SCIAMACHY V6.01 Nitrogen Dioxide Limb Validation

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1 Introduction

During the period 2002-2012 the SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) instrument on board of ENVISAT (European Environmental Satellite) has been performing global measurements of trace gases using three different viewing geometries: limb, solar occultation and nadir viewing (Burrows et al., 1995; Bovensmann et al., 1999). From the limb measurements of the scattered solar light vertical nitrogen dioxide (NO₂) profiles were retrieved.

The aim of this study is to document data quality of the ESA/DLR limb NO₂ profiles version 6.01 from SCIAMACHY by comparison to related limb and occultation satellite measurements. As NO₂ is characterised by strong diurnal variation the application of photochemical conversion is necessary. Below we provide not only the validation of ESA/DLR limb NO₂ profiles version 6.01 by means of limb and occultation measurements, but also provide advanced possibilities of performing photochemical convertions.

It was found that SCIAMACHY ESA/DLR limb NO₂ profiles version 6.01 are in good agreement with IUP retrievals version 3.1 (based on Level 1 version 6), with 1-5% relative difference in tropics and middle latitudes of Northern hemisphere (NH) in the altitude range 22-42 km (in middle latitudes Southern hemisphere, SH, at 25-42 km) and with only 1-2% differences at altitudes 28-40 km in the tropics and at NH middle latitudes, 26-36 km at SH middle latitudes (40-60°). At high latitudes differences are larger as was seen in the previous comparison of ESA/DLR NO₂ version 5.02 and IUP NO₂ version 3.1 (SCILOV-10, Weber et al. (2014)) and currently are within 10-20% in the altitude range 19-39 km NH and 15-19 km and 23-37 km SH.

2 Data and Instruments

SCIAMACHY ESA/DLR version 6.01 NO₂ profiles are validated in this work. SCIAMACHY ESA/DLR operational data was compared to SCIAMACHY IUP NO₂ data version 3.1 for the period of September 2002 - April 2012. August 2002 was skipped due to the reason of lack of data covering the whole month and further calculating collocations. Description of retrieval algorithm of scientific product of SCIAMACHY NO₂ profiles version 3.1 was provided by Rozanov et al. (2005) and validated by Bauer et al. (2012).

SCIAMACHY ESA/DLR operational data was also compared to MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) NO₂ profiles based on retrieval algorithm of the collaboration between Institute of Meteorology and Climate Research at the Karlsruhe Institute of Technology and the Instituto de Astrofisica de Andalucia (IMK-IAA) and on ESA retrieval scheme.

MIPAS IMK-IAA algorithm is described by von Clarmann et al. (2009) and Funke et al. (2014). MI-PAS ESA algorithm that produces the most recent data version 7.03 is described in a technical documentation available from https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/. The differences between MIPAS operational and scientific products are described in Wetzel et al. (2007). In our case only the period of January 2005 - April 2012 was used for the validation in order to avoid additional errors which might have been caused by switching the spectral resolution from 0.025 cm^{-1} and sampling time of 4.5 s to 0.0625 cm^{-1} and reduced sampling time of 1.8s due to the interferometer mirror slide anomaly. The same approach was used by Sheese et al. (2016) in the validation of ACE-FTS NO_y species.

In the validation here SCIAMACHY ESA/DLR operational data was also compared to occultation measurements of NO₂ from the SAGE II (Stratospheric Aerosol Gas Experiment, Chu et al. (1989)), which was on board the Earth Radiation Budget Satellite (ERBS) and launched in 1984. The overlap of SAGE II with SCHIAMACHY is from September 2002 to August 2005. In contrast to MIPAS

comparisons, the comparisons between SAGE II and SCIAMACHY requires prior photochemical corrections as SAGE II measured at sun rise/set time, while SCIAMACHY in the morning hours (around 10am).

3 Methods of Validation

The validation of SCIAMACHY ESA/DLR NO₂ profiles version 6.01 has been performed by collocating the NO₂ profiles within a specific spatio-temporal criteria described in Section 3 and interpolating NO₂ profiles measured by other instruments to the ESA/DLR vertical grid. The relative differences (RD) and standard deviations (STD) for individual pairs of collocated profiles were calculated as described in Dupuy et al. (2009). No sub-sampling of data was performed, which means all available profiles were included in the analysis.

