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Validation of SCIAMACHY limb ozone profiles with lidar

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Abstract

Validation of SCIAMACHY limb ozone profiles with lidar

The National Institute for Public Health and the Environment (RIVM) has examined the quality of SCIAMACHY measurements on the structure of the ozone layer of the entire atmosphere. SCIAMACHY is a measurement instrument onboard the environmental satellite ENVISAT. It gives information on the composition of the atmosphere, for example on the amount of ozone. De structure of the ozone layer is represented by ozone profiles. SCIAMACHY profile measurements are made by scanning the atmosphere horizontally layer by layer (limb measurements). Limb ozone profiles measured with SCIAMACHY have been validated by comparing them to very reliable ozone measurements from the ground (lidar). This validation shows that individual SCIAMACHY ozone profiles can differ from lidar measurements with 35 percent or more. The average difference is -8 to 5 percent.

Ozone concentrations, measured world wide and over a long time period, give information on the condition of the ozone layer and with that on the effectiveness of ozone reduction measures.

SCIAMACHY profile measurements are hampered because ENVISAT's attitude with respect to the earth is not sufficiently known. As a result, the accurate altitude at which SCIAMACHY measures is not well enough known. This leads to so-called altitude shifts that influence the results of the measurements. The investigation has shown for the first time with SCIAMACHY measurements that the altitude shifts are more complicated than thought before. This makes a correction on the measurements even more difficult. However, it gives more insight into the unclearness of ENVISAT's attitude with respect to the earth. If a solution is found, it can be implemented with retroactive effect (till 2002) on all SCIAMACHY profile measurements.

Keywords: validation, SCIAMACHY, ozone profiles, lidar, ENVISAT

Rapport in het kort

Validatie van SCIAMACHY limb ozonprofielen met lidar

Het RIVM heeft de kwaliteit onderzocht van SCIAMACHY-metingen van de opbouw van de ozonlaag in de hele atmosfeer. SCIAMACHY is een meetinstrument op de milieusatelliet ENVISAT. Het geeft informatie over de samenstelling van de atmosfeer, bijvoorbeeld over de hoeveelheid ozon. De opbouw van de ozonlaag wordt weergegeven met ozonprofielen. De profielmetingen van SCIAMACHY worden gedaan door de atmosfeer horizontaal laag voor laag te scannen (limbmetingen). De limb ozonprofielen die SCIAMACHY heeft gemeten, zijn vergeleken met zeer betrouwbare ozonmetingen vanaf de grond (lidar). Uit deze validatie blijkt dat de afzonderlijke SCIAMACHY-ozonprofielen 35 procent of meer kunnen afwijken van de lidarmetingen. De gemiddelde afwijking bedraagt -8 tot +5 procent.

Ozonconcentraties, gemeten over de hele wereld en over een langere tijdsperiode, geven informatie over de conditie van de ozonlaag, en daarmee over de effectiviteit van maatregelen om de afbraak van de ozonlaag te verminderen.

De profielmetingen van SCIAMACHY worden gehinderd doordat de stand van de ENVISAT-satelliet ten opzichte van de aarde niet voldoende bekend is. Hierdoor is de exacte hoogte waarop SCIAMACHY meet onvoldoende bekend. Dit leidt tot zogeheten hoogteverschuivingen, die de uitkomsten van de metingen beïnvloeden. Het onderzoek heeft voor het eerst met SCIAMACHY-metingen aangetoond dat de hoogteverschuivingen nog gecompliceerder zijn dan gedacht. Dit maakt een correctie op de metingen nog moeilijker. Wel geeft het meer inzicht in de onduidelijkheid over de stand van de ENVISAT-satelliet ten opzichte van de aarde. Indien een oplossing gevonden wordt, kan die met terugwerkende kracht (tot 2002) worden toegepast op de profielmetingen van SCIAMACHY.

Trefwoorden: validatie, SCIAMACHY, ozonprofielen, lidar, ENVISAT

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Samenvatting

Kennis van ozonconcentraties in de atmosfeer is cruciaal voor het bepalen van de conditie van de ozonlaag. Hiermee kunnen vragen beantwoord worden als: is de ozonlaag zich aan het herstellen en zo ja, waar en in welke mate? Ook kan hiermee de effectiviteit van maatregelen gericht op de reductie van ozonafbraak bepaald worden. Het werelddekkend monitoren van de ozonlaag gebeurt met satellietinstrumenten vanuit de ruimte. Het SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) instrument, aan boord van de milieusatelliet ENVISAT, voert metingen uit waaruit ozonprofielen gehaald kunnen worden. De meest geschikte metingen hiervoor zijn de limbmetingen waarbij horizontaal door de atmosfeer gemeten wordt. De betrouwbaarheid van verkregen ozonprofielen wordt bepaald door middel van validatie.

In het kader van de Nederlandse bijdrage aan de validatie van SCIAMACHY voor het Nederlands Instituut voor Vliegtuigontwikkeling en Ruimtevaart (NIVR) zijn in dit rapport de verschillende SCIAMACHY-ozonprofielprodukten gevalideerd. Hiertoe zijn de SCIAMACHY-ozonprofielen vergeleken met hoge-kwaliteit lidarmetingen van zeven stations verspreid over de wereld. Speciale aandacht is besteed aan eventuele afhankelijkheden, zoals locatie en oriëntatie van de satelliet, waardoor mogelijk niet alle ozonprofielen even betrouwbaar zijn.

De beste ozonprofielen zijn afkomstig van het IFE versie 1.62 produkt met fouten in ozonconcentratie variërend van -8% tot 5% voor het hoogtebereik 18-40 km en een vorm van het ozonprofiel die goed overeenkomt met het lidarvalidatieprofiel. Alle andere produkten geven aanzienlijk grotere fouten in ozonconcentratie en een van het lidarvalidatieprofiel afwijkende profielvorm. De fouten in ozonconcentratie van zelfs de beste profielen zijn significant groter dan die van ozonprofielen van andere satellietmetingen, bijvoorbeeld van GOMOS, ook een ENVISAT-instrument.
Daarnaast is er een azimutafhankelijkheid aangetoond in de reeds bekende hoogteverschuiving van SCIAMACHY-data. Deze afhankelijkheid maakt het corrigeren voor de hoogteverschuiving gecompliceerder, maar geeft tevens meer inzicht in het probleem dat de hoogteverschuiving veroorzaakt. Deze hoogteverschuiving blijft het belangrijkste probleem in het verkrijgen van bruikbare SCIAMACHY-ozonprofielen.

Summary

Knowledge about atmospheric ozone concentrations is crucial to determine the condition of the ozone layer. With this, answers can be given to questions like: is the ozone layer recovering and if yes, at which locations and to what extent? Also, the effectiveness of ozone depletion reduction measures can be determined with this. Monitoring the ozone layer on a global scale is done with satellite instruments from space. The SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmosphere CHartographY) instrument, onboard the ENVIronmental SATellite ENVISAT, performs measurements from which ozone profiles can be obtained. Most suitable measurements for this are the limb measurements for which horizontal scans through the atmosphere are made. The reliability of retrieved ozone profiles is determined by validation.

Within the framework of the Dutch contribution to the validation of SCIAMACHY on behalf of the Netherlands Agency for Aerospace Programs (NIVR) the different SCIAMACHY ozone profile products have been validated for this report. To this end, the SCIAMACHY ozone profiles have been compared with high-quality lidar measurements from seven stations around the world. Special attention has been given to possible dependencies, like location and orientation of the satellite, which might introduce variations in the reliability of different ozone profiles.

Best ozone profiles come from the IFE version 1.62 product with errors in ozone concentration of -8% to 5% for the altitude range 18-40 km and an ozone profile shape quite similar to that of the lidar validation profile. All other products give significantly larger errors in ozone concentration and a profile shape that differs significantly from that of the lidar validation profile. The errors in ozone concentration of even the best profiles are significantly larger than those of ozone profiles from other satellite measurements, for example from GOMOS, another ENVISAT instrument.
Furthermore, an azimuth dependency has been demonstrated in the well-known altitude shift present in SCIAMACHY data. This dependency makes correcting for the altitude shift more complicated, but it gives also insight into the problem causing the altitude shift. This altitude shift remains the most important problem in retrieving usable SCIAMACHY ozone profiles.

1. Introduction

In March 2002 the European Space Agency (ESA) launched the ENVIronmental SATellite ENVISAT in order to address outstanding environmental questions. One of these questions concerns the ozone layer. Both scientists and policymakers want to monitor the ozone layer to know whether the ozone layer is recovering and to measure the effectiveness of ozone depletion reduction measures. Together with two other ENVISAT instruments, GOMOS[1] and MIPAS[2], SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) investigates the concentrations and vertical distributions of ozone and related gases such as nitrogen dioxide, bromine oxide and chlorine dioxide.

