SCIAMACHY OZONE PROFILE VALIDATION

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ABSTRACT

A qualitative validation of SCIAMACHY ozone profiles retrieved using the off-line processor version 2.1 (DLR, April 2004, planned to become operational soon, hereafter OL2.1) is presented. The data are limited to the validation reference set (about 2000 states between July 2002 and December 2002) which is subject to altitude errors of up to about 3 km due to an ENVISAT pointing problem in 2002. In addition, ozone profiles retrieved using the non-operational Institute of Environmental Physics algorithm version 1.6 (von Savigny et al. 2004) (hereafter IFE1.6) were qualitatively validated. In addition to data in the second half of 2002, also data from March and August of 2003 are used. Comparisons have been performed for a selected set of SCIAMACHY profiles (both OL2.1 and IFE1.6) with ground-based and satellite data. SCIAMACHY ozone profiles agree to within about 10% to ground-based, and to within about 20% to satellite data. However, these good results are not consistent on a day-to-day basis, the rms values on the average differences are quite large (10-40%). Also, results vary from location to location. All comparisons are based on a small number of coincidences which also contain various problems that make drawing a quantitative conclusion difficult. A more thorough validation effort should be made after pointing corrections have taken place, or should be based on data from late 2003 onwards, that are not subject to large pointing errors. In addition, it should be repeated over a much larger timespan with a denser set of SCIAMACHY ozone profiles.

1. INTRODUCTION

SCIAMACHY is a limb and nadir mode viewing satellite instrument that measures the Earth reflectance between 240 and 2380 nm. In the limb mode, horizontal scans at about -3 to 92 km are made, with 3.3 km vertical intervals. From these scans, ozone profiles are retrieved. The DLR SCIAMACHY off-line ozone profile v2.1 algorithm (OL2.1) uses an optimal estimation code, with a fit window exclusively in the ultraviolet (319-333 nm). The IFE-Bremen SCIAMACHY ozone profile v1.6 algorithm (IFE1.6) (von Savigny et al. 2004) retrieves ozone profiles from Level 0, using 3 wavelengths of the Chappuis band and non-linear iterative optimal estimation with radiative transfer model SCIARAYS (Kaiser 2001). The retrieval works from about 15 km (or cloud top altitude, whichever is larger) to about 40 km. Above 45 km the SCIAMACHY signal is too low for the retrieval, and the SCIAMACHY profile will show only a-priori values.

2. DATA SETS

SCIAMACHY data sets: Selection of 383 limb states ("validation reference set") from July 18, 2002 through December 16, 2002 (OL2.1) and selection of limb states based on SCIAMACHY level 0 availability (average of 10 orbits per day) for July-December 2002 dates (IFE 1.6). Within the SCIAMACHY data, no implicit corrections for the altitude shifts due to ENVISAT pointing inaccuracies were made. Within this paper, provisional corrections will be made by shifting all profiles at a given location by a certain altitude (location-dependent, determined

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from initial comparisons with ground data).

Other SCIAMACHY ozone profile data that exist but were not validated within this paper are nadir profiles (R. van der A, KNMI), which currently are not useful due to the status of the radiometric calibration, differential slant column profiles (T. Wagner, Univ. Heidelberg), which are in an experimental status, mesospheric ozone profiles retrieved with an adapted version of the IFE Bremen stratospheric profile algorithm (Rohen et al. 2004a) and preliminary validated (Rohen et al. 2004b), and solar and lunar occultation profiles (coverage limited to 50-70° N, solar, and 30-90° S, lunar) retrieved by IFE Bremen. The ozone profiles from solar occultation are shown to be biased by about +10% with respect to SAGE II in the 15-35 km region (Amekudzi et al. 2004).

OL2.1 data were compared with satellite data, namely HALOE v19, SAGE II v6.2, SBUV/2, with groundbased data, namely lidar, microwave, and FTIR data, and with data from ozone sondes.

