POLE-TO-POLE VALIDATION OF SCIAMACHY OZONE PROFILES BY THE ENVISAT QUALITY ASSESSMENT WITH LIDAR (EQUAL) PROJECT

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ABSTRACT

The ENVISAT Quality Assessment with Lidar (EQUAL) project supports the long-term validation of ENVISAT's three atmospheric chemistry instruments. This ESA funded project started in 2004 and involves eleven, and since 2006 thirteen, lidar stations around the world measuring ozone and temperature profiles. Over the period 2002–2006 more than 4500 lidar profiles are available for correlative studies. The assessment here not only focuses on comparisons with lidar but it is extended with correlative data from ozonesondes and microwave radiometers. SCIAMACHY ozone profiles are assessed of ESA's offline processor with version IPF 3.00 and the scientific retrieval of IFE version 1.63. Applied collocation criteria, for the comparison between the two observations, were 500 km and 20 hours for the maximum allowed spatial and temporal difference, respectively. The validation results show a reasonable agreement of SCIAMACHY with correlative observations. In the altitude range 18–38 km the bias is negative and varies in magnitude from 5–20%. The precision is estimated to be smaller than about 10–15%. At 40-km altitude the bias peaks and is 25% negative. The bias in the Polar Regions is larger, and in all regions the ozone values at and below the ozone peak are underestimated by about 10–20%. SCIAMACHY data rely on a correct derivation of the tangent altitude which depend on accurate attitude information. We have estimated that there is still an altitude shift present in the data. Based on correlation with lidar and sonde data, we derive that SCIAMACHY ozone profiles require an average global altitude shift of about –800 m.

1 INTRODUCTION

In March 2002 the European Space Agency (ESA) launched the Environmental Satellite (ENVISAT) with on board three instruments measuring the Earth's atmosphere. Making use of a variety of measurement techniques, these three instruments should significantly enrich the number of detectable species and their vertical distribution. The Global Ozone Monitoring by Occultation of Stars (GOMOS) instrument is a medium-resolution star-occultation spectrometer operating in the ultraviolet–visible–near-infrared (UV-VIS-NIR) spectral range. The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) instrument is a Fourier transform spectrometer detecting the Earth's limb emission in the mid infrared. The Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY) instrument is an UV-VIS-NIR spectrometer allowing observations in nadir, limb-emission and solar-occultation mode.

An initial geophysical validation campaign has been carried out during the Commissioning Phase of the mission (covering originally the first six months after launch, later extended to a total of 9 months). The preliminary validation results of this campaign were presented during the ENVISAT validation workshop from 9–12 December 2002 in Frascati, Italy [1]. Validation results of a newer algorithm (IPF 2.1) were presented during the second workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2) from 3–7 May 2004 in Frascati, Italy [2]. A more extended validation exercise has been performed

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Table 1. Overview and details of stations and instruments that were used in this paper as correlative data. The details also include the network affiliation and the principle investigator (PI) of the instrument.

Location	Latitude	Longitude	Instrument	Instrument PI-name	Institute
Eureka (C,E)	80.05	–86.42	Lidar	S. Pal	SAAI & MSC
Ny-Ålesund (P,E)	78.92	11.93	Lidar	P. von der Gathen	AWI
Ny-Ålesund (P)	78.92	11.93	Microwave	K. Kunzi	IUP-Uni. Bremen
Ny-Ålesund (P)	78.92	11.93	Sonde	P. von der Gathen	AWI
Alomar (C,E)	69.30	16.00	Lidar	G. Hansen	NILU
Kiruna (C)	67.84	20.41	Microwave	U. Raffalski	IRF
Sodankylä (C,W)	67.37	26.63	Sonde	E. Kyrö	FMI
Jokioinen (W)	60.81	23.50	Sonde	E. Kyrö	FMI
Bremen	53.10	8.90	Microwave	J. Notholt	IUP-Uni. Bremen
Legionowo (C)	52.40	20.97	Sonde	B. Kois	IMWM
De Bilt (C,W)	52.10	5.18	Sonde	M. Allaart	KNMI
Uccle (C,W)	50.80	4.35	Sonde	D. De Muer	RMIB
Hohenpeissenberg (C,W,E)	47.80	11.02	Lidar	H. Claude	DWD
Hohenpeissenberg (C,W)	47.80	11.02	Sonde (BM)	H. Claude	DWD
Payerne (C,W)	46.82	6.95	Sonde	R. Stubi	MeteoSwiss
Payerne (C)	46.49	6.57	Microwave	N. Kaempfer	MeteoSwiss
Obs. Haute Provence (P,E)	43.94	5.71	Lidar	S. Godin-Beekmann	CNRS
Tsukuba (C,E)	36.05	140.13	Lidar	H. Nakane	NIES
Table Mountain (C,E)	34.40	–117.70	Lidar	I. S. McDermid	JPL
Mauna Loa (P,E)	19.54	–155.58	Lidar	I. S. McDermid	JPL
Mauna Loa (P)	19.54	–155.58	Microwave	A. Parrish	UMass & NIWA
Paramaribo (C,W,S)	5.75	–55.20	Sonde	M. Allaart	KNMI
La Reunion (C,E)	–20.8	55.50	Lidar	J.-L. Baray	RIVM & NIWA
Lauder (P,E)	–45.04	169.68	Lidar	D. Swart	RIVM & NIWA
Lauder (P)	–45.04	169.68	Microwave	A. Parrish	UMass & NIWA
Lauder (P)	–45.04	169.68	Sonde	G. Bodeker	NIWA
Rio Gallegos (C*,E)	–51.60	–69.30	Lidar	E. Quel	CEILAP