The SCIAMACHY instrument measures in the ultraviolet, visible and infrared part of the spectrum the earthshine radiance in limb and nadir viewing mode and the transmitted light trough the atmosphere in solar and lunar occultation viewing mode (Bovensmann et al., 1999). The large spectral range allows for the investigation of a relative large number of atmospheric trace gases, temperature and several cloud and aerosol parameters. Ozone profiles can be retrieved from both limb and nadir measurements, however for SCIAMACHY only limb ozone profiles are available at present. Ozone profile retrieval from nadir measurements is currently not possible because of large calibration errors.

The retrieval of ozone profiles from satellite measurements is quite complicated and depends on many parameters. It is therefore very important that the retrieved profiles are validated. In November 2004 two SCIAMACHY limb ozone profile products were available: the official ESA product developed for ESA by the German Aerospace Center (DLR), version 2.1 and the scientific product developed by Institute of Environmental Physics of the University of Bremen (IFE), version 1.6. Validation of both products has been performed by Brinksma et al. (2004). They concluded that for both products the profiles agreed within 10% in the altitude range 20-40 km compared with groundbased data and within 20% compared with satellite data. Standard deviations of the differences between SCIAMACHY and correlative ozone profiles were large (10-40%). The results were dominated by the attitude problem of the ENVISAT platform (section 2.1). The IFE version 1.6 product has also been validated by Bracher et al. (2005, comparison with satellite data), Segers et al. (2005, comparison with sonde data), Palm et al. (2005, comparison with microwave radiometer data), Kuttippurath et al. (2004, comparison with aircraft data) and De Clercq et al. (2005, comparison with sonde, lidar and microwave radiometer data) with similar conclusions.

[1] Global Ozone Monitoring by Occultation of Stars
[2] Michelson Interferometer for Passive Atmospheric Sounding

In the period November 2004 – December 2005 improved versions of both products became available: the ESA version 2.5 product and IFE version 1.61 and 1.62 products. Also, a selected number of profiles of four intermediate ESA products became available for pre-validation. This report describes the validation by intercomparison with lidar data of those three products and the pre-validation of the intermediate products. Part of the work performed for this report is published in Brinksma et al. (2006).

2. SCIAMACHY limb ozone profiles

In the limb viewing mode SCIAMACHY makes horizontal scans from 3 km below the horizon to typically 96 km above the horizon, with vertical intervals of 3 km. Each scan consists of four measurements (Bovensmann et al., 1999). From one complete limb measurement, called a state, four vertical profiles can be retrieved (Figure 1). A selection of the horizontal scans is used for ozone profile retrieval. The four different ozone profiles that can be retrieved from one limb state are referred to by their position within state: West, center-West, center-East and East profiles.

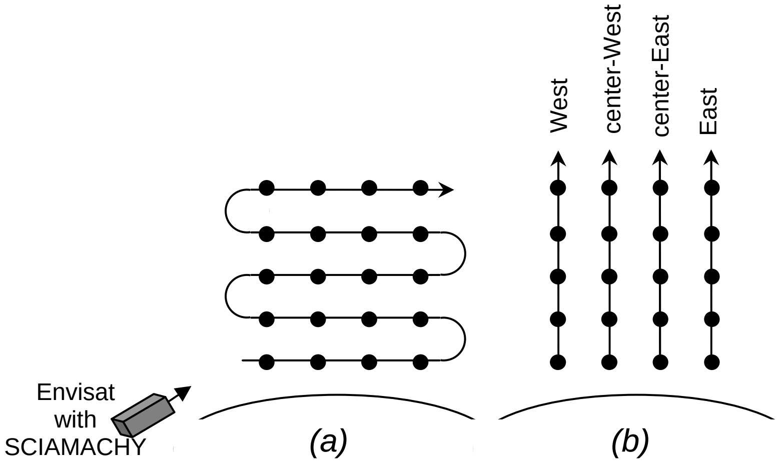

Figure 1a, b: Limb viewing mode of SCIAMACHY.
The dots indicate the positions of the individual measurements. A complete limb measurement, called a state, starts with a horizontal scan of four individual measurements pointing effectively 3 km below the horizon. This is followed by subsequent scans pointing higher in the atmosphere with intervals of 3 km. The last scan is made at about 96 km above the horizon (a). The four individual measurements within one horizontal scan can be used to retrieve four different vertical profiles from one limb state and are refered to as West, center-West, center-East and East profiles (b).

The position of the sun is a very important parameter in limb measurements. It determines to a large extent the signal-to-noise ratio. For small solar zenith angles the signal-to-noise ratio will be relatively large, whereas for large solar zenith angles the signal-to-noise ratio will be relatively small (Figure 2).

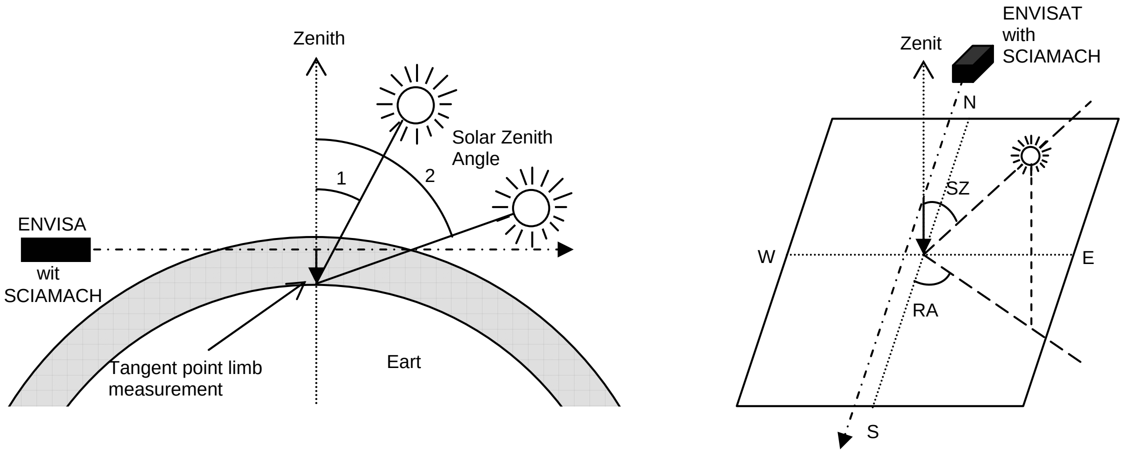

Figure 2: Solar zenith angle.

[Left figure shows ENVISAT measuring at small solar zenith angle (1) and at large solar zenith angle (2). The tangent point is the point at which SCIAMACHY effectively measures. Right figure shows the solar zenith angle and the relative azimuth angle at an ENVISAT measurement.]

2.1 Attitude problem

A precise knowledge of the effective altitude at which SCIAMACHY measures, the tangent height, is crucial for an accurate retrieval of ozone profiles. For example, an error of 500 m in tangent height leads to an error in the retrieved stratospheric ozone concentration of 10% (Von Savigny et al., 2005a). Unfortunately, SCIAMACHY tangent height errors are in the order of a few kilometers. This is due to an imprecise knowledge of the attitude of the ENVISAT platform: the actual attitude of the platform differs from the predicted attitude, the only known attitude. This difference between actual and predicted (known) attitude is not constant in time. It is therefore very difficult to correct for the tangent height offset afterwards. Largest inaccuracies in the tangent height offset result from inaccuracies in the elevation angle of the ENVISAT platform. Inaccuracies in the azimuth angle of the ENVISAT platform result in relatively small inaccuracies in the tangent height offset (Saavedra et al., 2005; Von Savigny and Lolkema, 2006).

A possible solution to correct for the tangent height offset afterwards is by use of the Tangent height Retrieval by UV-B Exploitation (TRUE)-method. The TRUE-method compares the maximum (i.e., the ‘knee’) in UV limb radiance profiles, present in the upper stratosphere / lower mesosphere, between 295 nm and 305 nm with an *a priori* ozone profile to determine the tangent height offset. This method is only applicable with relatively high precision in the tropics (between 20ºS and 20ºN) where stratospheric and mesospheric ozone is horizontally relatively homogeneous. At mid- and high-latitudes, stratospheric and mesospheric ozone is much more variable which can lead to significant errors in the determination of the tangent height offset. Therefore, for each orbit, only the mean tangent height offset in the latitude range 20ºS - 20ºN is determined and applied to all measurements in this orbit (Kaiser et al., 2004; Von Savigny et al., 2005a).

