

Cross comparisons of O₃ and NO₂ measured by the atmospheric ENVISAT instruments GOMOS, MIPAS, and SCIAMACHY

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Abstract

Vertical profiles of O₃ and NO₂ abundances from the atmospheric instruments GOMOS (Global Ozone Monitoring by the Occultation of Stars), MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) and SCIAMACHY (Scanning Imaging Spectrometer for Atmospheric Cartography) all on-board the recently launched European Space Agency (ESA) Environmental Satellite (ENVISAT) are intercompared. These comparisons contribute to the validation of these data products by detecting systematic deviations, for example, wrong tangent height determinations, spectroscopic errors, and others. The cross comparison includes GOMOS data products retrieved by the GOMOS prototype processor from ACRI (Sophia Antipolis, France), the scientific SCIAMACHY data products from the Institute of Environmental Physics at University of Bremen (IUP) and the scientific MIPAS data products from the Institute for Meteorology and Climate Research in Karlsruhe (IMK) and Institute of Astrophysics in Andalusia (IAA). Coincident measurements were identified by limiting the time difference to 100 min (duration of one orbit) and less than 500 km between two observation points. When lower stratospheric ozone is strongly depleted during polar spring, a homogeneity condition was further imposed on the satellite measurements by requiring an upper limit on the potential vorticity difference at the 475 K isentrope between both observations. Since geographically coincident NO₂ measurements of the three instruments are performed during different times of the day and NO₂ has a rather strong diurnal variability, matches of NO₂ profiles were compared only where the solar zenith angle difference was below 5°. First results of the cross comparison show an agreement within 15% between 21 and 40 km altitude for O₃ profiles and an agreement within 20% between 27 and 40 km altitude for NO₂ profiles among the GOMOS, MIPAS and SCIAMACHY measurements.

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1. Introduction

Climate change issues and global scale ozone depletion require global atmospheric observation platforms for long term monitoring. On March 1st 2002, the Environmental Satellite (ENVISAT) of the European Space Agency (ESA) was launched into a sun-synchronous orbit at about 800 km altitude with 98.55° inclination, performing 14.4 orbits per day. On board are the atmospheric chemistry instruments GOMOS (Global Ozone Monitoring by the Occultation of Stars), MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) and SCIAMACHY (Scanning Imaging Spectrometer for Atmospheric Cartography) measuring between 150 to 600 profiles of various atmospheric trace gases globally per day. These instruments monitor at least three common trace gases (O_3 , NO_2 , and H_2O), which complement each other and enable the global monitoring of the lower and middle atmosphere. Measurements are taken with different vertical and horizontal resolutions and during different times of the day: MIPAS measures the atmospheric limb emission spectra in the mid infrared region (during day and night) over the altitude range from 6 to 68 km (for details see Fischer and Oelhaf, 1996). SCIAMACHY measures ultraviolet (UV), visible (VIS), and near-infrared (NIR) radiation in the nadir, limb, and solar and lunar occultation geometries. Limb observations occur only during daytime since they require scattered sunlight (for details see Bovensmann et al., 2004). GOMOS measures in the UV–Vis range between 17 and 22 km and up to 80–100 km using stellar occultation (for details see Bertaux et al., 1991; Kyrölä et al., 2004). GOMOS favours nighttime measurements but can also observe brighter stars during daytime. The different trace gas information from the three instruments can be combined in order to provide insights on the global stratospheric distribution of these trace gases. Once these particular observations have been homogenized with other, already validated, atmospheric measurements, we can expect a significant improvement in the global understanding of many atmospheric processes. Before the trace gas profiles can be incorporated into numerical and chemical models or into climatological data bases, an extended validation, that demands a cross comparison between these data sets, is needed.

Since all three instruments, namely GOMOS, MIPAS and SCIAMACHY, are on the same platform, numerous spatial and time coincidences can be expected. Therefore, a cross comparison between these three sets of measurements provides a good statistical analyses within a fairly brief time period. It also permits the identification of zonal and seasonal peculiarities in the observed differences. So far, only a few operational O_3 and NO_2 limb profiles from SCIAMACHY are available, but all available SCIAMACHY level-0 and level-

1 data from 2002 to 2004 have been processed to extract O_3 and NO_2 profiles by the retrievals described in von Savigny et al. (2005) and Rozanov et al. (2005a), respectively, which we will thereof call the Institute of Environmental Physics (IUP) retrievals. In this study, we use these as the SCIAMACHY data products (Versions V1.6 for O_3 and V1 for NO_2), and for MIPAS we use the scientific data products from the Institute of Meteorology and Climate Research (IMK) at the Research Centre Karlsruhe and the Institute of Astrophysics in Andalusia at the Spanish Research Council (IAA), which we will thereof call the IMK/IAA retrievals (Versions V2_O3_2 for O_3 and V2_NO2_2 for NO_2). The IMK/IAA data have been limited to the short periods that determine the time frame for this cross comparison. This data set is based on a corrected tangent height retrieval in contrast to the operational MIPAS product (see von Clarmann et al., 2003a) where the operational ESA tangent heights are utilised. GOMOS trace gas profiles were taken from ACRI prototype level-2 data products (version GOPR – GOMOS Prototype processor data version – 6.0a). In this paper, we compare GOMOS, MIPAS and SCIAMACHY O_3 and NO_2 profiles from the period October to November 2003, where a MIPAS IMK/IAA data set is available. Before results from the intercomparison are presented, the problem of tangent height determination that affects the limb and occultation profile retrieval is discussed.

2. Data sets

2.1. Tangent height offset

Measurements from 2002 and 2003 indicate a slow drift in instrumental pointing towards higher tangent heights (TH; ~ 0.2 km/orbit) for SCIAMACHY (Kaiser et al., 2004) and towards lower TH for MIPAS (von Clarmann et al., 2003a). In addition, sudden TH discontinuities of up to 3 km due to an inaccurate on-board orbit analysis have been found during regular TH updates from the ground. Inaccuracies of the on-board orbit model however do not affect GOMOS tangent height retrievals as GOMOS uses star tracking for proper tangent height evaluation. Since December 2003, a correction scheme based on both engineering and orbit model updates has been provided by ESA that leads to improved limb pointing. Nevertheless, some residual pointing error still appears to be present in the data. For the MIPAS IMK/IAA data products a simultaneous retrieval of temperature and line of sight pointing is performed and tangent heights are derived from this information (von Clarmann et al., 2003a). For SCIAMACHY, an average correction ranging between 1 and 2 km for the entire data set is applied. In the present study, SCIAMACHY THs were shifted

down by 2 km. With this correction scheme applied to the SCIAMACHY limb profiles, inaccuracies in the determination of tangent height of up to 0.5 km still remain that can lead to errors of up to 20% at the altitude where the O₃ or NO₂ number densities peak. Further improvements are to be expected when the reprocessed SCIAMACHY 2002/2003 data sets, which will include further improved pointing information from ENVISAT, will be available (for further details see Duesmann et al., 2004).

2.2. SCIAMACHY

SCIAMACHY is the first satellite instrument making spectroscopic observations of the reflected, scattered and transmitted radiation at the top of the Earth's atmosphere in both viewing geometries of nadir and limb, as well as both solar and lunar occultation modes (Burrows et al., 1995; Bovensmann et al., 1999). SCIAMACHY senses in eight spectral channels between 240 and 2380 nm with a channel dependent spectral resolution between 0.2 and 1.5 nm. Latitudinal coverage depends on available sunlight and therefore on the solar zenith angle (SZA). Global coverage is reached after 6 days. For this study, data from SCIAMACHY limb observations performed during the day covering SZAs between 20° and 88°, which have an acceptable signal-to-noise ratio, have been used. In the limb scattering method, the line of sight follows a tangential path through the atmosphere. Solar scattered radiation is detected along the line of sight into SCIAMACHY's field of view and transmitted from the scattering point to the instrument. SCIAMACHY performs limb scans from -3 to about 100 km tangent heights in steps of about 3.3 km. At every tangent height step, a horizontal (azimuthal) scan is performed covering about 960 km across-track. The geometrical field of view (FOV) is about 2.8 km vertically and 110 km horizontally at the tangent point. The air volume sampled during one limb scan extends about 400 km in the along flight direction (the flight and viewing directions are identical).