3.1 Collocation criteria

The collocations are defined with the 'coincedence_tool' developed by Klaus Bramstedt, IUP, Bremen University, which defines the collocation pairs due to spatio-temporal criteria. The collocation criteria are chosen as a compromise between number of profiles, comparability, and coverage. Even if, in theory no collocation is required for the comparison of SCIAMACHY ESA and IUP, this program still was applied with the collocation radius of 60 km and the time difference 3.6 seconds to find identical profiles. For the comparison of SCIAMACHY ESA and MIPAS (both, IMK-IAA and ESA) the collocation radius was set to 300 km and 3 hours. For SCIAMACHY ESA and SAGE II comparison, the spatial difference was set to 500 km and temporal to 8 hours.

If several SCIAMACHY profiles were collocated with the profile of another instrument (e.g. MIPAS, SAGE-II), all were used, but if several profiles from the instrument were collocated with the same SCIAMACHY profile, only the one with the smallest spatial distance was used.

Two collocated profiles, where one profile is inside and the other is outside the polar vortex can have large (natural) differences. For this reason an additional criterion for collocation was that both profiles are either inside or outside the polar vortex, meaning have similar potential vorticity values. The modified potential vorticity (MPV) was calculated from ECMWF Interim reanalysis data for all profiles which were located polewards of 35° latitude. Those profiles, for which MPV was larger than 30 PVU (potential vorticity units) and smaller 40 PVU were not taken into account for the analysis as the profiles could not clearly be assigned being inside or outside the polar vortex. If the MPV differed by more than 3 PVU between two profiles, those profiles were also excluded to prevent the analysis of different air masses.

The estimation of the influence of cloud contamination on NO_2 profiles was done by Bauer et al. (2012). It was shown, that the application of cloud masking does not show significant improvements at the altitudes above 20 km; below this altitudes, error source can be significant, though, two thirds of all collocations are then sorted out. In current validation procedure, we do not apply any cloud masking in order to keep as many collocated profiles as possible. Thus, the analysis of tropical region below 20 km will be described with the account of possible error source from clouds.

3.2 Data gridding

The results of comparisons are presented as zonal means (arithmetic mean along longitudes) for the northern and southern hemispheres (NH and SH respectively) for the following latitude bands:

- Tropics (20° S 20° N)
- Middle latitudes I NH (20-40° N)
- Middle latitudes II NH (40-60° N)
- High latitudes NH (60-80° N)
- Middle latitudes I SH (20-40° S)
- Middle latitudes II SH (40-60° S)
- High latitudes SH (60-80° S)

These zones were chosen in order to be able to identify regional differences in NO_2 profiles. For all latitude bands computations were performed for average profiles from all years, time series, and the annual cycle.

3.3 Time series comparisons

Time series are provided for all available limb measurements and compared for altitudes between 15 and 45 km and comparison results are shown as difference profiles. For three selected altitudes (18, 28, and 38 km) the comparison was done for all available time periods (2002-2012 for SCIAMACHY ESA-SCIAMACHY IUP, 2005-2012 for SCIAMACHY ESA - MIPAS IMK-IAA, SCIAMACHY ESA - MIPAS ESA) and are shown as line plots. See Section 5 for details and results.

4 Photochemical conversion

 NO_2 being a photochemically active species has a pronounced diurnal variation. This makes comparisons of two profiles measured at different local times difficult. For the validation, the profiles should be scaled to the illumination conditions of the other profile. In this work we scaled NO_2 profiles from SAGE II, to the solar zenith angle (SZA) of SCIAMACHY ESA measurements. To do so, we first calculate scaling (conversion) factor *F* for each altitude *z* as follows:

$$F = \frac{MOD_{NO2}(\theta_{SCIA}, z)}{MOD_{NO2}(90, z)}$$
(1)

Here, MOD_{NO2} - modelled NO₂, θ - SZA, θ_{SCIA} - data at SZA of SCIAMACHY measurements.