2.2 Retrieval of ozone profiles

The retrieval of ozone profiles from limb as well as nadir uv-reflectance measurements is an ill-posed problem. Most retrieval schemes use an optimal estimation method in which an *a priori* ozone profile is updated with the measurement information. The retrieved ozone concentration at one altitude level depends not only on the measurement at that altitude level, but also on the measurements of one or more neighboring levels. How the retrieved, *a priori* and true ozone profiles are related is expressed by the averaging kernel matrix. The retrieved ozone profile depends on the *a priori* ozone profile, the true ozone profile and the averaging kernel matrix as follows (Rodgers, 2000):

$$X_{\mathrm{retrieved}} = X_{a\ priori} + A(X_{\mathrm{true}} - X_{a\ priori}) \tag{1}$$

With A the averaging kernel matrix and $X_{\mathrm{retrieved}}$, $X_{a\ priori}$ and X_{true} the state vectors of the retrieved, *a priori* and true ozone profile, respectively. In an ideal situation A is equal to the identity matrix and the retrieved profile will be identical to the true profile. In the opposite situation all elements of A are zero and the retrieved profile will be identical to the *a priori* profile (Meijer, 2005).

All SCIAMACHY limb ozone profile products analyzed for this report use for their retrieval an optimal estimation method as described above. It is important to realize that the tangent height offset present in SCIAMACHY limb measurements will result in relatively large errors in the retrieved ozone profile since the measurements are shifted in altitude and the *a priori* ozone profile is not.

3. Data

Within the period November 2004 – December 2005 improved versions of the previous ESA version 2.1 and IFE version 1.6 products became available: the ESA product version 2.5 and the IFE product versions 1.61 and 1.62. Also, a selected number of profiles of four intermediate ESA products became available for pre-validation. All these products have been analyzed. A description of these products and periods of available data are given below and summarized in Table 1.

ESA version 2.5

The ESA version 2.5 product is the current (at time of writing) operational ESA product. Ozone profiles are retrieved a few days after measurement. Data are available from December 7th, 2004 onward. Reprocessing of data before December 7th, 2004 is not intended for this product.

For this product, four different ozone profiles are retrieved per state. Ozone profiles can be retrieved between 12 and 65 km (Noël, 2005). The ozone concentrations are reported in volume mixing ratio, though these values should not be used. The ozone concentration in volume mixing ratio as reported in the product is subject to large errors since the ozone concentration is measured in number density and the temperature and pressure profiles, needed to convert number density to volume mixing ratio, are not independently retrieved. Correct approach is to calculate the ozone concentrations in number density from the partial column densities which are given in the product. No averaging kernels are available. The *a priori* ozone concentrations are not stored directly in the product but can be retrieved from the residuals of the different iteration steps used in the retrieval.

ESA version 2.8

The ESA version 2.8 product will be the new operational ESA product[3]. Main difference with the version 2.5 product is the retrieval algorithm which has been completely changed. In the process of developing this new version 2.8 product selected profiles of four intermediate products became available for pre-validation, all four based on different retrieval algorithms. One of these algorithms will be used for the new version 2.8 product. For this product, four different ozone profiles will be retrieved per state though for the intermediate products only one ozone profile per state has been retrieved. Hence, possible differences between the four ozone profiles that will be retrieved per state could not be investigated. Ozone profiles can be retrieved between 15 and 40 km according the disclaimer. The ozone concentrations will be reported in number density. The averaging kernels will be available though for the

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[3] Shortly before publication of this report ESA announced that the new operational ESA product will be version 3.0 in stead of version 2.8. The difference with the planned version 2.8 product will be a tangent height correction applied to the data.

intermediate products they were not. Hence, the averaging kernels could not be taken into account in the pre-validation. The *a priori* ozone concentrations are taken from the climatology of (McPeters, 1993) and are not stored directly in the product but can be retrieved from the residuals of the different iteration steps used in the retrieval, as with the version 2.5 product.

IFE version 1.61

The retrieval algorithm of the IFE version 1.61 product is basically the same as the one for the previous version 1.6 product. While the retrieval algorithm of the ESA version 2.5 product uses the measurements from a complete spectral band, the retrieval algorithm of the IFE product only uses the measurements at three wavelengths: the center and the wings of the Chappuis absorption bands of ozone (Von Savigny et al., 2005b). The radiative transfer model used is SCIARAYS (Kaiser, 2001; Von Savigny et al., 2005b). Data are available for the months January, March, May, September and November 2004. For this product, one ozone profile per state is retrieved. Ozone profiles can be retrieved between 15 and 40 km. Ozone concentrations are reported in number density. The averaging kernels are available. The *a priori* ozone concentrations can be retrieved from climatology files.

IFE version 1.62

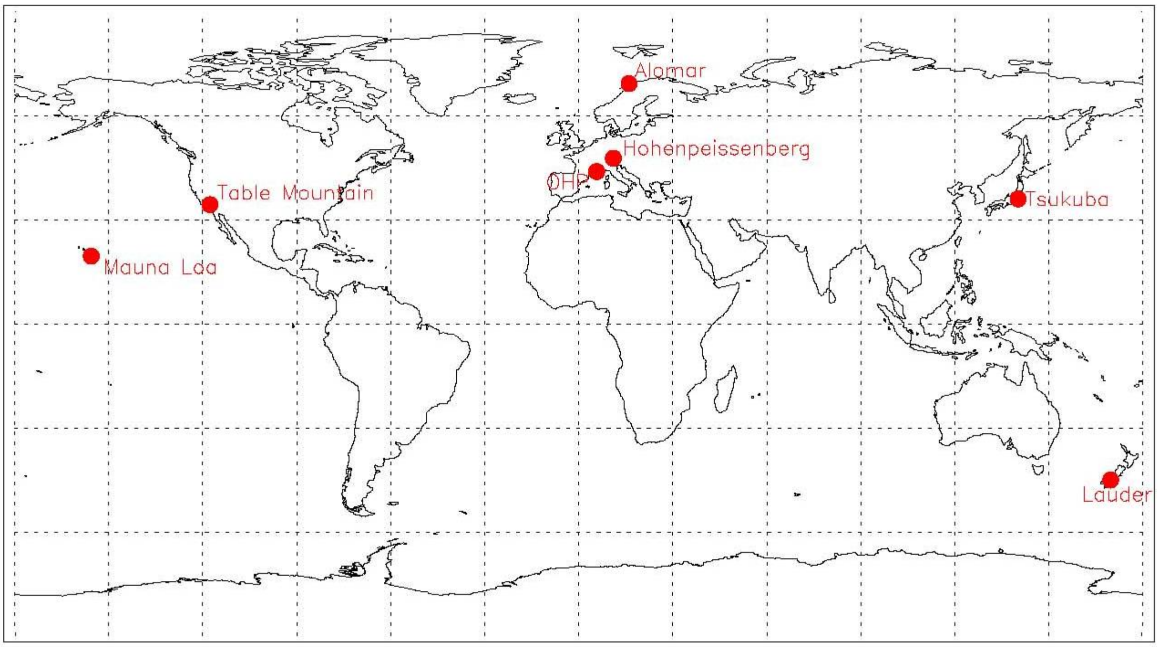
Main difference between the IFE version 1.62 product and the previous version 1.61 product is the use of the TRUE-method for the version 1.62 product, as described in section 2.2, to try to correct for tangent height errors resulting from the ENVISAT attitude problem. Data are available for the months September and October 2004. More data are currently being processed. For this product, four different ozone profiles per state are retrieved. Ozone profiles can be retrieved between 15 and 40 km. Ozone concentrations are reported in number density. The averaging kernels and *a priori* ozone concentrations are available.

Table 1: Characteristics of the different SCIAMACHY limb ozone profile products.

	ESA v2.5	ESA v2.8	IFE v1.61	IFE v1.62
Available data	Dec 7th 2004 -	-	Jan, Mar, May, Sep + Nov 2004	Sep + Oct 2004
# profiles per state	4	4*	1	4
Altitude range	12-65 km	15-40 km	15-40 km	15-40 km
Ozone conc. unit	Vol. mixing ratio	Number density	Number density	Number density
AVK available	-	+*	+	+
A priori available	+	+	+	+
*Not for the intermediate products.				

4. Validation method

The measurements of seven lidar stations around the world have been used to validate SCIAMACHY limb ozone profiles. These stations cover a wide range of latitudes (Table 2, Figure 3) and are all part of the Network for the Detection of Atmospheric Composition Change (NDACC, former NDSC). The NDACC guarantees and maintains high quality of these data. For stratospheric ozone lidar measurements accuracies lie within 2% for the altitude range 20-35 km and between 5-10% for the other altitudes (Keckhut et al., 2004).



Station name	Latitude	Longitude
Alomar	69.30	16.00
Hohenpeissenberg	47.80	11.02
OHP	43.94	5.71
Tsukuba	36.05	140.13
Table Mountain	34.40	-117.70
Mauna Loa	19.54	-155.58
Lauder	-45.04	169.68

Figure 3 and Table 2: Locations of the seven lidar stations from which measurements have been used to validate SCIAMACHY limb ozone profiles.