IUP O₃ profiles from SCIAMACHY limb measurements used in this study are retrieved from all available level-0 data by the method described in von Savigny et al. (2005) and are from data version 1.6. The retrieval uses three wavelengths (525, 600 and 675 nm) in the O₃ Chappuis band and a non-linear, iterative optimal estimation approach together with radiative transfer model (RTM) calculations from SCIAMACHY (Kaiser, 2001). It has been shown that IUP O₃ profiles agree with HALOE V19 data to within 10% (RMS scatter of about 15%) from a limited comparison of 61 profiles during March 2003 (Brinksma et al., 2004).

IUP NO₂ profiles from SCIAMACHY limb measurements used in this study are retrieved from all available level-1 Version 1 data as described in Eichmann et al.

(2004) and Rozanov et al. (2005a). The retrieval uses the spectral window between 420 and 490 nm and a ratio of limb measurements with limb data at 40 km tangent height as reference. The vertical profile is retrieved using an optimal estimation approach and weighting functions from the RTM SCIATRAN (Rozanov et al., 2005b). A pre-fit routine is applied to improve the radiometric calibration. Comparisons of SCIAMACHY-IUP NO₂ profiles with HALOE measurements, which were scaled to the SZA of the SCIAMACHY measurements using a 2D chemical transport model calculation, showed an agreement to within 15% (RMS 10–30%) between 22 and 33 km altitude (Bracher et al., 2005).

From the averaging kernels obtained in both O₃ and NO₂ retrievals (see Fig. 1), it can be concluded that significant information from the measurements is utilised between 15 and 40 km altitude with a vertical resolution of 3–4 km. The instrumental error is generally below 1%, but retrieval errors due to errors in the assumptions of albedo, aerosol profile and background atmosphere are generally larger. These systematic errors have not been determined for each single profile separately, but sensitivity studies have shown that these are the major systematic error sources and vary between <6% and 10% at 15–40 km altitude (Rozanov et al., 2003). Under these considerations, we have limited the comparisons of O₃ and NO₂ from SCIAMACHY to this altitude range and to SZAs below 88°.

2.3. MIPAS

MIPAS is a limb-viewing Fourier transform infrared (FTIR) emission spectrometer with 0.035 cm⁻¹ spectral resolution (unapodised), covering the mid-infrared region in five spectral bands from 685 to 2410 cm⁻¹ (14.5 to 4.1 μm; see, Fischer and Oelhaf, 1996). The FOV of MIPAS is 30 km in horizontal across-orbit and 3 km in vertical direction, while the along-track sampling rate is around 500 km. The measurements cover all latitudes with a latitudinal spacing of 5° and

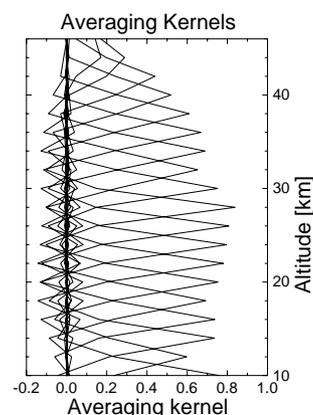


Fig. 1. Averaging kernels of an SCIAMACHY_IUP O₃ profile.

a longitudinal spacing of about 12.5° . The observations are performed during day and night (also polar night) and without any seasonal dependence. The data used in this paper were taken from the nominal observation mode, which consists of rearward limb scans covering the altitude range from 6 to 68 km with 17 steps. MIPAS limb radiance spectra at IMK/IAA are inverted to vertical profiles of atmospheric state parameters using constrained non-linear least squares fitting of the modelled to the measured spectra.

The general strategy of the IMK/IAA MIPAS retrievals is described in von Clarmann et al. (2003a,b,c). Aspects relevant to O_3 (data version V2_O3_2) are described in Glatthor et al. (2005). The retrieval grid is chosen to be constant, i.e., it does not depend on the actual tangent altitudes. This is necessary because firstly, the tangent altitudes themselves have to be retrieved, and secondly, permits an easier comparison of subsequent profiles without re-interpolation. In order to have a retrieval grid point close to each tangent altitude, wherever this real tangent altitude may prove to be, a 1-km retrieval grid is used. Since the measurements do not contain information at a 1 km, the retrieval problem is ill-posed, and a constraint is needed. A Tikhonov-like smoothing constraint is hence applied, which reduces the vertical resolution to around 4 km in the altitude range between 15 and 45 km. This provides a reasonably smooth profile, while unconstrained retrievals on the tangent altitude grid may lead to strong unreasonable oscillations (seen sometimes in ESA level-2 operational products). The precision of the retrieval is better than 6% and the systematic error at the O_3 maximum around 1–2 ppmv. Validation with HALOE (v19) showed an agreement to within 10% at 0.4–40 hPa (21–55 km, Kerridge et al., 2004).

For NO_2 (data version V2_NO2_2), the strategy described in Funke et al. (2005) is used. In this case, the retrieval is stabilized applying a Tikhonov-type regularization on an 1-km grid, under the consideration of non-LTE effects. It is important to account for non-LTE processes because assuming LTE emission in the retrieval would lead to an underestimation of upper stratospheric NO_2 of 2–10% between 40 and 50 km and up to 30% above (Funke et al., 2005). The vertical resolution at 15–50 km is around 4 km. The precision of the retrieval is between 0.2 and 0.3 ppb and the systematic error is at worst 1 ppb during daytime and 1.5 ppb during nighttime. Comparisons of MIPAS_IMK/IAA NO_x with HALOE (v19) NO_x agree to within 10–20% between 25 and 50 km with a positive bias of MIPAS NO_x above 30 km (Funke et al., 2005). These MIPAS-HALOE NO_x comparisons have been performed for MIPAS nighttime measurements, when essentially all NO is converted to NO_2 in the altitude region of interest. HALOE measurements have been photochemically corrected to the MIPAS measurement time as described

in Funke et al. (2005) in order to account for diurnal variations.

The measurement noise has been calculated for every collocated MIPAS O_3 and NO_2 profile and varies between 2% and 4%. A total error analysis on MIPAS_IMK/IAA-data has only been performed on the data from September–October 2002 (Glatthor et al., 2005; Funke et al., 2005). The largest contributions to the total error are spectroscopic, gain-calibration, instrumental line shape errors, and residual errors while determining the line-of-sight. For O_3 data at high and mid latitudes, the total error was below 20% at 0–60 km (below 10% at 10–55 km) and at the tropics below 20% at 20–65 km (below 10% at 20–60 km; Glatthor et al., 2005). For the NO_2 data, significant information from the measurements can be retrieved from the 15–65 km altitude. The relative accuracy, at the NO_2 peak altitude, is around 7–10% at 40 km for nighttime and 15–20% at 30 km for daytime measurements (Funke et al., 2005). Based on these estimates, we have only considered MIPAS data from the altitude ranges, where the total error was estimated to be below 20% for O_3 and from 15 to 65 km for NO_2 .

