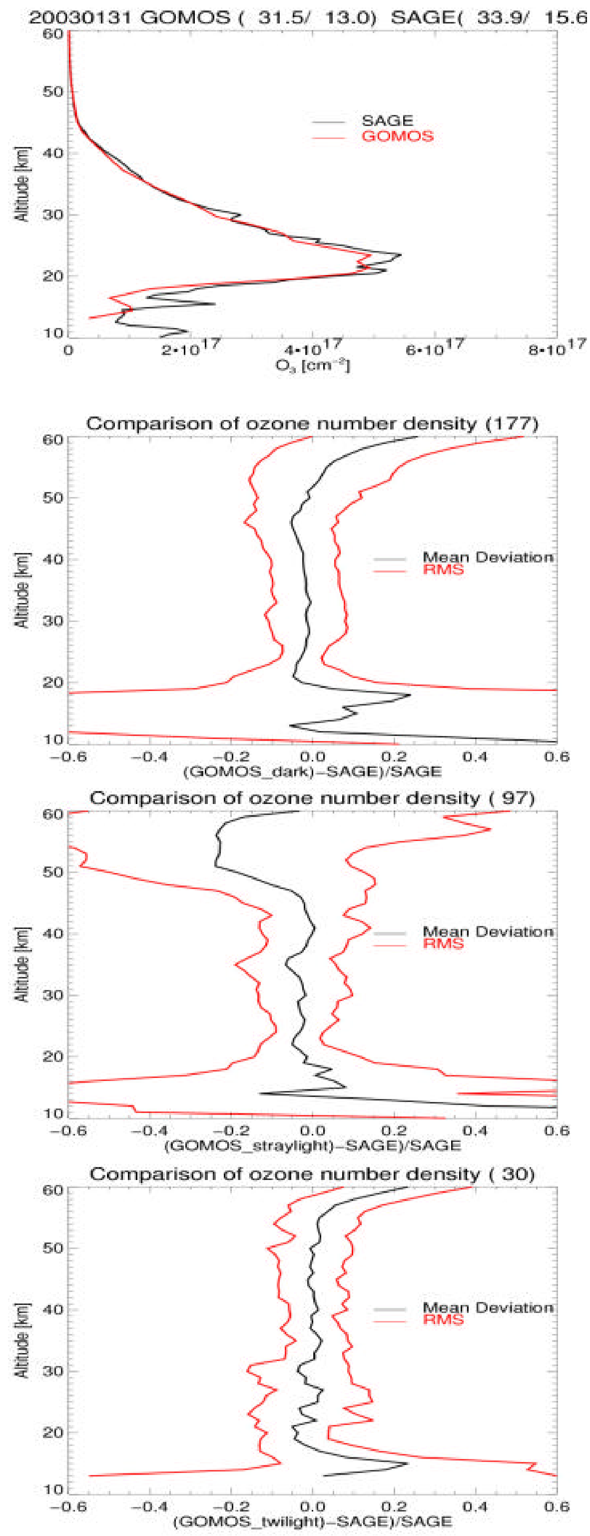

Fig. 10. Comparison of collocated GOMOS O_3 profiles with SAGE II from 20020901 to 20030331: Example of match where GOMOS measurement was taken in the dark (top). Below that the statistical results of these comparisons are shown where all GOMOS measurements taken in the dark (n=177, second top), under straylight only (n=97, second bottom) and twilight only (n=30, bottom)

Table 1. Mean relative deviation with RMS of the comparison of all collocated GOMOS O_3 profiles with SAGE II from 2002/09/01 to 2003/03/31 for the different GOMOS measurements taken in the dark, under twilight, straylight only, twilight and straylight and under daylight.

observation type	mean rel. deviation		RMS	n
dark	at 21 – 52 km	-5 – 0%	5 – 15%	177
twilight	at 17 – 57 km	± 5%	6 – 15%	30
straylight	at 20 – 45 km	-7 – 0%	6 – 15%	97
twi-+stralight	at 20 – 44 km	-8 – 2%	6 – 15%	56
daylight	at 17 – 58 km	±10%	3 – 15%	7

20 km and up to altitudes higher than 50 km. The statistical results of collocated O_3 profiles from GOMOS during all observation modes, also summarized in Table 1, show a very good agreement of GOMOS, within 5% (± 5 to 15%) to SAGE II at 17-20 to 45-55 km. Taking the accuracy of SAGE II O_3 profiles with 10% between 10 and 50 km [2], results show that above 17 to 20 km GOMOS O_3 number densities of high quality can be retrieved.

7 GOMOS NO2 PROFILES WITH SAGE II

As described in section 6, the complete GOMOS NO_2 profiles from 2002/09/01–2003/03/31 are searched for coincident measurements with SAGE II with the same coincidence criteria. 314 collocations are found, with 160 GOMOS measurements taken during darkness, 7 during daylight, 6 under twilight, 88 under straylight, and 53 under twilight and straylight. The photochemical correction as described in section 5 is also applied for the SAGE II NO_2 data. At SZA >100° the higher errors in the SAGE II measurements at altitudes > 45 km result in large errors at the Model output at GOMOS nighttime SZA.