Collocation criteria

Collocation criteria between a SCIAMACHY limb measurement and a lidar measurement have been a maximum distance of 800 km and a maximum time difference of 20 hours for the ESA version 2.5 and the IFE version 1.61 and 1.62 products. These collocation criteria are appropriate choices for comparisons of ozone profiles retrieved from satellite measurements with lidar measurements (Meijer et al., 2004). For the pre-validation of the intermediate ESA products the maximum distance has been increased to 1000 km to get a sufficient number of collocated pairs.

Averaging kernels

The lidar profile has a significantly higher vertical resolution than the SCIAMACHY profile. To compare both profiles it is common practice in satellite validation that the lidar profiles are convolved with the averaging kernel matrices and *a priori* ozone profiles according to equation 1 in section 2.3. The lidar profile is regarded then as the X_{true} state vector. This approach was first suggested by (Conner et al., 1991). Making use of convolved lidar profiles the averaging kernel matrices need also to be examined for one must not mistake a good comparison for a good retrieval while in fact two *a priori* profiles are compared (section 2.3). A measure for the amount of measurement information in the retrieval is the degrees of freedom for the signal (DFS) value. The DFS value is defined as the trace of the averaging kernel matrix (Meijer, 2005; Rodgers, 2000). For the comparisons of the IFE version 1.62 product the collocated lidar profiles have been convolved as described above with the averaging kernel matrices and *a priori* profiles that go with the product profiles. For these profiles the averaging kernel matrices have been examined and the DFS values have been computed. For the ESA version 2.5, intermediate ESA and IFE version 1.61 products the collocated lidar profiles have not been convolved. For the ESA version 2.5 and intermediate products no averaging kernels were available. For the IFE version 1.61 product the *a priori* ozone profiles were only supplied as climatology data: the retrieved ozone profiles did not come with an *a priori* ozone profile.

Altitude grid and range

For the comparisons, all ozone profiles have been brought to a common altitude grid of 200 m by means of linear interpolation. The comparisons have been limited to the altitude range 18-45 km for lidar measurements are best used in this altitude range for ozone profile validation (Meijer et al., 2004). Since for the intermediate ESA products and the IFE version 1.61 and 1.62 products ozone profiles can only be retrieved with relatively high accuracy between 15 and 40 km altitude, comparisons for those products have been focused on the altitude range 18-40 km. Pairs of collocated SCIAMACHY and lidar measurements have only been compared within their overlapping altitude range.

Tangent height offset

The tangent height offset is a major problem in retrieving SCIAMACHY limb ozone profiles. The retrieved profile will contain large errors and will be shifted in altitude. To be able to compare the retrieved profiles with correlative data, the SCIAMACHY ozone profiles have been shifted in altitude with a constant offset. Remember that the tangent height offset is not constant in time. Best approximation for the average tangent height offset is -1500 m (Brinksma et al., 2006). This altitude shift has been applied to the profiles of the ESA version 2.5, IFE version 1.61 and intermediate ESA products. The IFE version 1.62 product employs the TRUE-method to correct for the tangent height offset. The average TRUE-shift for the

IFE version 1.62 data-set is -800 m. An additional altitude shift of -700 m (equal to the difference between the average tangent height offset and the average TRUE-shift) has been applied to the profiles of the IFE version 1.62 product. Note that the averaging kernel matrices will contain an intrinsic tangent height offset. In convolving the collocated lidar profiles for the IFE version 1.62 product no tangent height corrections have been made.

Comparisons

For all products, comparisons have been made on sets of all available collocated measurement pairs for that one product. For those products that retrieve four different profiles per state, the measurements for each profile state position (i.e. West, center-West, center-East or East) form different sets.

Subsets

Besides the comparisons on sets of all collocated measurements, comparisons on subsets have been made to investigate the influence on the retrieval of different measurement conditions. Intercomparisons have been made between subsets of different profile state position: West, center-West, center-East and East. The same is done for subsets of different geographical location: polar regions, mid-latitudes (Northern and Southern hemisphere) and tropical regions. To investigate the influence of the position of the sun, intercomparisons have been made between subsets of different solar zenith angle range: 0°-30°, 30°-60° and 60°-90° and between subsets of different relative azimuth angle range: 0°-45°, 45°-90°, 90°-135° and 135°-180°. Not all subsets contain enough collocated measurement pairs to perform a meaningful comparison.

Collocation numbers

The numbers of collocated measurement pairs for the different products and subsets are given in Table 3. Note that hardly any collocations were found in the polar regions and for solar zenith angle range 0°-30°.

Table 3: Numbers of collocated measurement pairs for the different products and subsets. For the ESA version 2.5 and IFE version 1.62 products four numbers are given for each subset referring to the West, center-West, center-East and East profiles within state respectively. Grey numbers indicate that for the specific subset the numbers of collocated measurements were not well enough distributed to perform a valuable comparison on this subset. 'Interm. ESA' refers to the intermediate ESA products provided for pre-validation. Used abbreviations: lat = latitude, sza = solar zenith angle and raa = relative azimuth angle.

		ESA v2.5	interm. ESA	IFE v1.61	IFE v1.62
	All	77 / 81 / 86 / 94	32	228	78 / 82 / 74 / 65
polar	|lat| > 66.5º	-	-	-	3 / 3 / 3 / 2
mid-lat NH	23.5 < lat < 66.5	38 / 41 / 45 / 51	25	125	44 / 47 / 42 / 37
mid-lat SH	-66.5 < lat < -23.5	15 / 17 / 19 / 20	5	30	14 / 15 / 14 / 13
tropics	-23.5 < lat < 23.5	24 / 23 / 22 / 23	2	73	17 / 17 / 15 / 13
SZA range	0°-30°	-	2	37	- / - / 2 / 5
	30°-60°	49 / 51 / 53 / 55	23	153	68 / 73 / 64 / 53
	60°-90°	28 / 30 / 33 / 38	7	38	10 / 9 / 8 / 7
RAA range	0°-45°	21 / 35 / 46 / 61	not calcu-lated	31	11 / 25 / 38 / 39
	45°-90°	40 / 29 / 21 / 13		144	53 / 42 / 21 / 13
	90°-135°	9 / 9 / 14 / 17		26	-
	135°-180°	7 / 8 / 5 / 3		27	14 / 15 / 14 / 13

5. Results

For the ESA version 2.5 product the comparison between all collocated retrieved and lidar ozone profiles showed that the retrieved ozone profiles differ less than 10% from the lidar profiles in the altitude range 25-40 km. Outside this range differences can be as large as 25%. A striking feature of the retrieved ozone profiles is that the its shape differs significantly from the shape of the lidar profiles (Figure 4).
The analyses performed on the four different intermediate ESA products all gave similar results. The comparison between the profiles retrieved with the algorithm that will be used for the new version (2.8) of the ESA product and collocated lidar profiles showed that the profiles of this intermediate product underestimate ozone considerably over the whole altitude range. The profiles of this intermediate product demonstrate a sharp bend near the ozone maximum (Figure 5).
For the IFE version 1.61 product the comparison between all collocated retrieved and lidar ozone profiles showed that the differences are within the range -15% to 10% for both the altitude range 18-45 km as the altitude range 18-40 km. The retrieved ozone profiles demonstrate two sharp bends, one near the ozone maximum and one a few kilometers above the ozone maximum (Figure 6).
For the IFE version 1.62 product the comparison between all collocated retrieved and lidar ozone profiles showed that the differences are within the range -8% to 5% for the altitude range 18-40 km. The shape of the retrieved profile does not demonstrate any striking features (Figure 7). The averaging kernels are quite sharp (Figure 8). The median and standard deviation of the DFS values is 10.02 ± 0.59 which means that the amount of measurement information in the retrieval is quite large and constant.

Subsets

Intercomparisons between the sets of different profile state position demonstrated an increase in the tangent height offset from West to East measurements, indicating an azimuthal dependence of the tangent height offset (Figure 9). Intercomparisons between the subsets of different geographical location showed for the ESA version 2.5 product large differences in the shape of the difference profile (Figure 10). For the IFE version 1.61 product no large differences have been observed. Intercomparisons between the subsets of different solar zenith angle ranges showed for the ESA version 2.5 product large differences in the profile shape (Figure 11). For the IFE 1.61 product ozone concentrations are significantly underestimated for the solar zenith angle range 60°-90° (Figure 12). Intercomparisons between the subsets of different relative azimuth angle ranges showed that for the IFE version 1.61 product ozone concentrations are significantly underestimated for the relative azimuth angle ranges 0°-45° and 135°-180° (Figure 13).