NO₂ profiles from occultation measurements (measured at 90° SZA) were scaled to the SZA of SCIAMACHY measurements NO₂(θ , z) by multiplying occultation profiles by model based conversion factor *F*.

$$NO_2(\theta, z) = NO_2(90, z) \times F$$
⁽²⁾

Below we provide analysis of recently tested methods of NO₂ photochemical conversion, discuss their advantages and disadvantages and discuss which conversion scheme is best in our opinion.

4.1 Pratmo model

The photochemical box model developed at the University of California, Irvine, (Prather, 1992; McLinden et al., 2000), also known as Pratmo, was recently used for the validation of limb and occultation measurements. (e.g. Sheese et al., 2016). Model is written in Fortran. Unfortunately, we were not able to get the original code of the model, although, we received the C++ version, developed at the University of Saskatchewan (http://odin-osiris.usask.ca/). We performed two different experiments to model the NO₂ diurnal variation for selected days using the Pratmo C++ version:

- using simplified meteorological fields introduced to the model as look-up tables and
- actual profiles of temperature and pressure from ECMWF and O₃ measured by SCIAMACHY.

Results are shown in Fig. 1. The relative difference between two approaches is within 10-15% in the altitude range 10-45 km. It is expected that PRATMO model simulates better NO₂ diurnal variation with the O₃ data from SCIAMACHY measurements used as input to the model.

Disadvantages. C++ version of PRATMO model is developed and operated on a Windows system.



Figure 1: Comparison of NO₂ [vmr] diurnal variation in PRATMO with simplified climatology (left plot), with ECMWF meteorology and SCIAMACHY O₃ (middle plot) and their relative difference (right plot), middle latitudes Northern hemisphere on 11 July 2004.

Application of the model thus requires transfer of all data sets to Windows machines from our data depository hosted in a Linux cluster, which is time consuming. Another possibility would be the use of the original Fortran code, which is currently not available.

4.2 Pratmo look-up tables

For 3 days in each month (1st, 11th and 21st) the complete diurnal cycle of NO₂ is modelled by the Pratmo model for each 2.5° latitude within altitude range from 8 to 56 km. The same method was applied by Brohede et al. (2007) in the validation of Odin/OSIRIS NO₂. The uncertainty of the photochemical conversion using look-up tables is approximately 20% (Bracher et al., 2005; Bauer et al., 2012). To further reduce the uncertainties introduced by look-up tables the application of a more sophisticated method is required.

In Fig.2 we present conversion factors delivered for NO₂ from the comparison of the Pratmo model (blue and yellow) and look-up tables (green). We compare 4 different dates and different locations: a) 11 January 2004, tropics, scaling from 90° to 35° SZA, b) 11 April 2004, tropics, scaling from 90° to 45° SZA, c) 11 July 2004, SH middle latitudes, scaling from 90° to 84° SZA, and d) 11 October 2004, NH middle latitudes, scaling from 90° to 70° SZA. Blue line indicates conversion factor received with Pratmo model driven by simplified climatology (look-up tables of temperature and pressure distribution), yellow line - Pratmo model driven by meteorology from ECMWF and SCIAMACHY O₃ and green line - look-up table, derived from Pratmo model. The largest differences in conversion factors from these approaches occur mostly below 15-20 km and above 40 km.



Figure 2: Comparison of scaling factors for NO₂ with PRATMO model driven by simplified climatology (blue), PRATMO model with meteorology from ECMWF and SCIAMACHY O₃ (yellow) and look-up tables (green) for a) 11 January 2004, tropics, scaling from 90° to 35° SZA, b) 11 April 2004, tropics, scaling from 90° to 45° SZA, c) 11 July 2004, SH middle latitudes, scaling from 90° to 84° SZA, d) 11 October 2004, NH middle latitudes, scaling from 90° to 70° SZA.

Disadvantages. Rather coarse temporal resolution of provided NO₂ conversion profiles (3 days per month) introduce additional uncertainties. Also, latitudinal step of 2.5° may be rather coarse while matching measurements and model.

4.3 B3DCTM

B3DCTM stands for Bremen Three Dimensional Chemistry-Transport Model and was developed by Sinnhuber et al. (2003) and is based on the SLIMCAT model (Chipperfield et al., 1993; Chipperfield, 2006). B3DCTM is driven by ECMWF (European Centre for Medium-Range Weather Forecasts) meteorological reanalysis ERA-Interim (EI) at a spatial resolution of 2.5° lat x 3.75° lon, using 29 isentropic levels in the vertical, ranging from 335K to 2726K (about 11-55 km). Horizontal transport is calculated from meteorological wind fields, and the vertical transport from EI diabatic heating rates using the Prather advection scheme.