(P): NDACC primary station (Network for the Detection of Atmospheric Composition Change)
(C): NDACC complementary station, *station is candidate for this status
(E): lidar station is part of the EQUAL project
(W): WOUDC station (World Ozone and Ultraviolet Radiation Data Center)
(S): SHADOZ station (Southern Hemisphere Additional Ozonesondes)
(BM): Brewer/Mast ozonesonde type

on SCIAMACHY ozone profiles using ozonesondes, lidar and microwave instruments which involved SCIAMACHY data of ESA's IPF version 2.5 and scientific data of IFE version 1.6 [3, 4]. Later the ESA algorithm was furthermore refined after an analysis of different processing algorithms settings [4]. The resulting processor version (IPF 2.8) was then extended to include a correction for the tangent height offset, which changed its version number to 3.00. The data of this new processor are presented in this paper.

Geophysical validation activities now rely on projects that are part of the long-term validation program of ENVISAT. The ENVISAT Quality Assessment with Lidar (EQUAL) project is part of this program and is described in section 2. In section 3 details about the satellite and the correlative observations are provided. In section 4 the analysis approach and results are presented of the comparison with lidar, balloon-sonde, and microwave radiometer data. In section 5 a methodology and results are presented for estimating a possible remaining altitude shift. In section 6 we present the conclusions.

2 EQUAL PROJECT

The ENVISAT Quality Assessment with Lidar (EQUAL) project supports the long-term validation of ENVISAT's three atmospheric chemistry instruments. This ESA-funded project started in 2004 and involves eleven, and since 2006 thirteen, lidar stations around the world measuring ozone and temperature profiles. The participating stations are (from north to south) located in Eureka, Ny Ålesund, Alomar, Esrange, Hohen-peissenberg, Observatoire Haute Provence (OHP), Tsukuba, Table Mountain, Mauna Loa, La Reunion, and Lauder. In 2006 two additional lidar stations, located in Rio Gallegos (Southern Argentina) and Dumont d'Urville (Antarctic), joined the consortium (see Tab. 1 and Fig. 1). Over the period 2002–2006 in total over 4500 lidar data files have been submitted and are available in the ENVISAT Cal/Val database at NILU.