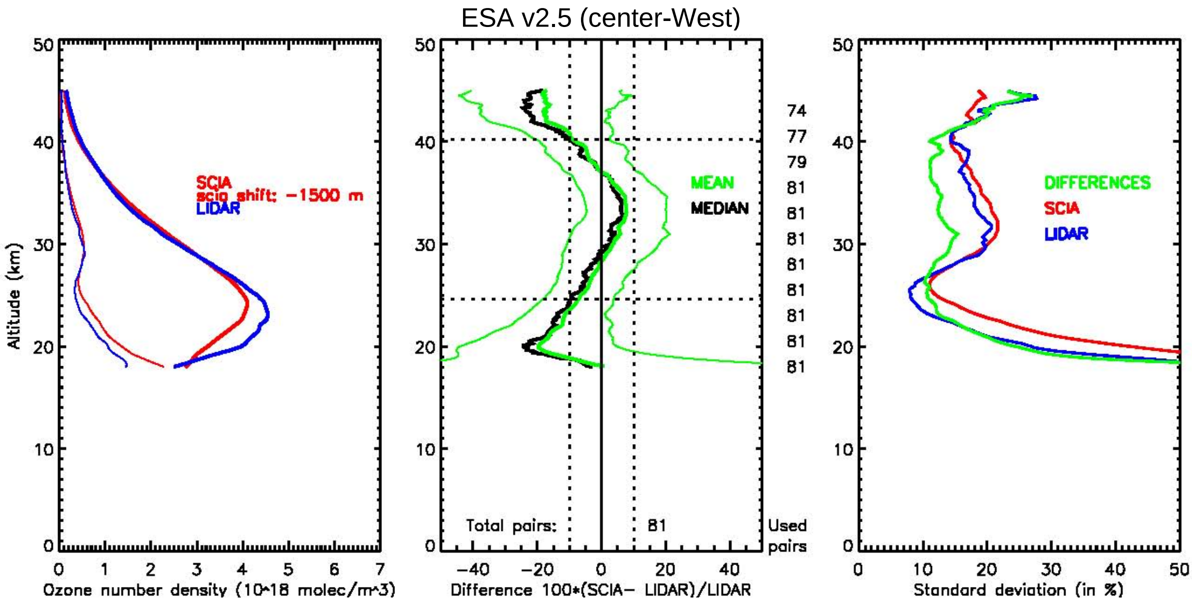


Figure 4: Analysis of the ESA version 2.5 product for the center-West profiles.

Left panel: averaged ozone profile and standard deviation of the collocated SCIAMACHY measurements (red) and of the collocated lidar measurements (blue). Middle panel: mean and standard deviation (green) and median (black) of the differences between the SCIAMACHY and lidar profiles, relative to the lidar profiles. Right panel: relative standard deviation of the differences (green), SCIAMACHY profiles (red) and lidar profiles (blue). The numbers placed at the different altitude levels between the middle and the right panels give the number of collocated measurement pairs for that one altitude level. The vertical dotted lines in the middle panel indicate the ±10% range of the differences and the horizontal dotted lines in the middle panel indicated the altitude range for which the median of the differences lies within this ±10% range.

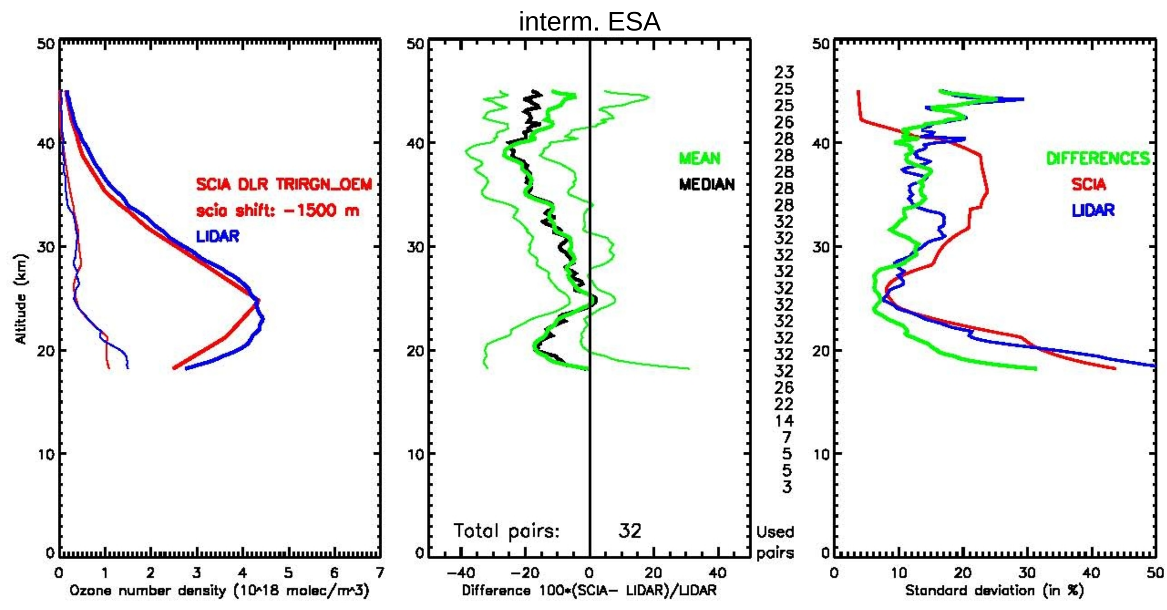


Figure 5: Analysis of the intermediate ESA product which retrieval algorithm will be used for the new version (2.8) of the ESA product. Panels as in Figure 4.

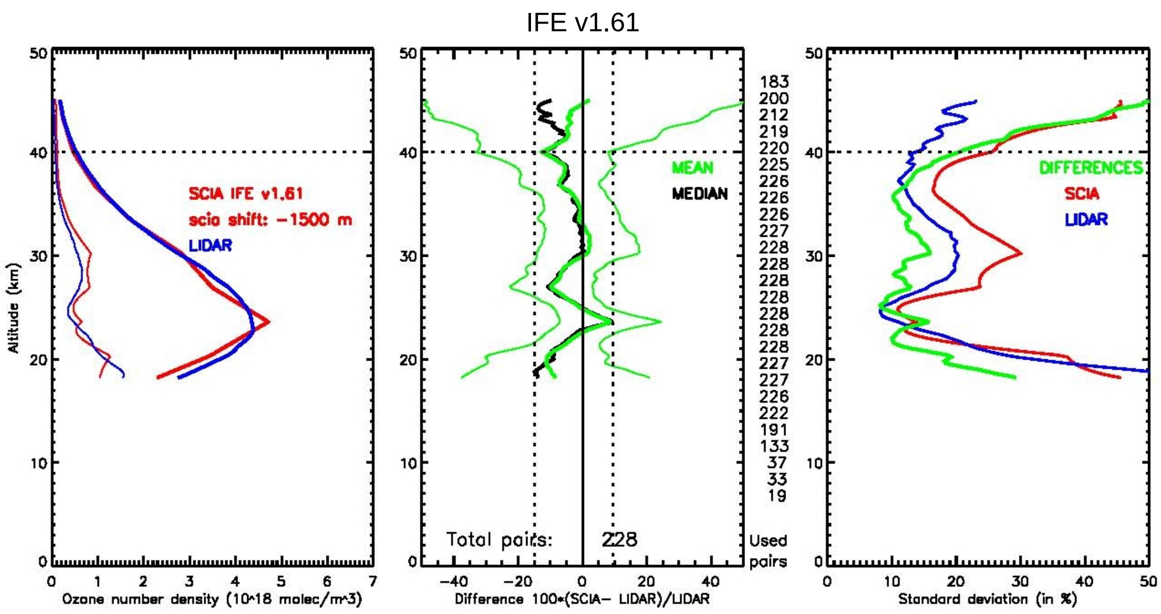


Figure 6: Analysis of the IFE version 1.61 product.

Panels as in Figure 4. The horizontal dotted line indicates the 40 km altitude level below which ozone profiles can be retrieved with relatively high accuracy. The vertical dotted lines in the middle panel indicate the minimum and the maximum of the median of the differences within the altitude range 18-40 km.