We established model runs for specific days with 15 minutes output. To improve the photolysis in the model to better estimate NO₂ variations at sunrise and sunset, the original scheme of Meier et al. (1982) was replaced by SCIATRAN radiative transfer model (RTM) actinic fluxes. More details about SCIATRAN RTM can be found here: http://iup.uni-beremen.de/sciatran and Rozanov et al. (2014). In Fig.3 we present comparisons of NO₂ diurnal variation from PRATMO model with SCIAMACHY O₃ fields (orange line), B3DCTM with standard Meier scheme (purple) and with implemented SCIATRAN actinic fluxes (light blue) for 11 January 2004, SH middle latitudes, at 38 km altitude (left plot), 35 km (middle plot), and 30 km (right plot). Significant differences between models occur around times of local sunrise and sunset. Such differences can be explained by the simulated time step of B3DCTM, which is too coarse during sunrise/sunset. Therefore, further improvement of B3DCTM is needed by reducing the time sampling. A higher temporal sampling can be achieved by using also the 1 dimensional (1D) Box model.



Figure 3: NO₂ diurnal variations from PRATMO model (orange), B3DCTM with standard Meier scheme (purple) and B3DCTM with SCIATRAN actinic fluxes (blue) for 11 January 2004, SH middle latitudes, in altitudes 38 km (left plot), 35 km (middle plot) and 30 km (right plot).

Disadvantages. Coarse time sampling in B3DCTM becomes crucial for the times of sunrise and sunset affecting the accuracy of the conversion factor.

4.4 SLIMCAT and related 1D model

The SLIMCAT (Chipperfield et al., 1993) chemical-transport model (CTM) initially developed by Prof. Chipperfield at Météo France, comprises troposphere and stratosphere, is driven by reanalysis data. It uses different vertical coordinates: potential temperature levels for the stratosphere and pressure levels for the troposphere and different methods of treating key processes, e.g. vertical transport (Chipperfield, 2006).

To scale SAGE-II profiles measured at 90° SZA to the SZA of SCIAMACHY measurements and to compare collocated occultation-limb profiles the 1D version of the SLIMCAT stratospheric model was applied. The procedure of photochemical conversion comprises the following steps:

- Collect output data of full-chemistry (3D) SLIMCAT simulation for all available SAGE-II measurements (for the period 09.2002-09.2005 with 13418 measurements)
- Initialise 1D model with the output from SLIMCAT and run the model to reproduce NO₂ diurnal variation for each SAGE-II measurement with the time step of 1 minute. An example of NO₂ diurnal variation (simulated over 2 days) for location 0.5° S and 156.4° E is shown in Fig.4 for 1 January 2005 at four altitudes: 40 km (red), 35.3 km (purple), 29.5 km (blue), and 25.3 km (green), with the red shadings indicating sunrise (when NO₂ concentrations rapidly decrease) and sunset (when NO₂ concentrations rapidly increase).



Figure 4: NO₂ diurnal variations (0.5° S, 156.4° E) from SLIMCAT-related 1D model simulated for 1 January 2005 at different altitudes: 40 km (red), 35.3 km (purple), 29.5 km (blue), and 25.3 km (green). Red shadings indicate sunrise/sunset periods. Usually such models are run for several days, see Bracher et al. (2005) due to spin-up. We checked whether a drift between profiles is observed from the first to the second day for the case shown in Fig.4. From Fig.5 it is apparent that the differences between profiles are small and negligible. Therefore, it is sufficient to run 1D model for one day only.



- Figure 5: NO₂ profiles for 0.5° S, 156.4° E from SLIMCAT-related 1D model simulated for 1 January 2005 at 89.4° SZA (black first simulation day, pink second simulation day) and at 40° SZA (yellow first simulation day, green second simulation day)
 - Calculate conversion factors as shown in Eq.1 and 2 from modelled profiles of NO₂ at SCIAMACHY-ESA SZA and SAGE-II SZA (90°).