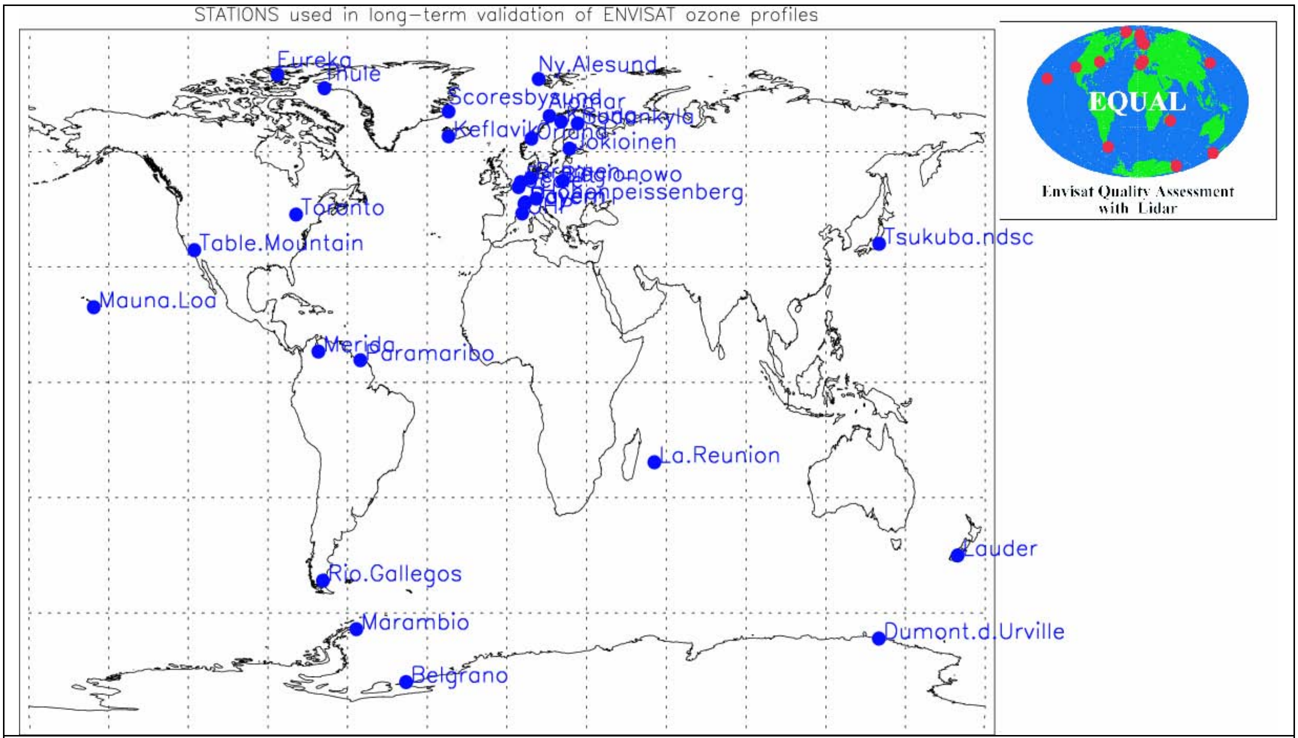

Figure 1. Geolocation of lidar, sonde and microwave stations used in the analyses of SCIAMACHY ozone profiles. Lidar stations are part of the ENVISAT Quality Assessment with Lidar (EQUAL) project (logo is shown on the right).

Besides the required coordination of the data acquisition, this project involves dedicated validation activities to assess the data quality. The data under investigation are the ozone and temperature profiles of GOMOS, MIPAS and SCIAMACHY. The main focus will be on the quality of the operational ESA products, in which the data quality is monitored during the satellite's lifetime (health of instruments and processing chain), and new data releases (processor upgrades) are validated. The focus might sometimes also change toward products of scientific institutes exploring retrieval algorithms of (potential) future operational products. The vast amount of lidar data covering several latitudinal regions allows the analysis for possible dependencies of these data on several geophysical (e.g., latitude) and observational (e.g., solar position) parameters. In this paper the analysis results will be presented of SCIAMACHY ozone profiles.

3 SCIAMACHY AND CORRELATIVE DATA

3.1 SCIAMACHY Measurements

3.1.1 SCIAMACHY Data Availability

SCIAMACHY performs observations in nadir- and limb-viewing, and solar/lunar occultation-viewing mode employing an UV-VIS-NIR spectrometer. Its retrieved ozone profiles are in the altitude range (typically) 15–50 km with 3–4 km vertical resolution. Some scientific retrievals indicate that there is also mesospheric ozone profile information in the data. The retrieval of pressure and temperature profiles was originally foreseen by using the spectral observations of the NIR-channels, but this retrieval is obstructed by ice built up which corrupts the retrieval. Since the start of the SCIAMACHY measurements in 07–2002, there have been no major interruptions of its operations.

Data from the operational processor (IPF) using version 2.5 are available since 11–2004 until 07–2006, compromising about 7,000 orbit files (70 GB). Since then the new version (3.00) took over the processing. For validation purposes this processor has also been used to process the, so-called, validation reference set. This set comprises a sub-selection of the SCIAMACHY measurements which all have collocated correlative measurements connected to them and is generated for (preliminary) validation studies. The data used in this paper come from this new operational version IPF 3.00.

In addition to the ESA processed data, we have also analyzed the data processed by the Institute of Remote Sensing (IFE) at the University of Bremen, Germany. The algorithm used to process the validation reference set, and used in this paper, has version 1.63.

3.1.2 SCIAMACHY Limb Pointing

The retrieval of ozone profiles from limb-viewing measurements is highly dependent on an accurate knowledge of ENVISAT's attitude. This information is required to derive the tangent altitude of the retrieved profile. Since its launch there have been problems to get the accuracy and precision of the attitude to within acceptable ranges for limb measurements. For the limb data products this has been the major source of error. In contrast to SCIAMACHY, the limb measurements of MIPAS can rely on the retrieved pressure as the vertical coordinate. In the latest processor version, that generates the level-1 (spectral) data, a fixed altitude offset is introduced of –1000 m and an attitude correction scheme. These level-1 data were the basis for both the IPF 3.00 and IFE 1.63 retrieved ozone profile retrievals.