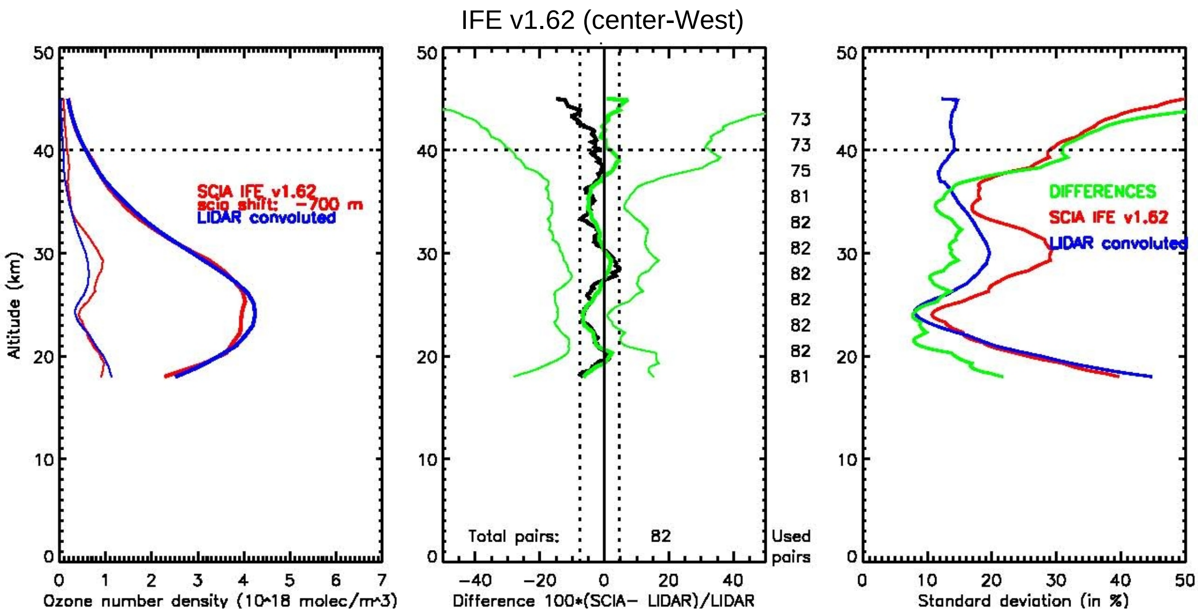


Figure 7: Analysis of the IFE version 1.62 product for the center-West profiles.

Panels as in Figure 4. The horizontal dotted line indicates the 40 km altitude level below which ozone profiles can be retrieved with relatively high accuracy. The vertical dotted lines in the middle panel indicate the minimum and the maximum of the median of the differences within the altitude range 18-40 km.

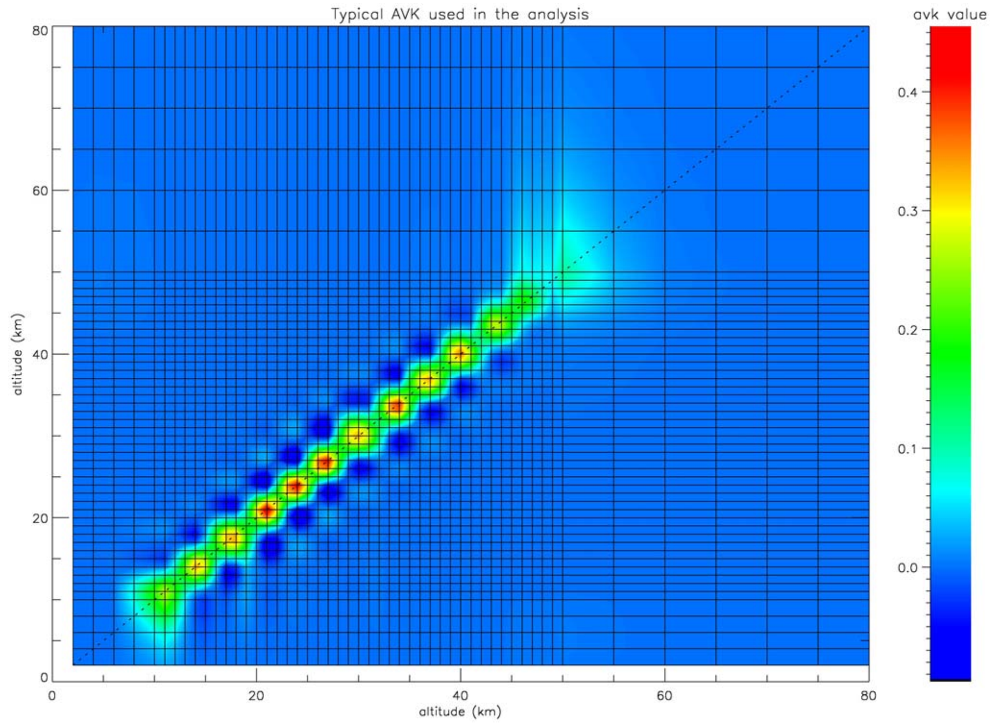


Figure 8: Typical averaging kernel matrix of the IFE version 1.62 product.

Horizontal axis: ozone in this level contributes to other levels. Vertical axis: contribution of each level to this level. Colors indicate the weighting factors: from -0.10 (dark blue) to 0.46 (red). Black horizontal and vertical lines represent the altitude levels. The dotted line represents the one-to-one line.

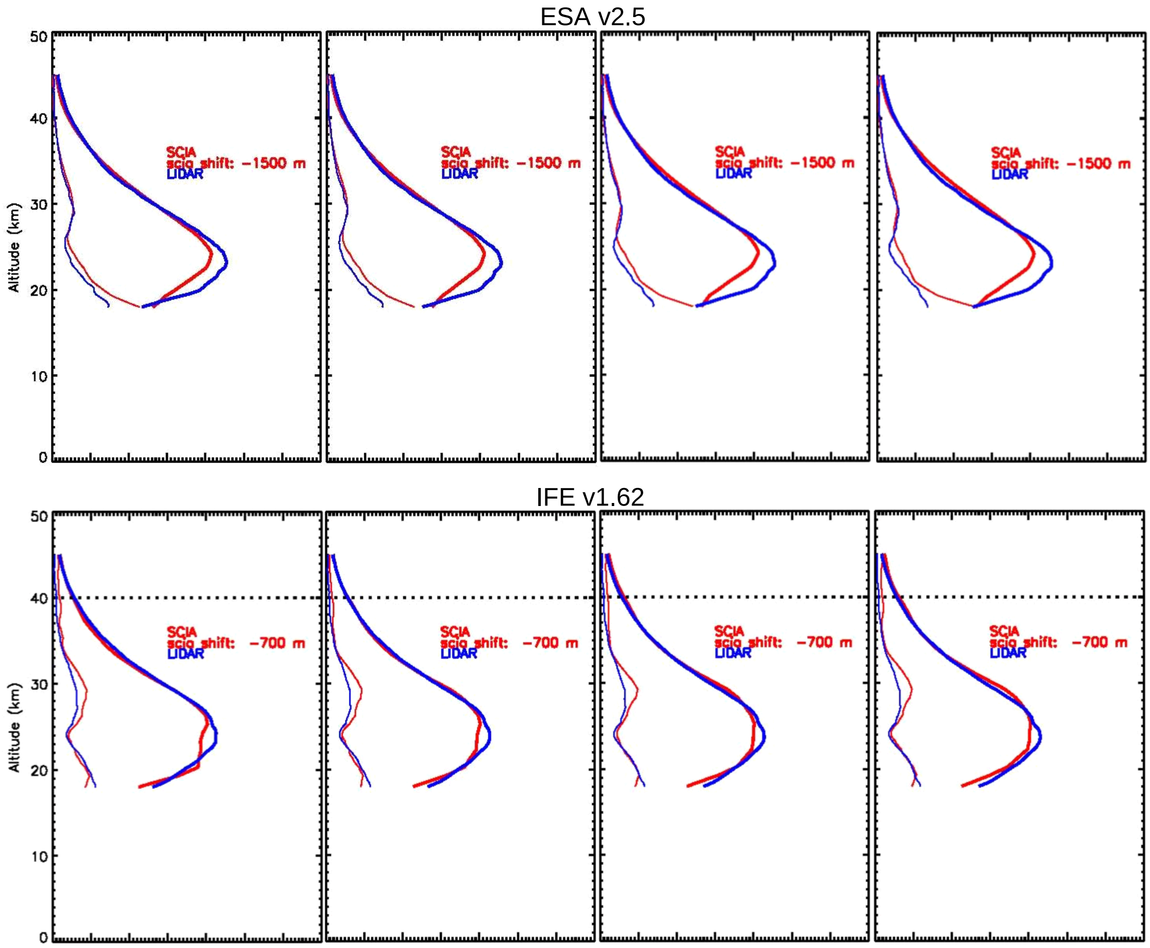


Figure 9: Averaged ozone profiles and standard deviations of SCIAMACHY (red) and lidar (blue) for the ESA version 2.5 product (top) and the IFE version 1.62 product (bottom).

From left to right for the West, center-West, center-East and East measurements. Numbers of collocated pairs for the ESA version 2.5 product are 77, 81, 86 and 94, respectively. Numbers of collocated pairs for the IFE 1.62 product are 78, 82, 74 and 65, respectively.