2.4. GOMOS

GOMOS exploits the stellar occultation technique for the detection of temperature, atmospheric O_3 and NO_2 , and other trace gases such as NO_3 and H_2O . This technique allows measurements of atmospheric transmission spectra with a vertical spatial resolution of 2–3 km and 180–280 km horizontal resolution. Its principle is based on the alternating spectrum of a stellar light source observed outside, and transmitted through, the Earth's atmosphere. Using the acquired spectra and the known molecular cross-sections, the vertical trace-gas profiles are retrieved (more details in Bertaux et al., 1991; Kyrölä et al., 2004). Inherent to the sun-synchronous orbit of ENVISAT, the same star can be observed 14 times per day at different longitudes and more or less the same latitude. In the course of one month the latitudes change. The geographical coverage depends on the availability of suitable stars, which of course varies as the Earth progresses in its orbit around the sun. In 2003, the minimum and maximum observed latitudes were -79.9° and 89.7° , respectively. As seen in Fig. 3 in Meijer et al. (2004), a global coverage within this latitudinal range is reached with a small spacing ($<1^\circ$) between individual observation points within the course of one month.

Nominally, the GOMOS data products should be generated and distributed by ESA's ENVISAT Payload Data Segment (PDS), which is their operational processing chain. So far, the data could not be provided to the calibration and validation teams because of data generation and dissemination problems. ESA has arranged

for an alternative data supply using the prototype processing chain at ACRI (Sophia Antipolis, France). The O₃ profiles from the newest data version (GOPR 6.0a) showed a small negative bias between 0 and 5% (RMS between 5% and 15%) at 21–52 km to collocated SAGE II (v6.2) profiles and the NO₂ profiles a bias of 30–50% at 25–45 km with photochemically corrected collocated SAGE II measurements (Bracher et al., 2004a). The previous O₃ data product GOPR 5.4 b from GOMOS dark observations validated by Meijer et al. (2004) already produced a good data quality with an insignificant negative bias, from 2.5% to 7.5%, with standard deviations of 11–16% between 19 and 64 km, to the correlative global data set of balloon and ground-based measurements.

According to the method applied by Meijer et al. (2004) for the previous GOMOS ACRI data product GOPR 5.4 b, only GOMOS data points, where the error estimate given in the data product was below 20%, were included. In order to avoid a possible random selection of data points at the edges, a consistent profile, which had at least a vertical extension of 4 km, was required. Generally, GOMOS observations are performed between 20° and 150° SZA, but besides some exceptions, only the twilight and dark observations covering SZAs larger than 108° are usable (Bertaux, 2004; Meijer et al., 2004).

3. Collocation criteria

All available SCIAMACHY, MIPAS, and GOMOS data sets from 21 October 2003 to 12 November 2003 were searched for near coincident measurements. The time period for the intercomparison was chosen because for the period around the solar storms of October–November 2003 numerous MIPAS IMK/IAA data products are available. The coincidence criteria were two: one, that measurements took place within one orbit from each other and second, that the mean tangent points of a GOMOS or MIPAS observation were within 500 km of the centre of the nearest SCIAMACHY limb scan. This ensured that the GOMOS or MIPAS tangent points lie within the SCIAMACHY limb scan.

Validation at the edge of different air masses is more difficult, because of gradients in the horizontal distribution of the gases due to transport processes, for example, near the polar vortex or at the upper troposphere lower stratosphere (UTLS) region. An additional criterion was selected to ensure that collocations were within the same air masses. Among the collocated measurements used in this study, only a few SCIAMACHY-MIPAS collocations were found within the southern hemispheric polar vortex. For these collocations the PV criterion, as described in Bracher et al. (2004b), was applied. The potential vorticity (PV) values were taken from the United Kingdom Meteorological Office (UKMO) assimilated meteorological dataset available in a 3.75° × 2.5° (longitude–latitude) grid resolution (Swinbank and O'Neill, 1994) and spatially interpolated to the observation points. Due to the large horizontal limb scan (across- and along-track) of a retrieved SCIAMACHY profile, the corner coordinates of the limb scan for each SCIAMACHY profile were checked for homogeneity in PV. The four corners of a SCIAMACHY limb scan and the collocated MIPAS or GOMOS tangent point must be either completely inside or outside the polar vortex, excluding measurements across the vortex edge region. Observation points inside the polar vortex were identified by PV values less than –40 PVU and outside the polar vortex for PV values higher than –30 PVU at the isentropic level of 475 K. This screening method is cost-effective and Bracher et al. (2004b) have shown that imposing this atmospheric dynamics criterion for the selection of collocated measurements improves significantly individual comparisons.

Because of the strong diurnal cycle of stratospheric NO₂, matches of NO₂ profiles were compared only where the difference of SZAs during the time of measurement was less than 5°. Since all collocated measurements compared in this study were taken at SZAs less than 85° (for SCIAMACHY and MIPAS matches) or higher than 116° (for GOMOS and MIPAS matches), no additional photochemical corrections were needed.

In order to enable a statistical analysis between collocated measurements, which have different vertical resolutions, the collocated O₃ and NO₂ profiles of all three ENVISAT instruments were interpolated from the ground to an altitude of 40 km (for comparisons of GOMOS with MIPAS up to 60 km) with a 1-km spacing. Comparisons are based on number densities (ND), because SCIAMACHY and GOMOS trace gas values are retrieved in ND. MIPAS trace gas values on the other hand are retrieved in volume mixing ratios (VMR). Since temperature and pressure profiles are also retrieved from MIPAS measurements, MIPAS trace gas VMR can be easily converted into ND. The vertical resolution and averaging kernels are different for all three instruments (MIPAS has the coarsest vertical resolution with 3–5 km and GOMOS the finest resolution with 2–3 km when accounting for chromatic scintillation). SCIAMACHY and GOMOS profiles have hence been convolved with the MIPAS averaging kernels. In order to use the MIPAS averaging kernels and a priori information, GOMOS and SCIAMACHY O₃ concentrations (in ND) had to be converted into VMR using the MIPAS temperature and pressure profiles. The MIPAS temperature and pressure profile retrieval has been extensively described by von Clarmann et al. (2003a) and validated by Wang et al. (2004, 2005), showing that those profiles should be preferred over climatological or met analysis information. No interpolation of these profiles in time and location of the collocated

SCIAMACHY and GOMOS profile were performed because of the tight collocation criterion imposed.

In addition to the direct comparison of trace gas profiles, O₃ subcolumns from 15 to 40 km for MIPAS and SCIAMACHY matches, from 20 to 40 km for GOMOS and SCIAMACHY matches, and from 20 to 50 km for MIPAS and GOMOS matches have been compared. NO₂ subcolumns from 20 to 40 km for MIPAS and SCIAMACHY matches and from 25 to 45 km for MIPAS and GOMOS matches have been also compared. The subcolumn altitude range was selected according to the maximum information content in the pair of measurements as discussed earlier. The dataset of all coincident measurements was divided into subsets of zonal bands and solar zenith angle ranges. For each collocation pair the relative deviation (RD) from two

of the instruments (X1 and X2) was determined at each altitude grid, or subcolumn level (h), as follows:

$$RD(h) = \frac{X1(h) - X2(h)}{(X1(h) + X2(h)) \cdot 0.5} \quad (1)$$

For each subset the mean relative deviation (MRD), the root mean square of the relative deviation (RMS) and the uncertainty in the mean relative deviation (RMS divided by the square root of the number of comparisons between all measurement pairs) was calculated.