3.2 Stratospheric Ozone Lidar Measurements

Stratospheric ozone lidar systems measure the atmosphere between about 15- and 50-km altitude. These measurements are performed between 1 and 3 times per week, which is dependent on weather and atmospheric conditions. Lidar systems are usually operated at night under clear-sky conditions, but some lidars have been adapted for daytime use in Polar Regions. Stratospheric ozone lidar instruments use a special lidar system, which is called a Differential Absorption Lidar (DIAL) system [5, 6]. These systems simultaneously emit two light pulses at different wavelengths with different ozone absorption cross sections. The differences in light intensity backscattered from different altitudes can be directly related to the local ozone concentrations. Data are provided as ozone number densities as a function of geometric altitude and hence no conversion is necessary.

3.3 Additional Ozone Measurements

In addition to the lidar measurements coming from the EQUAL project, we have incorporated additional ozone measurements which are available in the ENVISAT Cal/Val database. These data (mainly) come from a similar project as EQUAL which is called Technical Assistance to ENVISAT (TASTE) validation. This project is run by BIRA in Brussels, Belgium. Ozone profile data come from measurements using balloon-borne sondes and ground-based microwave radiometers, see Tab.1 and Fig. 1 for their details and locations.

3.3.1 Balloon-borne Ozonesondes

The lower part of the atmosphere, between ground and 30-km altitude, is sampled by Electrochemical Concentration Cell (ECC) ozonesondes based on small balloons. These soundings are performed between 1 and 3 times per week as part of routine and special (validation) campaign observations. In the ECC sondes, air is pumped through a chemical cell containing an aqueous solution of potassium iodide [7, 8]. The chemical reaction with ozone results in molecular iodine that can be detected and directly related to the ozone abundance in the outside air. Data are therefore provided as partial ozone pressure as a function of air pressure. The use of the ideal gas law and the assumption of hydrostatic equilibrium, which requires the additionally measured pressure and temperature information, yield the conversion to the common units for comparison. Some of the ozonesonde data used in this study were measured by a Brewer-Mast sonde, which mainly differs from the ECC sonde in the concentrations of the electrolyte and the design of the cell.

3.3.2 Microwave Radiometer Ozone Measurements

Ozone in the stratosphere and mesosphere can be measured with microwave radiometers. These measurements are performed almost continuously during both daytime and nighttime and are largely unaffected by clouds. These systems detect the microwave emissions of atmospheric ozone using a millimeter wave receiver and multi-channel spectrometer [9]. In the observed spectrum ozone lines and their pressure-broadened shape can be used to reveal altitude-resolved ozone information, which is based on the optimal estimation technique of Rodgers [10]. Data are provided as volume mixing ratios as a function of air pressure, and in addition these data come with averaging kernels and a priori information. The conversion to the common units is performed by assuming hydrostatic equilibrium and applying the ideal gas law, which requires the use of the provided pressure and temperature information.

4 QUALITY ASSESSMENT

4.1 Comparison Approach

For the ozone analysis results we have compared SCIAMACHY data measured within 500 km distance and within 20 hours of a correlative observation. These criteria result in 805 collocations. This data set will now be analyzed for its quality and further sub-divided in selections involving certain situations.

4.2 Ozone Profile Validation Results

The overall, global comparison results are shown in Fig. 2, showing in the left panel the average profiles and