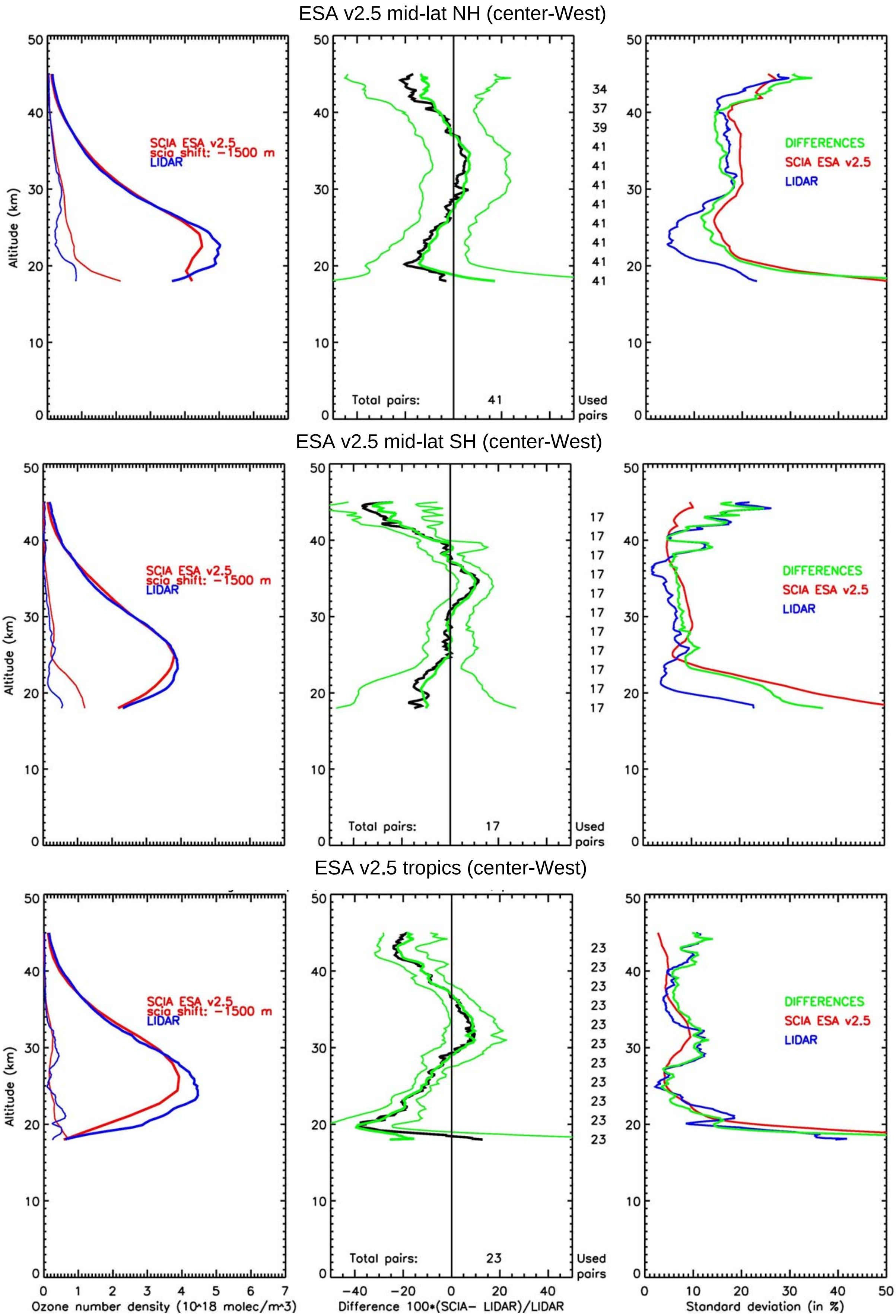


Figure 10: Analysis of the ESA version 2.5 product for the center-West profiles for the subsets mid-latitudes Northern hemisphere (top), mid-latitudes Southern hemisphere (middle) and tropical regions (bottom).

Panels as in Figure 4. Note the large differences in the shape of the difference profile (middle panels) for the different subsets.

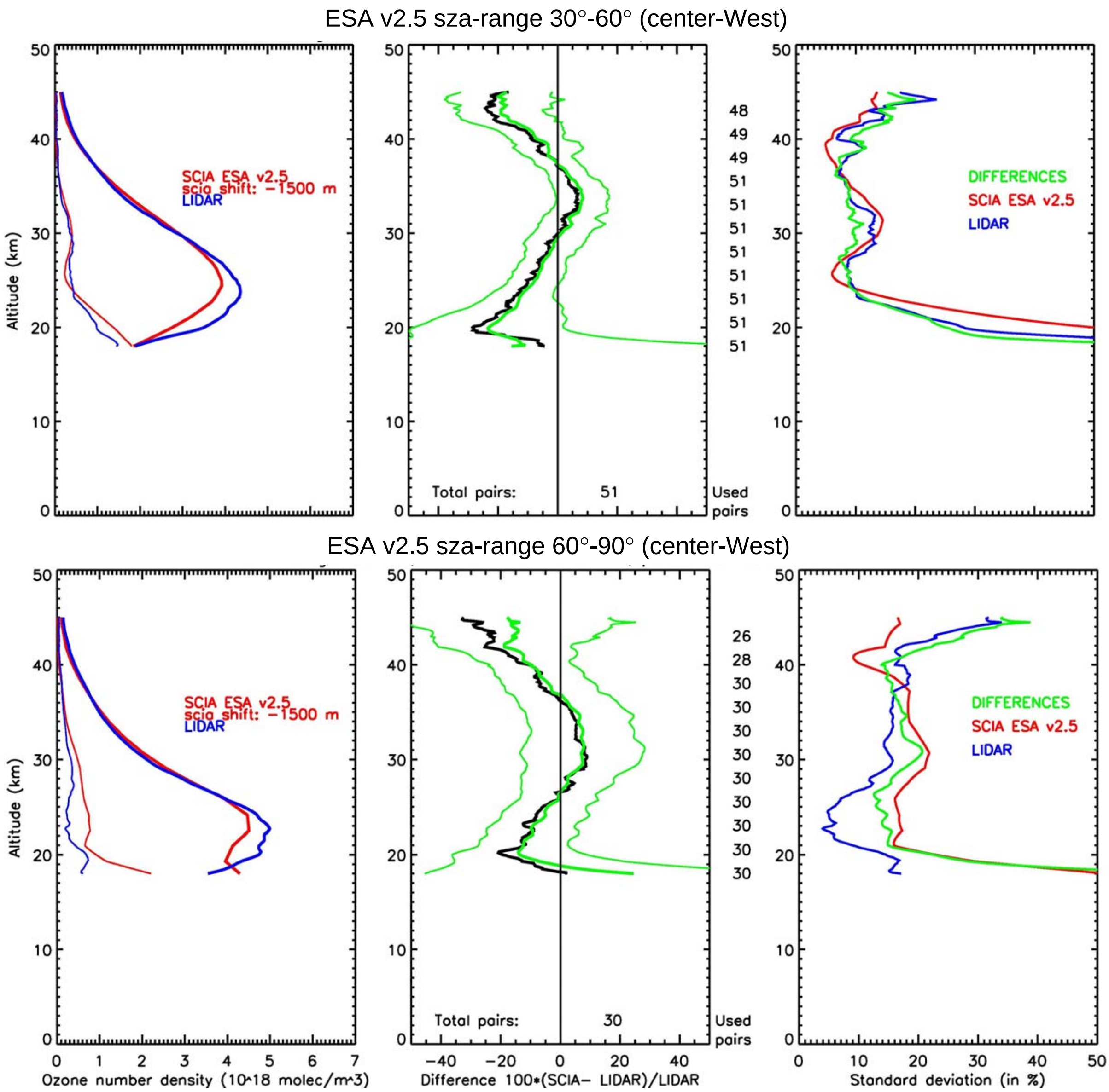


Figure 11: Analysis of the ESA version 2.5 product for the center-West profiles for the subsets solar zenith angle range 30°-60° (top) and solar zenith angle range 60°-90° (bottom).

Panels as in Figure 4. Note the large differences in the shape of the difference profile (middle panels) for the different subsets.