4. ENVISAT O₃ comparisons

For the October–November 2003-time period, 2154 collocated MIPAS and SCIAMACHY O₃ measurements

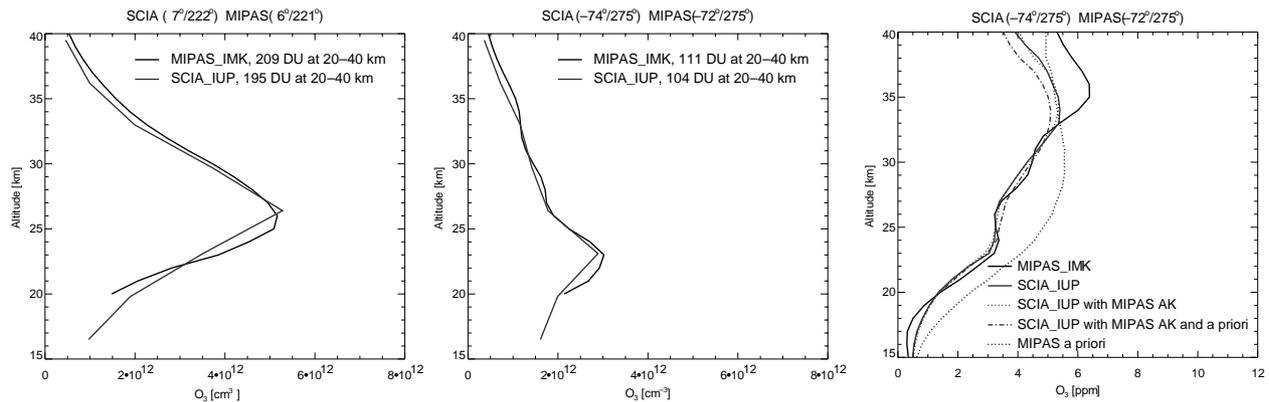


Fig. 2. Comparisons of O₃ profiles from collocated MIPAS_IMK (black) and SCIAMACHY_IUP (=SCIA_IUP; grey) measurements. Examples from October 30th and November 1st 2003, respectively, in the tropics (left panel) and high southern latitudes (middle panel) in number densities are shown. The 20–40 km subcolumn amounts are given in the legend. The subcolumn altitude range roughly corresponds to where, for both SCIAMACHY and MIPAS profiles, information content from the measurements is maximum. Right panel: the high latitude example in VMR where in addition to the MIPAS_IMK (black, solid) and SCIA_IUP (grey, solid) profile, the MIPAS_IMK a priori (black, dotted), the SCIA_IUP profile which has been convolved using MIPAS averaging kernels (grey, dotted) and MIPAS a priori information (grey, dashed-dotted) have been plotted.

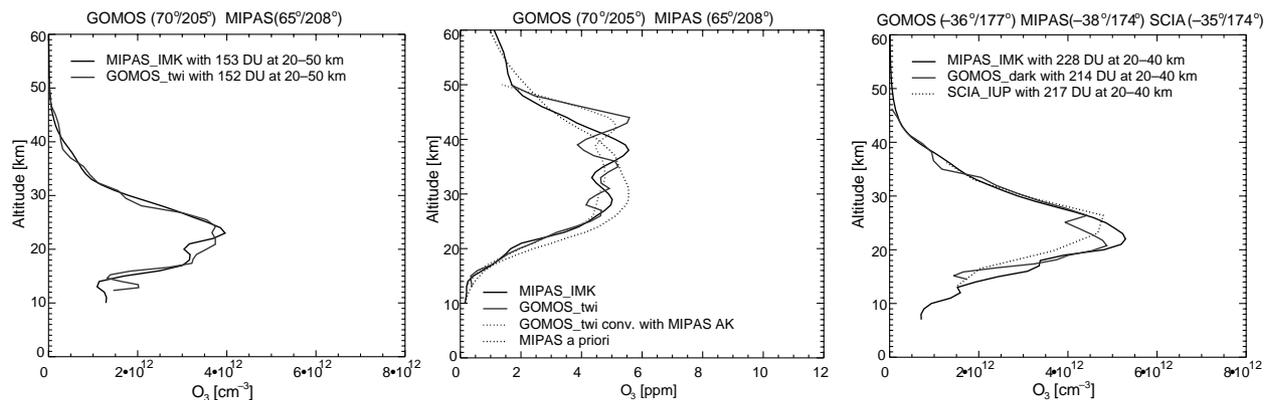


Fig. 3. Comparisons of number density O₃ profiles from collocated MIPAS_IMK (black) and GOMOS (grey) measurements. Examples are shown from the 30th and the 22nd of October 2003, respectively, in the Arctic region (left panel) using GOMOS twilight observations (=GOMOS_twi), and from a triple collocation of MIPAS_IMK (black, solid), SCIAMACHY_IUP (=SCIA_IUP; black dotted) and GOMOS (using GOMOS dark observations (=GOMOS_dark, grey)) in the southern subtropics (right panel). The 20–50 km (left panel) and 20–40 km (right panel) subcolumn values of each measurement are given in the legend. The subcolumn altitude range roughly corresponds to where, for all GOMOS, SCIAMACHY and MIPAS measurements, independent information is retrieved. Middle panel: the example in the Arctic region plotted in VMR where, in addition to the MIPAS_IMK (black, solid) and GOMOS (grey, solid) profiles, the MIPAS_IMK a priori profile (black, dotted) and the GOMOS profile convolved with the MIPAS averaging kernels and a priori information (grey, dotted) have been plotted.

Table 1
Statistical results using Eq. (1) for the Envisat O₃ product comparisons between SCIAMACHY_IUP limb (=SCIA), MIPAS_IMK (=MIPAS) and GOMOS profiles including all type of pair wise matches for specific latitudes bands are shown

O ₃ matches	Latitudes	N	MRD (RMS) for SC	Uncert.	MRD (RMS) for altitudes in ND	MRD (RMS) for GOMOSconv. in VMR
SCIA-MIPAS	60°S–84°S	517	–10% (12%) at 20–40 km	<0.8%	–15% to +7% (14–20%) at 23–38 km	
SCIA-MIPAS	30°S–30°N	1337	–3% (5%) at 20–40 km	<0.5%	–10% to +7% (6–15%) at 20–38 km	
SCIA-MIPAS	30°N–45°N	300	–9% (5%) at 20–40 km	<0.9%	–13% to –4% (6–15%) at 20–38 km	
SCIA-MIPAS	All	2154	–6% (8%) at 20–40 km	<0.5%	–15% to +5% (10–16%) at 22–38 km	
SCIA-GOMOS_dark	23–39°S	57	+1% (6%) at 20–40 km	<1.7%	–10% to +8% (8–13%) at 22–38 km	
SCIA-GOMOS_twi	40–50°N	11	–6% (5%) at 20–40 km	<5%	–10% to +2% (4–15%) at 22–38 km	
SCIA-GOMOS	All	68	~0% (7%) at 20–40 km	<1.5%	–10% to +6% (8–12%) at 22–38 km	
GOMOS_dark-MIPAS	30°S–44°S	188	–4% (4%) at 20–50 km	<0.9%	–7% to +2% (4–14%) at 21–43 km	–6% to +3% (6–11%) at 22–44 km
GOMOS_dark-MIPAS	18°S–30°S	142	–5% (5%) at 20–50 km	<1%	–7% to +4% (6–13%) at 22–48 km	–7% to +5% (5–12%) at 22–48 km
GOMOS_dark-MIPAS	18°S–44°S	330	–4% (5%) at 20–50 km	<0.8%	–6% to +3% (7–14%) at 21–44 km	–7% to +1% (5–13%) at 22–44 km
GOMOS_twi-MIPAS	40–50°N	27	–4% (3%) at 20–50 km	<2.3%	–7% to +4% (5–11%) at 20–44 km	–6% to +4% (4–11%) at 22–46 km
GOMOS_twi-MIPAS	65–75°N	31	–3% (6%) at 20–50 km	<2.8%	–5% to 0% (7–11%) at 21–41 km	–4% to +1% (6–9%) at 21–41 km
GOMOS_twi-MIPAS	40–75°N	58	–3% (5%) at 20–50 km	<2%	–6% to 0% (8–15%) at 20–41 km	–6% to 0% (7–15%) at 21–42 km
GOMOS-MIPAS	All	388	–4% (5%) at 20–50 km	<0.7%	–6% to +2% (7–14%) at 21–43 km	–6% to +1% (6–13%) at 22–44 km