The application of SLIMCAT and related 1D model is a preferred choice for the validation of limb NO₂ profiles. Expected error for this conversion should not exceed 15-20 %, though, further validation of new method is required. Clear advantage of suggested method is based on possibility calculating conversion factor for time and location of each particular collocated profile, which is not provided by e.g. Pratmo look-up tables. The results of this method are shown in Section 5.4. Though, photochemical conversion is not the only source of errors in NO₂ retrievals. NO₂ profiles can be affected by errors in temperature and pressure, aerosol particles, clouds, etc.

5 Results

5.1 SCIAMACHY ESA vs. SCIAMACHY IUP NO2

Profile comparisons

The ESA/DLR and IUP profile comparisons of NO₂ [molecules /cm³] were performed in the altitude range 15-45 km. The results for all latitude bands are presented in Fig.6. For each latitude band the left panels of Fig.6 show mean NO₂ profiles and the standard deviation of the mean as shaded areas, while the right panels show relative differences and the STD as shaded areas. Fig.6 shows that the relative difference of collocated profiles does not exceed 1-5% in tropics and NH middle latitudes at 22-42 km (at SH middle latitudes at 25-42 km). Relative differences of only 1-2% are observed at altitudes 28-40 km in the tropics and NH middle latitudes, and 26-36 km at 40-60° S. At high latitudes the differences are larger as was seen in the previous comparison of ESA/DLR NO₂ version 5.02 and IUP NO₂ version 3.1 and currently are within 10-20% in the altitude range 19-39 km for NH and 15-19, 23-37 km for SH. The largest differences are observed below 20 km for all latitude bands.

Time series comparisons

The ESA/DLR and IUP NO₂ time series are compared in the altitude range 15-45 km. In Fig.7 time series at selected altitudes are presented (18, 28, and 38 km). At high latitudes the relative differences can reach more than 50%, and those time series were not plotted. One of possible reasons for such differences can be a too high regularization in SCIAMACHY ESA retrievals. In contrast, quite good agreement is observed in the tropics and middle latitudes of both hemispheres at 28 km. Relative differences mostly do not exceed 6%. This is also observed at 38 km in tropics (Fig.7, green line) and 20-40° of both hemispheres (red and blue lines respectively). Larger discrepancies (mostly around 40%) are observed at 18 km. As mentioned in Section 3.1, no cloud masking was applied in order to save available collocations, which could have effect profiles in tropical region below 20 km. Though, shown in Fig.7 relative differences in tropics at 18 km are smaller in comparison with middle latitudes. The 18 km differences for SH and NH are in phase, which also was shown in previous validation of ESA/DLR NO₂ version 5.02 (SCILOV-10, Weber et al. (2014)). The potential reason of observed seasonality in Fig.7 is the difference in the choice of the smoothness constrain for the two retrievals.

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Figure 6: Comparison of the retrieved NO₂ profiles from SCIAMACHY ESA V6.01 and IUP V3.1 for different latitude bands. Left panels: mean absolute NO₂ profiles [mol /cm³] and standard deviation of the mean (shaded). Right panels: mean and de-biased standard deviation.



Figure 7: Time series of the relative difference of retrieved NO₂ from SCIAMACHY ESA V6.014 and IUP V3.1 for different altitudes:18, 28, and 38 km.

5.2 SCIAMACHY ESA vs. MIPAS IMK-IAA NO₂

Profile comparisons

SCIAMACHY ESA/DLR and MIPAS IMK-IAA profile comparisons of NO₂ were performed in the altitude range 17-45 km. In general MIPAS IMK-IAA NO₂ is lower in area of its maximum in comparison with SCIAMACHY ESA (see Fig. 8): NO₂ decreases more rapidly below the NO₂ peak altitude for MIPAS than for SCIAMACHY, that means the peak is sharper for MIPAS. The relative difference between the two data sets does not exceed \pm 20% at altitudes 20-45 km, except in the tropics and 20-40° N (where relative difference exceeds 20% at 23-27 km). Better agreement is observed in the altitude range 30-45 km in the tropics, where relative difference is \pm 10%. Also, relative difference does not exceed 6% for altitudes 30-35 km in the tropics and at middle latitudes. The increase of relative difference with altitude within 31-41 km is observed in the NH and at high latitudes SH.