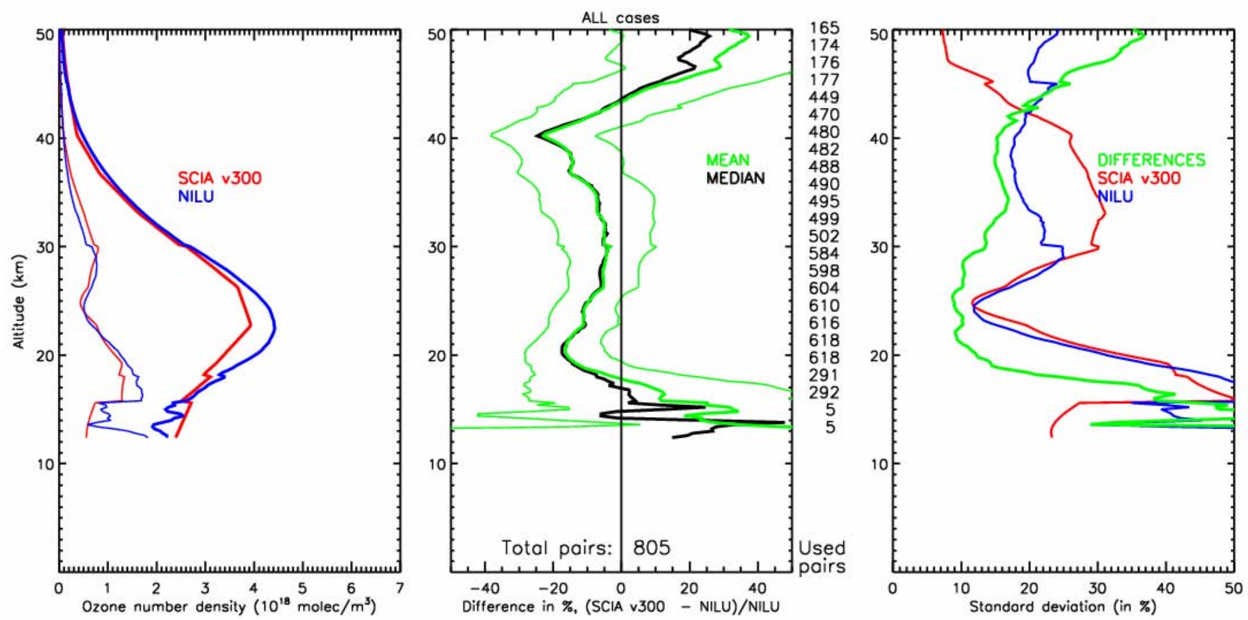

Figure 2. Intercomparison results of GOMOS and lidar, sonde and microwave ozone profiles (from the NILU database). Left panel shows the mean GOMOS (bold red line) and lidar (bold blue line) ozone profiles and their standard deviations (thin lines in corresponding colors). Middle panel shows the mean (green line) and median (black line) differences between all the paired GOMOS and NILU data as a percentage of the latter. For the mean profile, we also plotted the (1 σ) standard deviation of the differences (thin green line). Numbers at the right of the middle panel indicate, for some altitude levels, the number of pairs used at that level. Right panel shows a comparison of the standard deviation of the differences (green line) and the standard deviation of all GOMOS (red line) and NILU (blue line) ozone profiles.

their standard deviations, in the middle panel the average and median differences, and in the right panel a comparison of the standard deviations. If the median results deviate from the mean results then the distribution is skewed (i.e., not Gaussian), which is, for example, the case below about 18-km altitude.

4.3 Influence of Geolocation

SCIAMACHY data have been assessed for a possible dependency of the results on the global region in which the measurements were obtained. The paired data have been sub-divided in profiles measured in polar (66.5°–90°), mid-latitude (23.5°–66.5°) and tropical (0°–23.5°) regions, shown in Fig. 3 top, middle and bottom panel, respectively. Note that we have grouped the results obtained in either the Southern or Northern Hemisphere.

4.4 Influence of Solar Zenith Angle

SCIAMACHY data have been assessed for a possible dependency of the results on the solar zenith angle. The measurements have been sub-divided in profiles obtained from measurements in different SZA ranges (not shown). The results for these different selections show no clear dependency.

4.5 Influence of Correlative Instrument

In order to check the quality of the correlative instruments we have selected those collocations that only involve sonde, lidar and microwave data, and the results are presented in the left, middle and right top panels of Fig. 4, respectively.

4.6 Analysis Results of IFE 1.63 Ozone Profiles

The ozone profiles retrieved using the IFE version 1.63 algorithm were also analyzed (see bottom panels of Fig. 4). This algorithm retrieves four profiles per state, instead of one for IPF 3.00, resulting in more collocated measurement pairs.

5 ALTITUDE SHIFT ANALYSIS

5.1 Methodology

In order to avoid misinterpretation by visual inspection due to the presence of a bias [11], we have set up an analytical methodology based on correlation. In steps of 200 m we shift the SCIAMACHY profile in altitude ranging from –5 to +5 km. For each step the correlation