The number of collocations (N), the mean relative deviation (MRD) and the root mean square of the relative deviation (RMS) for a specific subcolumn (MRD (RMS) for SC), and MRD and RMS in number densities for a specific altitude range (MRD (RMS) for altitudes in ND) are given. The uncertainty in the mean relative deviation for a specific altitude range (Uncert.) is also given. The MIPAS-GOMOS matches are also divided into subsets where MIPAS matches either GOMOS dark or twilight observations. In addition, statistical results from the comparison in volume mixing ratio (VMR) of MIPAS to GOMOS O₃ profiles convolved using MIPAS averaging kernels and a priori information (MRD (RMS) for GOMOSconv. in VMR) are given.

have been found. The distribution is highly biased towards the low latitudes (30°S–30°N) with 1337 matches found in this region. The remaining collocations are distributed in high southern latitudes (84°S–60°S) with 517 matches and in northern mid latitudes (30°N–45°N) with 300 matches. Fig. 2 (left and middle panels) shows two examples of collocated O₃ profiles from MIPAS and SCIAMACHY in the tropics and the high southern latitudes, respectively. In these examples, SCIAMACHY and MIPAS agree well between 20 and 40 km although SCIAMACHY values are generally lower than MIPAS. The observed bias in the subcolumn amounts between 20 and 40 km ranges from 7 to 14 DU. Below 20 km, larger deviations are observed in the Antarctic profiles (Fig. 2, middle panel). The right panel of Fig. 2 shows the same profiles as in the middle panel, but as VMR profiles. In addition, the right panel also shows the SCIAMACHY profile convolved with the MIPAS averaging kernels (AK) and the MIPAS a priori profile. At all altitudes, the agreement between MIPAS and the convolved SCIAMACHY profile is about the same as compared to the unconvolved SCIAMACHY profile. This is expected because of the quite similar vertical resolution of both instruments. In the following, we only performed the statistical analysis with SCIAMACHY profiles without MIPAS AKs.

For the same time period, only 388 collocated MIPAS and GOMOS O₃ measurements were found. In 330 cases, GOMOS measurements were night time observations and all matches were located between 18°S and 44°S. Fifty eight of the matches contained GOMOS measurements under twilight conditions, of which 27 matches were between 40°N and 50°N and 31 at arctic latitudes (65°N–75°N). For GOMOS and SCIAMACHY, only matches with GOMOS daylight observations were found which were not usable due to the lack of solar scattered straylight corrections in the GOMOS retrieval. For this reason, we relaxed the collocation criteria and looked within the sample of all 388 MIPAS-GOMOS collocations for matches with SCIAMACHY measurements from the same day (from different orbits) that were located within a radius of 500 km. All in all, 68 triple comparisons were found, 57 comparisons in southern subtropics containing GOMOS nighttime observations and 11 comparisons at northern mid latitudes with GOMOS observations during twilight conditions. Examples from a GOMOS-MIPAS match at northern high latitudes are shown in the left panel and from a triple comparison in the southern subtropics are shown in the right panel of Fig. 3, respectively. There is good agreement between GOMOS and MIPAS, but the GOMOS profile shows some oscillations that are particularly visible near the O₃ number density maximum peak. The middle panel of Fig. 3 shows the match at the high northern latitude example (in VMR), including the GOMOS profile convolved

with MIPAS AKs. The agreement between MIPAS and GOMOS slightly improves with the convolved GOMOS O₃ profile. No difference between convolved and original profiles has been seen in comparisons between GOMOS and SCIAMACHY matches (not shown). The 20–50-km subcolumns in the example from the Arctic (Fig. 3, left) agree to within 1 DU, but in the triple comparison (Fig. 3, right) GOMOS subcolumns are lower than MIPAS by 14 DU. In the triple comparison shown, both SCIAMACHY and MIPAS profiles seem to agree slightly better than GOMOS with SCIAMACHY or MIPAS.

Statistical results from the ENVISAT comparisons are summarized in Table 1. Cross comparisons at their respective original vertical resolutions are given in ND. Since the GOMOS number density (ND) profiles were converted into VMR using the same MIPAS temperature and pressure profiles as for the conversion of the collocated MIPAS VMR profiles, the statistical results for the comparison of GOMOS and MIPAS at their original vertical resolutions are identical for ND and VMR. The table also shows the statistical results of the comparison of convolved GOMOS profiles to MIPAS VMR profiles that only show small statistical differences compared to the unconvolved GOMOS profiles. The uncertainty in the mean relative deviation for a specific altitude range is given in Table 1 and is below 1% when the number of compared collocation pairs is above 100. If the number of pairs is between 20 and 100, the uncertainty is below 3% and for less than 20 pairs it is below 5%. The uncertainty in the mean relative deviation for the specific subcolumn was also calculated and it is generally less than 50% of the uncertainty given for the particular altitude range. The values of uncertainty indicate that the results for the MRD of all com-

parisons are significant. Both statements are also true for the statistical results of the comparison of NO₂ profiles.

Looking at zonal differences, the largest deviations are observed in the Antarctic region where SCIAMACHY O₃ concentrations are biased by –15% to +7% (RMS of 10–15%) with respect to MIPAS, between 23 and 38 km. A mainly negative bias is also observed for the 20–40 km subcolumns with a mean of –10% (RMS 12%). In the tropical region (30°S–30°N), the bias decreases to –10% to +7% (RMS of 6–15%) at a broader altitude range between 20 and 38 km. SCIAMACHY 20–40-km subcolumns are 3% lower than MIPAS (RMS 5%). In the northern subtropics, the SCIAMACHY profiles show a clear negative bias of 4–13% in comparison to MIPAS at 20–38 km altitudes and of 9% for the 20–40-km subcolumns.

For the GOMOS–SCIAMACHY comparisons, the SCIAMACHY profiles in the southern subtropics are within 10% at 22–38 km and +1% for the 20–40-km subcolumns compared to GOMOS dark observations, but at northern mid latitudes a negative bias (–10% to 2% at 22–38 km altitude and –6% for the subcolumns) compared to GOMOS twilight observations is found (Table 1). These different deviations can be either due to differences in the number of collocations in each region or in the GOMOS observation mode (dark and twilight).

No variations in the statistical differences are observed as a function of latitude and observation modes in the comparisons of collocated MIPAS and GOMOS profiles, either convolved or at their original resolution (Table 1). A different behaviour was found only below 22 km and above 47 km in the comparisons of MIPAS profiles to convolved and original GOMOS profiles (Fig. 4, right panel). At these altitudes O₃ concentrations