Time series comparisons

The ESA/DLR and MIPAS NO₂ time series are compared in the altitude range 17-45 km. In Fig.9 time series at selected altitudes are presented (18, 28, and 38 km). For the time series near 28 km relative difference is rather stable and varies within 10-20% for middle latitudes of Northern and Southern Hemispheres. For tropical region at this altitude it varies mostly within 20-30%. Larger discrepancies (mostly up to 50%, for 20-40° S exceeds 50%) are observed at 18 km middle latitudes in both hemispheres. The 6-months phase shift at 18 km in NH and SH is observed: possible reasons of this pattern are still under consideration and require further analysis. At 38 km relative difference is stable (within 0-20%) for all latitude bands, except 40-60° S. Time series at high latitudes were not included due to too high differences.

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Figure 8: Comparison of the retrieved NO₂ profiles from SCIAMACHY ESA V6.01 and MIPAS IMK-IAA V5R for different latitude bands. Left panels: mean absolute NO₂ profiles [mol/cm³] and standard deviation (shaded). Right panels: mean percental difference and de-biased standard deviation.



Figure 9: Time series of the relative difference of retrieved NO₂ from SCIAMACHY ESA V6.014 and MIPAS IMK-IAA V5R for different altitudes:18, 28, and 38 km.

5.3 SCIAMACHY ESA vs. MIPAS ESA NO₂

Profile comparisons

During comparison of SCIAMACHY ESA and MIPAS ESA data very similar features were observed as described in Section 5.2 for MIPAS IMK: MIPAS NO₂ below the NO₂ peak (around 30 km) is lower than SCIAMACHY. This feature is observed in the tropics and at middle latitudes. The agreement between the two data sets is generally good: relative difference does not exceed 20% in the altitude range 23-45 km in the tropics and at SH middle latitudes, 20-45 km at NH middle latitudes, and around 24-38 km at high latitudes of both hemispheres. Below 20 km the differences are higher, than those, seen in the comparison to MIPAS IMK (Fig.8). High variability of STD points out to the wide spread of MIPAS ESA NO₂ values below 20 km, which requires further improvement. A better agreement to MIPAS ESA than to MIPAS IMK is observed in the tropics and $20-40^{\circ}$ N, where differences to SCIAMACHY ESA retrievals are smaller and do not exceed 20%.

Time series comparisons

Significantly higher variability of time series at altitudes 18, 28, and 38 km is seen from the Fig.11 in comparison with the Fig. 9, where SCIAMACHY ESA profiles were compared to MIPAS IMK-IAA. Large variability is seen at 18 km altitude (Fig. 11, lowermost plots), where during 2005-2007 relative difference was changing much more, in comparison with later years. At NH middle latitudes at 28 and 38 km the difference was mostly within $\pm 20\%$. For the tropics and SH middle latitudes these differences are higher and are changing around $\pm 30\%$ at both altitudes.

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Figure 10: Comparison of the retrieved NO₂ profiles from SCIAMACHY ESA V6.01 and MIPAS ESA V7.03 for different latitude bands. Left panels: mean absolute NO₂ profiles [mol/cm³] and standard deviation (shaded). Right panels: mean percent difference and de-biased standard deviation.



Figure 11: Time series of the relative difference of retrieved NO₂ from SCIAMACHY ESA V6.01 and MIPAS ESA V7.03 for different altitudes:18, 28, and 38 km.

5.4 SCIAMACHY ESA vs. SAGE II NO₂

The occultation instrument used in this study was SAGE II Version 7.00A. The period for the analysis comprised all available collocated measurements within 2002-2005 in the altitude range 20-43 km following the recommendation of Damadeo et al. (2013). Also, following (Damadeo et al., 2013), only sunset collocated event were taken into account. This results to limited amount of data in SH, since almost all collocated SAGE II profiles were observed during sunrise. Also, due to coarse collocation spatial criterion and data fragmentation, no time series are provided.

Profile comparisons

The ESA/DLR and SAGE-II profiles comparison of NO₂ were performed in the altitude range 20-43 km. In order to compare two data sets correctly, the photochemical conversion scheme as described in Section 4.4 (1D Box model) was applied.