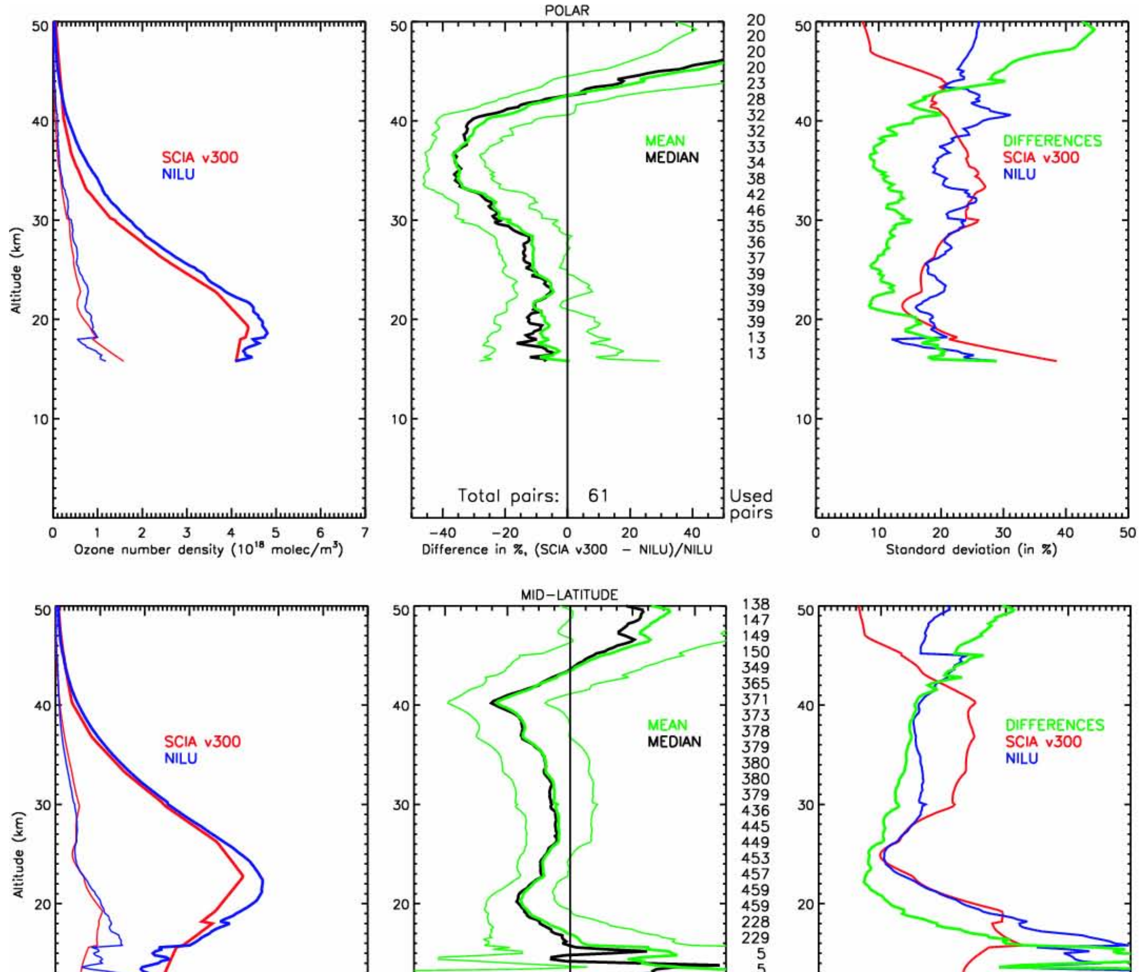

Figure 3. Same panel definitions as in Fig. 2. but now showing the results of the sub-selection of the paired data which were measured in the polar (top), the midlatitude (middle) and the tropical (bottom) regions.