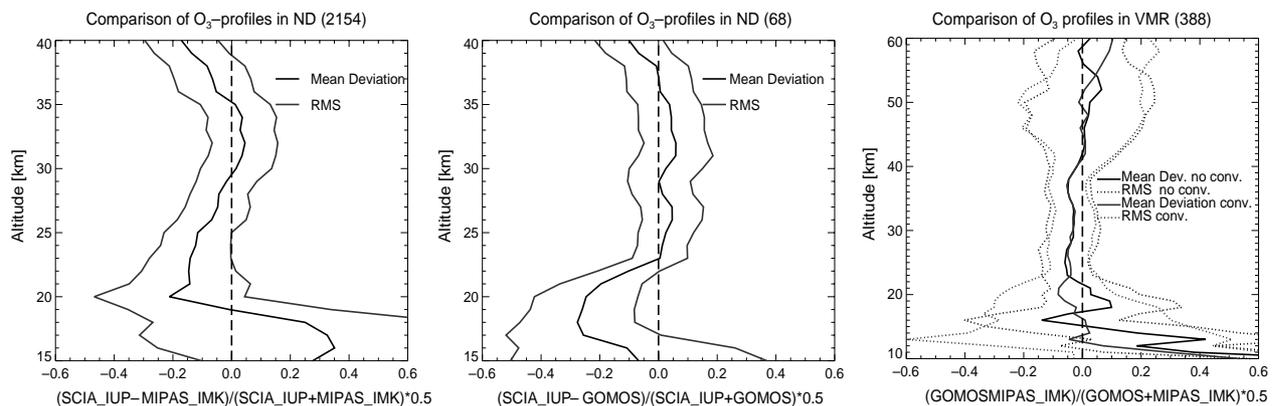


Fig. 4. Statistical results of collocated O₃ profile comparisons with mean relative deviation (mean deviation; black) and root mean square of mean relative deviation (RMS; grey) determined from Eq. (1) for all collocated MIPAS_IMK and SCIAMACHY_IUP (SCIA_IUP) number density profiles (left panel) and SCIAMACHY_IUP and GOMOS ND profiles (middle panel). Right panel: Statistical results (mean deviation = straight line, RMS = dotted line) of the comparison in volume mixing ratio (VMR) of MIPAS_IMK to GOMOS O₃ profiles in their original resolution (black) and convolved using MIPAS averaging kernels a priori information (grey). The number of compared collocations is given in brackets in the title of each figure.

Table 2

Statistical results using Eq. (1) for the Envisat NO₂ product comparisons between SCIAMACHY_IUP limb (=SCIA) and MIPAS_IMK (=MIPAS), and MIPAS and GOMOS profiles at specific solar zenith angle ranges (SZA ranges) are shown

NO ₂ matches	SZA range	N	MRD (RMS) for SC	Uncert.	MRD (RMS) for altitudes in ND	MRD (RMS) for GOMOSconv. in VMR
SCIA–MIPAS	24°–40°	722	–12% (8%) at 20–40 km	<0.9%	–26% to +6% (10–28%) at 27–38 km	
SCIA–MIPAS	40°–60°	497	–13% (8%) at 20–40 km	<0.9%	–13% to +3% (12–26%) at 27–38 km	
SCIA–MIPAS	60°–85°	96	–12% (8%) at 20–40 km	<2%	–8 to +14% (14–29%) at 25–37 km	
SCIA–MIPAS	All	1315	–12% (8%) at 20–40 km	<0.8%	–20 to +4% (13–27%) at 27–38 km	
GOMOS_dark–MIPAS	116°–122°	29	–8% (8%) at 25–45 km	<5%	–15% to 0% (11–30%) at 25–41 km	–13% to 0% (9–26%) at 25–40 km
GOMOS_dark–MIPAS	122°–130°	153	–9% (13%) at 25–45 km	<2.5%	–9% to +2% (13–29%) at 25–41 km	–10% to –1% (12–33%) at 25–41 km
GOMOS_dark–MIPAS	130°–140°	107	–10% (12%) at 25–45 km	<3%	–11% to +3% (11–30%) at 25–41 km	–13% to +1% (11–31%) at 25–41 km
GOMOS_dark–MIPAS	140°–147°	41	–6% (9%) at 25–45 km	<5%	–14% to +8% (13–36%) at 26–41 km	–14% to +4% (12–33%) at 27–41 km
GOMOS_dark–MIPAS	116°–147°	330	–9% (12) at 25–45 km	<1.7%	–10 to 0% (13–29%) at 26–41 km	–11% to 0% (12–30%) at 26–41 km
GOMOS_twi–MIPAS	116°–122°	6	–7% (18%) at 25–45 km	<16%	–30% to +27% (13–33%) at 25–39 km	–30% to +25% (8–44%) at 25–39 km
GOMOS_twi–MIPAS	140°–147°	27	–13% (24%) at 25–45 km	<7%	–22% to +11% (15–32%) at 26–41 km	–23% to +8% (13–33%) at 26–42 km
GOMOS_twi–MIPAS	116°–147°	33	–12% (22%) at 25–45 km	<6%	–24% to +16% (17–32%) at 26–41 km	–24% to +13% (15–32%) at 26–41 km
GOMOS–MIPAS	116°–122°	35	–10% (11%) at 25–45 km	<5%	–15% to 0% (11–30%) at 25–41 km	–13% to 0% (9–30%) at 25–41 km
GOMOS–MIPAS	140°–147°	68	–8% (12%) at 25–45 km	<5%	–14% to +9% (13–34%) at 26–41 km	–14% to +7% (12–33%) at 27–41 km
GOMOS–MIPAS	116°–147°	363	–10% (15) at 25–45 km	<1.6%	–10% to 0% (13–29%) at 26–41 km	–11% to 0% (12–30%) at 26–41 km

The number of collocations (N), the mean relative deviation (MRD) and the root mean square of the relative deviation (RMS) for a specific subcolumn (MRD (RMS) for SC), and MRD and RMS in number densities for a specific altitude range (MRD (RMS) for altitudes in ND) are given. SZA differs among a collocation pair by no more than 5°. The MIPAS–GOMOS matches are also divided into subsets where MIPAS matches either GOMOS dark or twilight observations. The uncertainty in the mean relative deviation for a specific altitude range (Uncert.) is also given. In addition, the statistical results of the volume mixing ratio (VMR) comparison of MIPAS to GOMOS NO₂ profiles convolved using MIPAS averaging kernels and a priori information (MRD (RMS) for GOMOS conv. in VMR) are given.

decrease rapidly and the comparison of MIPAS to convolved GOMOS profiles seems more appropriate. For all MIPAS–GOMOS matches, GOMOS shows a negative bias of 4% in the 20–50-km subcolumns and up to 6% (RMS <15%; uncertainty of <0.7%) between 21 and 43 km when comparing convolved and original profiles to MIPAS profiles (Fig. 4, right panel). From 43 up to 60 km, the mean relative deviations between collocated measurements remain within 6% for the original and 10% for the convolved profiles, but the uncertainty increases up to 25%.

Deviations are largest between collocated MIPAS_IMK and SCIAMACHY_IUP O₃ profiles among all three cross comparisons. SCIAMACHY agrees at 22–38 km within –15% to +5% (RMS of 10 to 16%; uncertainty of <0.5%) with respect to MIPAS (Fig. 4, left), and within –10 to +6% (RMS of 8–12%; uncertainty of <1.5%) with respect to GOMOS (Fig. 4, middle). Deviations between GOMOS and MIPAS profiles are lower. In general, MIPAS_IMK V2_O3_2 seems to be slightly higher (4–10%) than GOMOS GOPR 6.0a and SCIAMACHY_IUP V1.6 in both profile and subcolumn comparisons.

5. ENVISAT NO₂ comparisons

For the October–November 2003-time period, only SCIAMACHY–MIPAS and MIPAS–GOMOS matches for NO₂ have been found using the additional solar zenith angle (SZA) criterion of less than 5°. For GOMOS and SCIAMACHY measurements, the only matches with GOMOS daylight observations that have been found are not usable, like in the case of the O₃ comparisons. The statistical results are summarized in Table 2. The uncertainty in the mean relative deviation for a specific altitude range is below 3% when the number of compared collocation pairs is above 95. If this number is in between 25 and 70 pairs (as it happens in some subset comparisons of GOMOS to MIPAS) the uncertainty is below 7% and for less than 10 pairs it is below 16% (in subset comparisons of GOMOS twilight to MIPAS at 166° to 122° SZA). The values of uncertainty indicate that the results for the MRD of all comparisons are significant.