Fig. 11 presents four examples, the best ones, of the comparisons of SAGE II, including photochemical corrections, and GOMOS NO_2 profiles, taken under different light conditions. The statistical results of

Table 2. Mean relative deviation and RMS of the comparison of all collocated GOMOS NO_2 profiles with SAGE II from 20020901 to 20030331 for the different GOMOS measurements taken in the dark, under twilight, straylight only, twilight and straylight and under daylight.

observ. type	mean rel. deviation		RMS	n
dark	at 25 – 45 km	-25 – -75%	10 – 30%	160
twilight	at 23 – 46 km	+10 – -50%	5 – 25%	6
straylight	at 25 – 45 km	-30 – -70%	20 – 35%	77
twi-+stralight	at 22 – 38 km	-15% – 30%	25 – 50%	53
daylight	at 20 – 40 km	-30 – -60%	10 – 25%	7

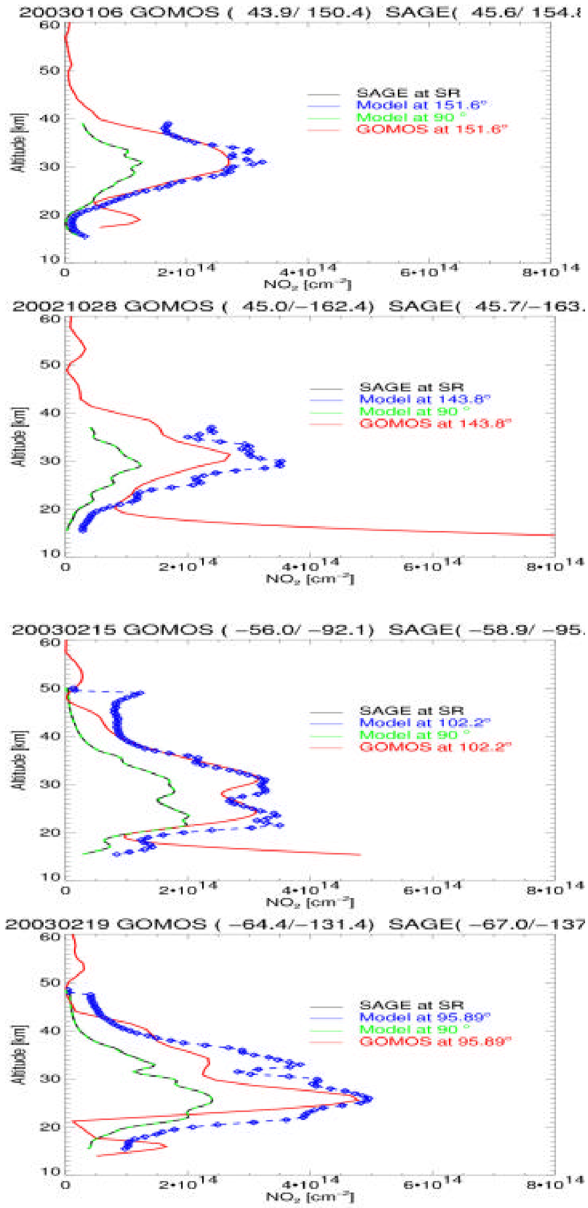

Fig. 11. Comparisons of NO_2 profiles from SAGE II (black) and GOMOS (red) from 2002/09/01 to 2003/03/31 with results from model runs described in [6]: Model at 90° (green) signifies where model NO_2 values are scaled to correspond to SAGE II NO_2 at 90°. Model at GOMOS SZA (blue): here Model at 90° NO_2 values are scaled to GOMOS SZA. Examples (from top to bottom) where GOMOS measurement is taken under dark, straylight only, twi- and straylight, and daylight conditions.

collocated NO_2 profiles from GOMOS during all observation modes, with SAGE II are summarized in Table 2. For all observation modes GOMOS NO_2 values still largely deviate from SAGE_Model at GOMOS SZA by 30 to 70% (RMS of 5 to 30%) and we suggest to further improve the retrieval of NO_2 from GOMOS.

8 CONCLUSIONS

The new data version 5.1 SCIAMACHY O_3 and NO_2 columns show a high quality, as can be concluded from comparisons with GOME 3.0. Also the first released version (2.1) of SCIAMACHY O_3 profiles show reasonable results (within 20%) above 20 km as we can conclude from first comparisons with SAGE II and HALOE. Opposed to that, SCIAMACHY NO_2 profiles (v2.1) show large deviations to photochemically corrected HALOE NO_2 profiles. GOMOS O_3 profiles GOPR 6.0a compared to a large data set of SAGE II profiles show a very good agreement and reliable O_3 data are derived from GOMOS measurements above 20 km. Opposed to that, GOMOS NO_2 profiles still show large deviations from 30 to 70% to photochemically corrected SAGE II profiles. Still all these validation results presented here, are preliminary due to the limited availability of GOMOS and SCIAMACHY data sets. Reprocessing of all available data sets will enable a much larger validation leading to more reliable validation results.

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