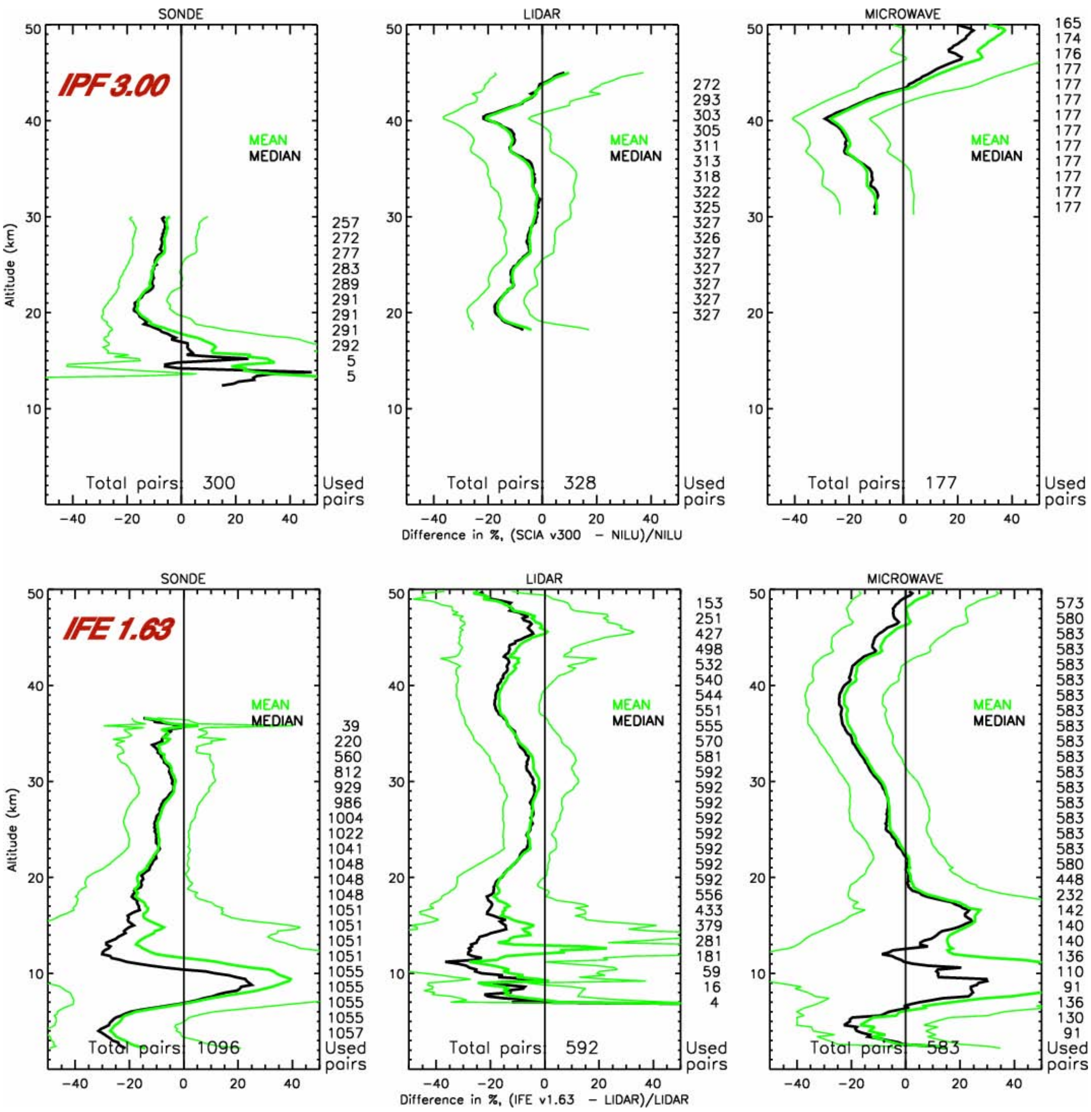

Figure 4. Same as middle panel of Fig. 2. but now only showing the results of one type of correlative instrument. Collocations of SCIAMACHY with (left) sonde, (middle) lidar and (right) microwave radiometer observations. Results are shown for the (top) ESA processing with IPF version 3.00 and (bottom) IFE processing with version 1.63.

km between the shifted SCIAMACHY and the correlative (lidar or sonde) ozone profile. Note that we have omitted the microwave data for its coarse vertical resolution. The altitude range for the calculation has been limited at the top because of the 40-km reference height in the IPF 3.00 retrieval and at the bottom because the SCIAMACHY profile rapidly deteriorates in quality. The optimal altitude shift has been defined as the shift which demonstrates the highest correlation coefficient of all shifts.

5.2 Optimal Altitude Shift Results

Initially we have checked the method by calculating the optimal shift in comparison between lidar and sonde profiles with the *a priori* profiles that were used in the SCIAMACHY retrieval. The results of all optimal shifts as a function of latitude are shown in the top panel of Fig. 5. As expected, this provides a mean optimal shift of about 0 km with a large scatter due to the natural variability which increases toward the poles. The optimal shifts for the correlation with retrieved profiles using IPF 3.00 and IFE 1.63 are shown in the middle and bottom panel of Fig. 5, respectively.

In analyses performed after the validation workshop we found a bug in the software. This bug included values in the derivation of the mean optimal shift that reached the shift boundaries (±5 km). Excluding these (corrupt) values result in a mean shift of about –800 m for both retrievals, instead of the previous reported value of about –1000 m during the ACVE-3.