A total of 1315 collocated MIPAS and SCIAMACHY NO₂ measurements have been found. Like in the case of ozone, the majority of collocations (930

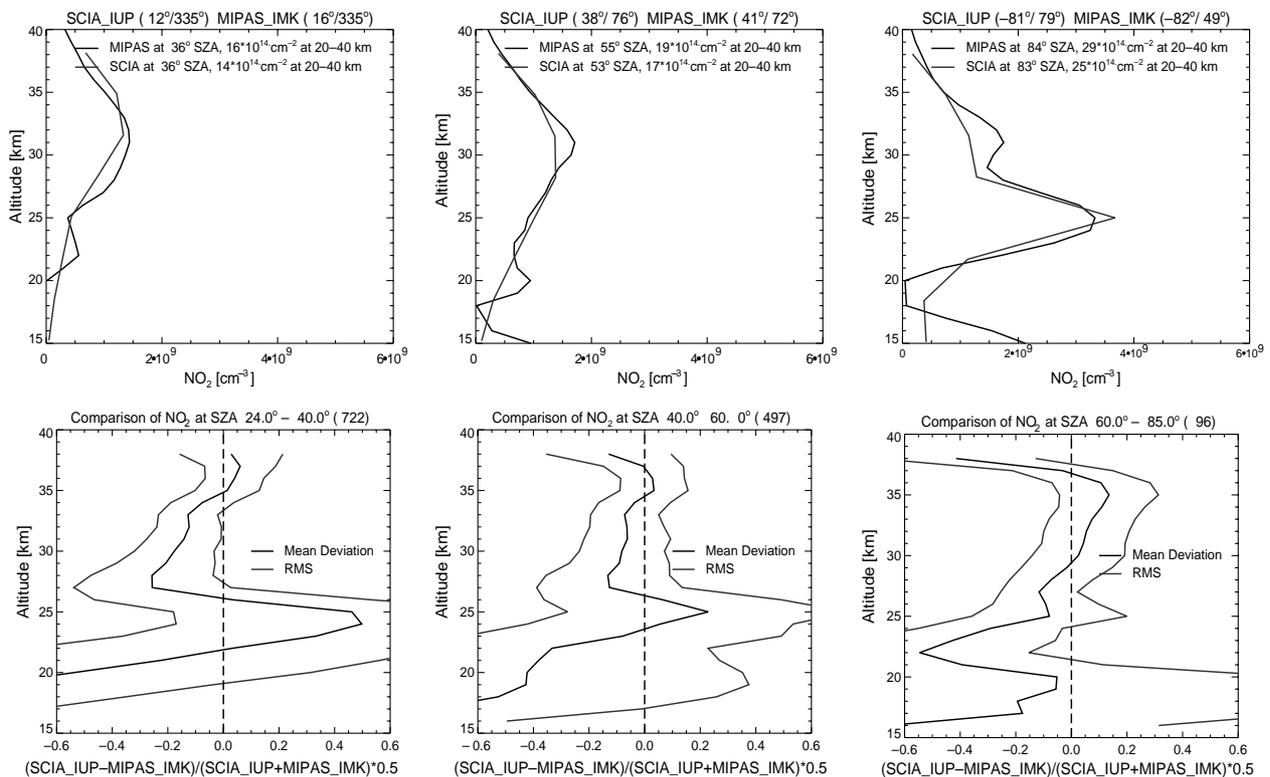


Fig. 5. Comparisons of NO₂ profiles from collocated MIPAS_IMK (black) and SCIAMACHY_IUP (=SCIA; grey) measurements. Top panels: examples from the 25th, 21st and 26th of October 2003, respectively, at different solar zenith angles (SZA) ~36° (left), ~54° (middle), ~84° (right). The 20–40 km subcolumn value of each measurement is indicated in the legend. The subcolumn altitude range roughly corresponds to where from both the vertical SCIAMACHY and MIPAS measurements, independent information is retrieved. Bottom panels: statistical results using Eq. (1) with the mean relative deviation given in black and the root mean square of mean relative deviation given in grey. These were determined for different SZA ranges, 24–40° (left panel), 40–60° (middle panel), and 60–85° (right panel). The number of collocations is given in brackets in the title of each figure.

matches) were at low latitudes (30°S–30°N), the remaining being distributed within 30°N–45°N (273 matches) and within 84°S–60°S (112 matches). Most matches in the tropics were in the SZA range of 24°–40°, the remaining in the range from 40°–85° SZA (see Table 2). Fig. 5 (top) shows three examples of collocated NO₂ profiles from MIPAS and SCIAMACHY in the tropics at around 36° SZA, at northern mid latitudes at around 55° SZA and above Antarctica at around 84° SZA. In all three examples, SCIAMACHY NO₂ subcolumns are between 2×10^{14} and 4×10^{14} molecules/cm² lower than MIPAS. In the lowermost stratosphere, deviations in the profiles get larger. In the tropical example (Fig. 5 top left), the SCIAMACHY profile seems to show a tangent height offset of about 1–2 km when compared to MIPAS. The statistical results of all comparisons show that the observed differences depend on SZA (Fig. 5 bottom) with deviations

being largest in the SZA range of 24°–40° with a bias of SCIAMACHY of between –26% and +6% at 27–38 km. At all three SZA ranges, the mean relative deviation between SCIAMACHY and MIPAS alternates from a low bias near the NO₂ number density maximum to a high bias at higher altitudes. Most likely, the positive tangent height offset in the SCIAMACHY profiles, caused by the pointing problem, partly explains this disagreement. Statistical results are better for comparisons of SCIAMACHY to MIPAS in the SZA range of 40°–60° with a smaller bias of –13% to +3% at the same altitude range and of –8 to +14% down to 25 km at high SZA angles (60°–85°). Including all matches in the statistical analysis, results in SCIAMACHY NO₂ values at 27–38 km are rather low (MRD of –20 to +4% with RMS of 13–27%) and the 20–40 km NO₂ subcolumns show a negative bias of 12% (RMS 8%) with respect to MIPAS (Table 2).