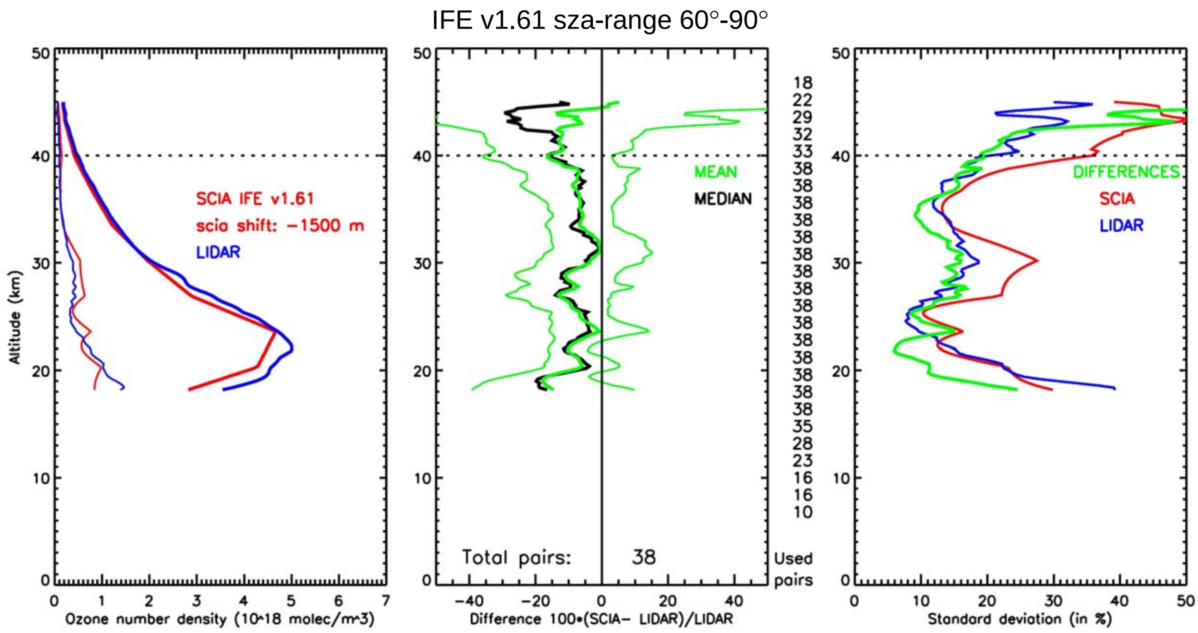


Figure 12: Analysis of the IFE version 1.61 product for the subset solar zenith angle range 60°-90°. Panels as in Figure 4. Ozone concentrations are significantly underestimated.

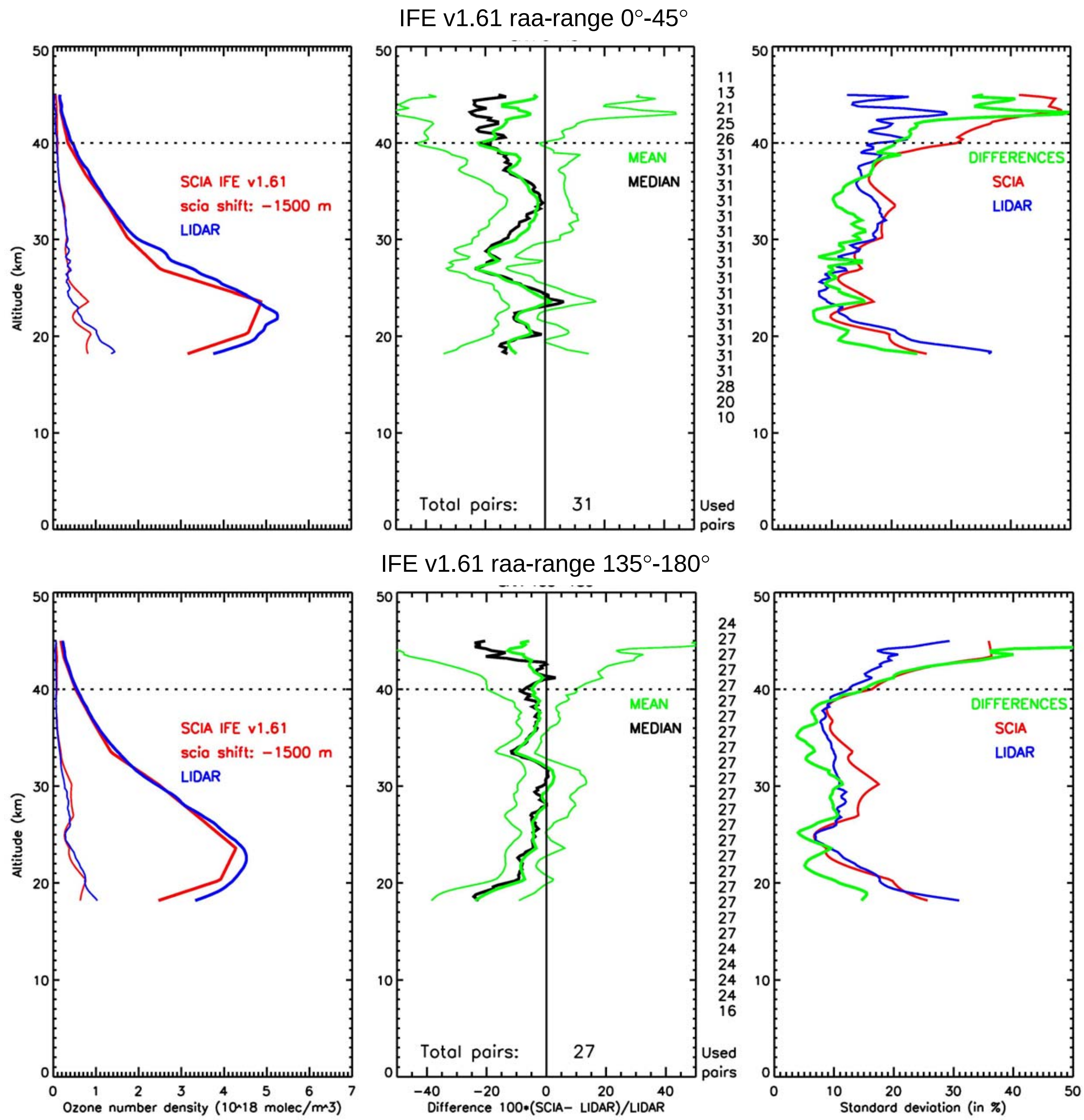


Figure 13: Analysis of the IFE version 1.61 product for the subsets relative azimuth angle range 0°-45° (top) and relative azimuth angle range 135°-180° (bottom). Panels as in Figure 4. Ozone concentrations are significantly underestimated.

6. Discussion and conclusions

All SCIAMACHY limb ozone profile products that have become available for validation in the period November 2004 – December 2005 have been validated with high quality lidar data covering a wide range of latitudes. Intermediate ESA products have been pre-validated and the results have been considered in the development of the new version of the ESA product. Most products have been compared with unconvolved lidar data in stead of convolved lidar data since the accompanying averaging kernel matrices and *a priori* profiles were not supplied. Though comparisons with convolved lidar data are to be preferred above comparisons with unconvolved lidar data discrepancies between the retrieved ozone profile and the unconvolved lidar profile should be small for good ozone profile retrieval.

Validation results for the ESA version 2.5 product are consistent with the validation results for this product with SAGE[4] II and microwave radiometer data. The results of the comparison for the IFE version 1.61 product differ slightly from the results of the comparison for this product with SAGE II and SAGE III data. This might well be explained by the difference in distribution over the different solar zenith angles for the collocated SAGE II and the collocated lidar data. Both the comparison with lidar data as the comparison with SAGE II data show a solar zenith angle dependence for the IFE version 1.61 product. The sharp bends present in the retrieved ozone profiles of the IFE version 1.61 product are not explained by the shape of the averaging kernel matrices as the convolved SAGE II and SAGE III ozone profiles do not demonstrate these sharp bends (Brinksma et al., 2006).

An azimuthal dependence of the tangent height offset has been observed in the SCIAMACHY limb ozone profile data for the products that retrieve different ozone profiles for different profile state positions. This azimuthal dependence has already been observed in ENVISAT data other than SCIAMACHY data (Saavedra et al., 2005) but it is the first time it has been seen in SCIAMACHY ozone profile data (Von Savigny and Lolkema, 2006).

Best SCIAMACHY limb ozone profile product up to now is the IFE version 1.62 product. It is the first product that retrieves the shape of the ozone profile quite well. The errors in ozone concentration are of -8% to 5% in the altitude range 18-40 km. This is significantly larger than those of ozone profiles of other satellite measurements, for example from GOMOS, another ENVISAT instrument. Main problem in retrieving SCIAMACHY limb ozone profiles is the imprecise knowledge of the attitude of the ENVISAT platform. Up to now, an effective solution has not been found. Both IFE and DLR on behalf of ESA are still working on the improvement of their ozone profile retrievals from SCIAMACHY limb measurements. Both institutes try to correct for the tangent height errors resulting from the ENVISAT

[4] Stratospheric Aerosol and Gas Experiment

attitude problem, but errors in the retrieved ozone concentrations can only become small when the attitude problem itself will be solved.

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