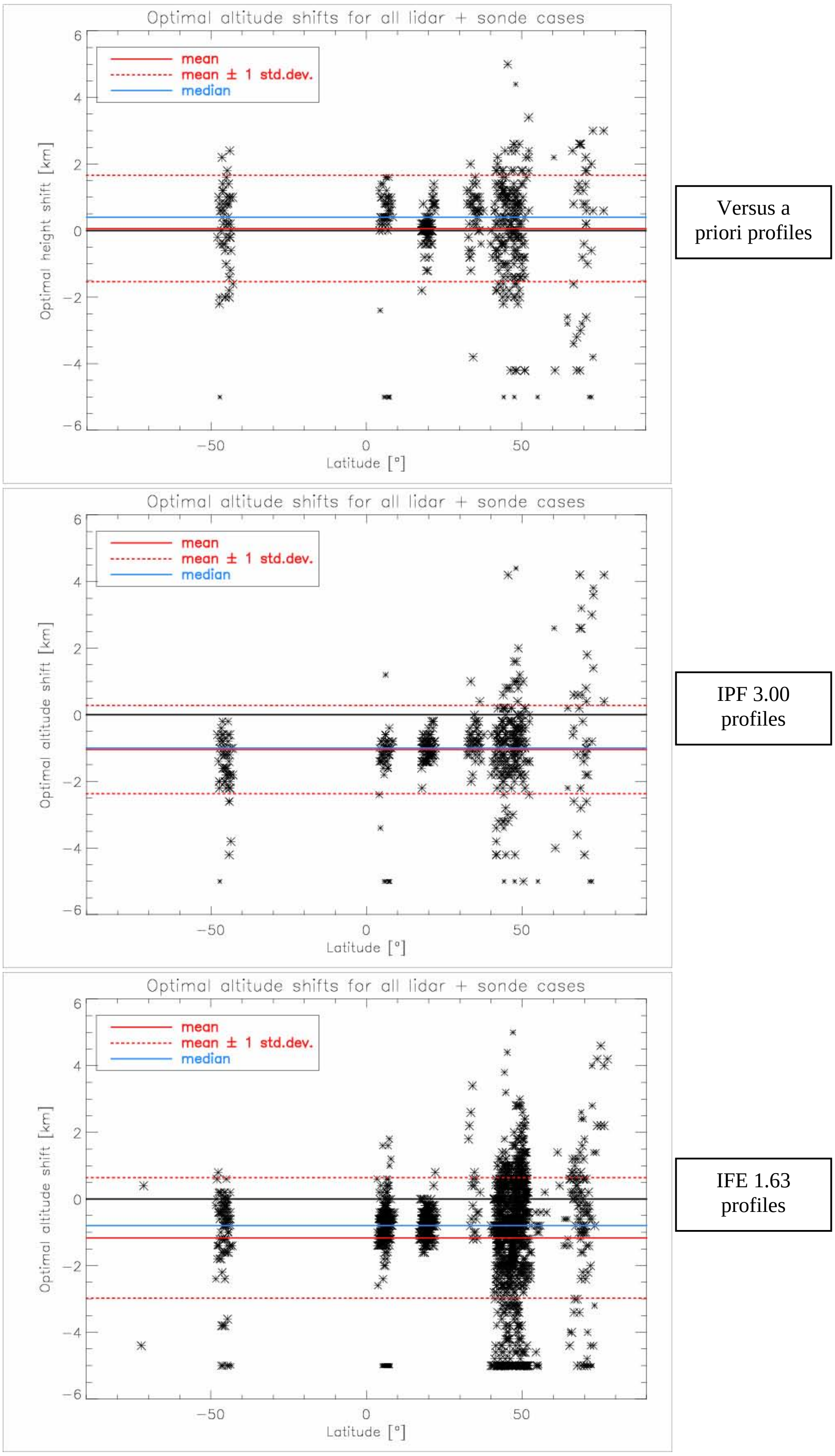

Figure 5. Optimal altitude shifts derived from correlation with lidar and sonde profiles of (top) a priori ozone profiles, and retrieved ozone profiles of (middle) of IPF version 3.00 and (bottom) IFE version 1.63. The mean (red line), mean ±1 standard deviation (red dotted lines) and median (blue line) of the optimal shifts are also shown.

6 CONCLUSIONS

SCIAMACHY ozone profiles from the validation reference data set (IPF version 3.00) show a reasonable agreement with lidar, sonde and microwave data. There is a negative bias of 5–20% in the altitude range 18–38 km with the smaller values in the range 25–35 km. At 40-km altitude there is a 25% negative bias in the SCIAMACHY profiles. Comparisons in the altitude range 18–38 km show that the precision of SCIAMACHY is better than 10–15%.

In the Polar Regions the SCIAMACHY ozone profiles show a larger negative bias above the ozone peak. In general for all regions, the high ozone concentrations in the ozone peak and the profile just below the peak are underestimated by about 10–20%.

The validation results do not indicate a clear dependence of the derived bias on solar zenith angle and validation instrument. The data retrieved using the IFE 1.63 algorithm show similar validation results and are consistent with IPF 3.00.

In addition to the validation study, we have also estimated a possible remaining altitude offset in the SCIAMACHY profiles. Initially (presented during the meeting and shown in the Fig. 5) we derived a larger global average altitude shift, but this has been recalculated and now has a value of about 800 m upward. Hence a shift in the profiles is required of –800 m. This is in line with previous results [2, 3, 4] which assumed a shift of –1500 m but were based on level-1 data which were not corrected with a fixed –1000 m shift.

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