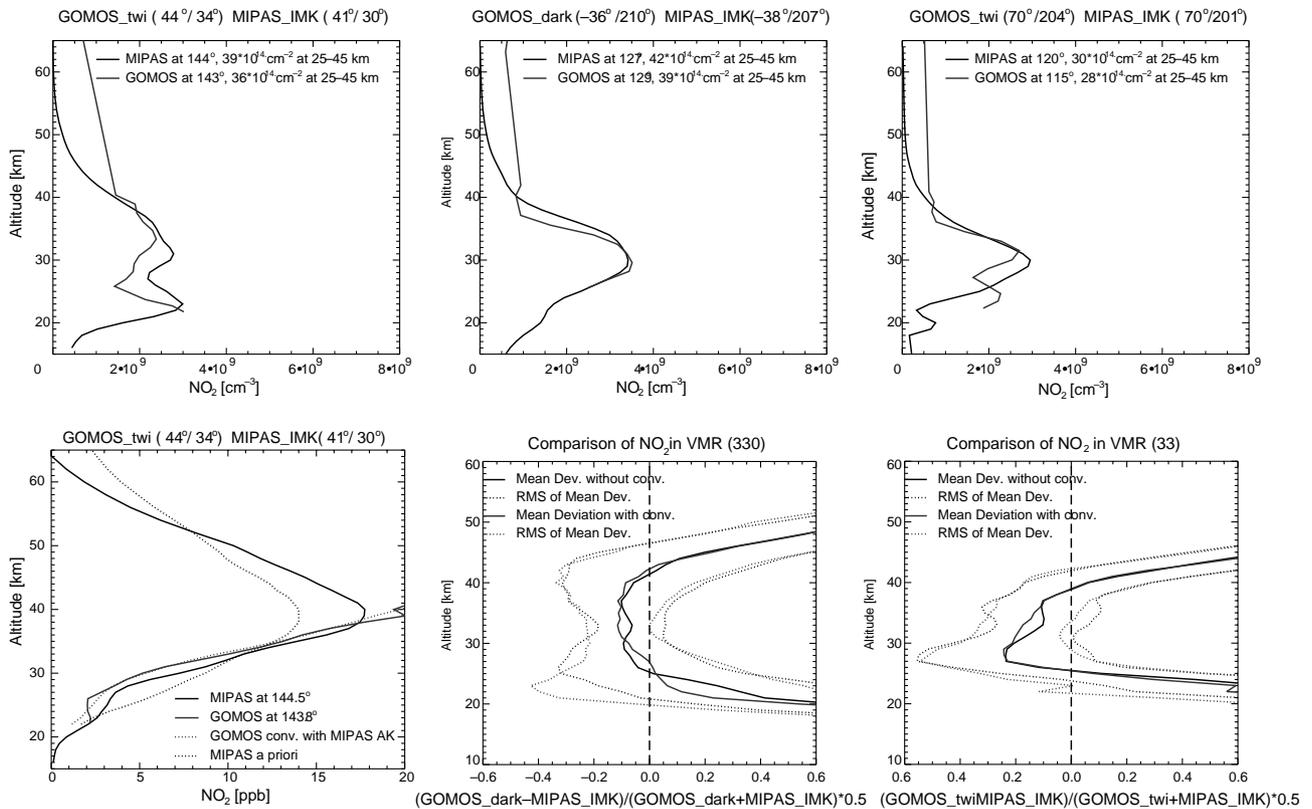


Fig. 6. Comparisons of NO₂ profiles from collocated MIPAS_IMK (black) and GOMOS (grey) measurements. Examples are shown from the 24th (top left panel), 26th (top middle and right panel) October 2003 in number densities for solar zenith angles at ~144° with GOMOS twilight observations (top left panel), ~128° with GOMOS dark observations (top middle panel), and ~118° with GOMOS twilight observations (top right panel). The 25–50 km subcolumn value of each measurement is given in the legend. The subcolumn altitude range roughly corresponds to where independent information is retrieved in both GOMOS and MIPAS vertical profiles. Bottom left panel: the example at 145° SZA in VMR where, in addition to the MIPAS_IMK (black, solid) and GOMOS (grey, solid) profile, the MIPAS_IMK a priori (black, dotted) and the GOMOS profiles (convolved using MIPAS averaging kernels and a priori information) (grey, dotted) have been plotted. Statistical results from the comparison in volume mixing ratio (VMR) are shown in the bottom right (MIPAS_IMK and GOMOS_twilight) and bottom middle (MIPAS_IMK and GOMOS_dark) panels. The statistics were performed using Eq. (1) and the mean relative deviations (mean deviation = straight line) and root mean square of mean relative deviations (RMS of mean deviation = dotted line) are presented. The black lines depict the NO₂ profiles in their original resolution and the grey lines depict GOMOS NO₂ profiles convolved using the MIPAS averaging kernels and MIPAS a priori information. The number of collocations is given in brackets in the title of each figure for both statistical results.

For the time period investigated 361 collocated MIPAS and GOMOS NO₂ measurements have been found. Three hundred and twenty eight of them were dark observations from GOMOS and all these matches fall within 18°S and 44°S. The other 33 matches include GOMOS twilight profiles (27 matches at 40°N–45°N and 5 matches at Arctic latitudes from 65°N to 75°N). In Fig. 6, three examples of collocated NO₂ profiles from MIPAS and GOMOS at northern mid latitudes at around 144° SZA (top left), at southern mid latitudes at around 128° SZA (top middle), and in the Arctic at around 117° SZA (top right) are shown. Overall, between 25 and 40 km, GOMOS profiles are lower than MIPAS. Also, the GOMOS 25–45 km NO₂ subcolumns are lower by 2×10^{14} – 3×10^{14} cm⁻². Above 40 km GOMOS NO₂ values seem unrealistically high. The bottom left panel of Fig. 6 shows the same profile at 144° SZA as the top left panel if Fig. 6 but in VMR, including the convolved GOMOS profile which is obviously not in any better agreement with MIPAS compared to the original GOMOS profile. Statistical results of the comparisons of MIPAS to GOMOS convolved profiles are quite similar to the comparisons to the original GOMOS profiles. Statistical results showed only marginal differences for different subsets based on latitudinal or SZA ranges. However, larger differences are observed when the results were separated by the GOMOS observation types (Table 2 and Fig. 6, bottom middle). While NO₂ values from GOMOS dark observations showed a negative bias compared to MIPAS which ranges between 11% and 0% (RMS 13–29%; uncertainty of <2%) at 26–41 km and of 9% for the 25–45 km subcolumns, the GOMOS twilight observations showed a larger bias ranging between –24 and +13% (RMS 15–32%; uncertainty of <6%) between 26 and 41 km and –12% for the 25–45 km subcolumn (Fig. 6 bottom right). Looking at all GOMOS–MIPAS matches, GOMOS values are lower by 11–0% (RMS 12–30%) for the same altitude range and by 10% for the 25–50 km subcolumn as compared to MIPAS (Table 2).

In summary, both SCIAMACHY_IUP V1 and GOMOS GOPR 6.0a NO₂ profiles are only comparable to MIPAS_IMK between 27 and 38 km and 26 and 41 km altitude, respectively, and are lower by 10–20% than MIPAS V2_NO2_2 NO₂ profiles.

6. Conclusions

In this study, cross comparisons between the new SCIAMACHY_IUP (V1.6 for O₃ and V1 for NO₂), MIPAS_IMK (V2_O3_2 for O₃ and V2_NO2_2 for NO₂) and GOMOS (GOPR 6.0a) O₃ and NO₂ data products from October–November 2003 have been performed. Results show an agreement for ozone within 15% at 21–40 km altitudes between these different Envi-

sat O₃-products. GOMOS agrees to within –6% to +1% and SCIAMACHY within –15% to +5% with respect to MIPAS, and SCIAMACHY agrees to within –10% to +6% with GOMOS. All three data sets showed reasonable results in previous comparisons with satellite data from the SAGE II (V6.2) and HALOE (V19) experiments.

Comparisons of SCIAMACHY and GOMOS NO₂ products to MIPAS products with a difference of less than 5° in SZA between collocated measurements show agreement within 10–20% for the 27–40 km altitude range, with the values of MIPAS profiles higher than GOMOS and SCIAMACHY profiles. Also comparisons of the 20–40 km subcolumns for SCIAMACHY–MIPAS matches and of the 25–45 km subcolumns for GOMOS–MIPAS matches show a positive bias of around 10% between MIPAS and the two other data sets. So far, no direct comparisons between GOMOS nighttime and SCIAMACHY NO₂ daytime products were possible due to the different timing of both measurements. The comparison of GOMOS and SCIAMACHY NO₂ profiles measured at different times of a day and within a radius of 500 km is planned by applying a photochemical correction based on the method described by Bracher et al. (2005).

From this study, we can conclude that first results of Envisat O₃ and NO₂ data product intercomparisons show a reasonable agreement within a specific altitude range. The SCIAMACHY IUP products are still suffering from a tangent height offset resulting from an incorrect Envisat orbit model. Recently, a method by Kaiser et al. (2004; see further details in von Savigny et al., 2004) has been developed to correct the tangent height offset in limb profiles for tropical measurements which is based upon the Tangent Height Retrieval by UV-B Exploitation (TRUE) using calculations with the radiative transfer model (RTM) SCIRAYS by Kaiser (2001). Improvements for these data products are expected after the TRUE method is applied to correct for the tangent height offset to all measurements from the same orbit. Also, the reduction of SCIAMACHY horizontal resolution to 240 km across-track will improve the comparability to the other two data sets. After these improvements to the SCIAMACHY data set, more validations and cross comparisons of these data products from the three Envisat instruments can be achieved.

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