Results for all latitude bands are presented in Fig.12. Good agreements between SCIAMACHY ESA and SAGE-II within 20% is observed in the tropics in the altitude range 29-40 km, for 20-40° at altitudes 23-38 km in the NH and 29-38 km in the SH, for 40-60° both hemispheres at around 26-35 km. At 60-80° N relative difference around 30% is observed within the altitude range 20-34 km. Overall, NO₂ photochemically corrected sunset profiles from SAGE-II are higher than SCIAMACHY ESA. Similar, Bauer et al. (2012) compared SCIAMACHY scientific NO₂ product with SAGE-II V.6.2, although his results can not be compared to our findings due to the following reasons: 1) different data versions, 2) application of sunrise data in Bauer et al. (2012) and 3) large differences between sunrise and sunset profiles within one data version and between different versions.



Figure 12: Comparison of the retrieved NO₂ profiles from SCIAMACHY ESA V6.01 and SAGE-II V7.0 for different latitude bands. Left panels: mean absolute NO₂ profiles [mol/cm³] and standard deviation of the mean (shaded). Right panels: mean and de-biased standard deviation.

6 Conclusions

This document reports on the validation of SCIAMACHY NO₂ profiles ESA version 6.01 over the full mission from September 2002 to April 2012. Comparison of SCIAMACHY ESA and IUP retrievals showed good consistency in the tropics and at middle latitudes NH with relative differences within 1-5% in the altitude range 22-42 km (at SH middle latitudes between 25 and 42 km), and with only 1-2% differences at 28-40 km in the tropics and NH middle latitudes, and 26-36 km in 40-60° S.

Comparison of SCIAMACHY ESA and MIPAS IMK-IAA NO₂ also showed good agreement in the tropics in the altitude range 30-45 km with relative differences around \pm 10%. Also, relative difference does not exceed 6% for the altitudes 30-35 km for tropics and middle latitudes. At other latitude bands the relative difference between the two data sets did not exceed \pm 20% in the altitude range 20-45 km, except for the tropics and 20-40° N, where relative difference exceeded 20% at 23-27 km.

Both, MIPAS ESA NO₂ data and MIPAS IMK-IAA are lower than SCIAMACHY below the NO₂ peak altitude (around 30 km) in the tropics and at middle latitudes. Though, the differences between SCIAMACHY ESA and MIPAS ESA do not exceed 20% in the altitude range 23-45 km in the tropics and SH middle latitudes, 20-45 km at NH middle latitudes, and around 24-38 km at high latitudes of both hemispheres. Below 20 km high variability of MIPAS ESA STD points out to the wide spread of retrieved NO₂ values, which require further improvement. A better agreement between SCIAMACHY ESA and MIPAS ESA than SCIAMACHY ESA and MIPAS IMK is observed in the tropics and 20-40° N in the altitude range 20-30 km, where differences do not exceed 20%.

We also showed several possibilities of photochemical conversion that allows to compare NO₂ profiles measured under different illumination conditions (e.g. SAGE II at sunset/sunrise and SCIAMACHY local time). We applied SLIMCAT and related 1D model to scale SAGE-II profiles to the SZA of SCIAMACHY measurements. Scaled sunset SAGE-II profiles agree with SCIAMACHY-ESA within 20% in the tropics in the altitude range 29-40 km, at 20-40° N in the altitude range 23-38 km, at 20-40° S in the range 29-38 km, and at 40-60° of both hemispheres in the range 26-35 km.

Generally, comparison of SCIAMACHY ESA stratospheric NO_2 profiles with correlated limb measurements showed good agreement to within 20% between 20 and 45 km. Larger deviations were observed below 20 km and at high latitudes. One of possible reasons of these differences can be a too high regularization in SCIAMACHY ESA retrievals. Thus further data improvement is needed.

Comparison of SCIAMACHY ESA stratospheric NO₂ profiles with collocated occultation measurements is also in a good agreement within 20% in the altitude range around 23-40 km. Below 25 km, the differences exceed 20-25%, which can be mainly the consequence of the diurnal effect error and photochemical conversion. We are further validating newly applied conversion method (SLIMCAT and related 1D model), but expected error should not exceed 15-20 %.

7 References

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