IFE1.6 data were compared with HALOE version 19 and SAGE III satellite data, with an airborne lidar, ozone sondes, and with ground-based lidar and microwave data. In addition, a substantial amount of comparisons of the IFE1.6 retrievals are being performed with BreRAM (the Bremen microwave radiometer), a RAM (also MW) in Spitzbergen, with the Bremen FTS, and the aircraft-borne ASUR (MW), but unfortunately time was too short to include all these results in this paper.

3. VALIDATION WITH LIDAR AND OZONE SONDES

OL2.1 data were compared to collocated (within 1000 km from any of the state corners, and within 18 hours) lidar and sonde data. Collocations for one lidar or sonde profile are always with four SCIAMACHY profiles, namely those within the same state. In principle, all data for these instruments in the ENVISAT-NILU correlative database were read. However, in some cases automatic reading did not always succeed, and averaging was not possible. Data for these locations were therefore inspected by eye, but not averaged, and are not shown here. Table 1 shows the results of these comparisons. Fig. 1 shows an illustration for De Bilt sondes, Fig. 7 for the lidar and sondes in Lauder, and Fig. 8 for the lidar in Mauna Loa. The shifts mentioned were applied to all OL2.1 data, the size of the shifts was judged by eye to yield the best average comparisons.

IFE1.6 ozone profiles were compared to collocated (within 1000 km from any of the state corners, and within 18 hours) lidar and sonde data. Table 2 shows the results of these comparisons. Fig. 2 shows an illustration for De Bilt sondes, Fig. 3 for a Hohenpeissenberg sonde, Fig. 9 for the lidar in Lauder, and

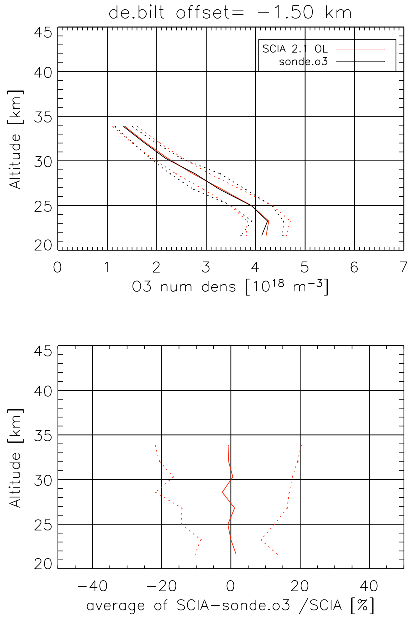

Figure 1. Comparisons between OL2.1 and De Bilt ozone sondes (13 coincidences). Top panel: Averaged ozone profiles. Bottom panel: Relative differences (SCIA-sonde)/SCIA in %. An altitude shift of -1.5km ('offset') is applied to the SCIAMACHY profiles.

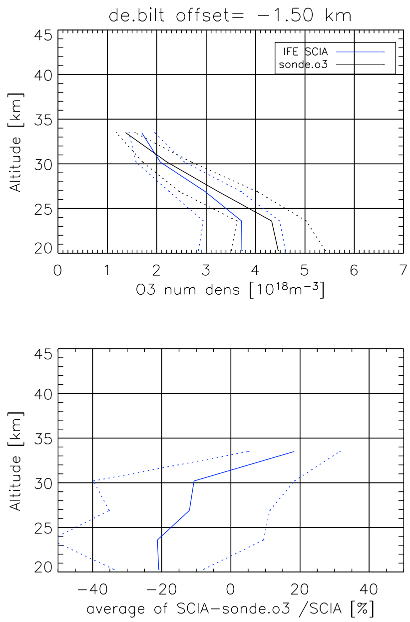

Figure 2. Comparisons between IFE1.6 and De Bilt ozone sondes (18 coincidences). Top panel: Averaged ozone profiles. Bottom panel: Relative differences (SCIA-sonde)/SCIA in %. An altitude shift of -1.5km ('offset') is applied to the SCIAMACHY profiles.

Table 1. OL2.1 compared with lidar and ozone sondes. The average difference ('av.diff.') is taken over the altitude range (sondes up to burst altitude) and over all coincidences.

Location	av.diff (StDev)[%]						Nr./4	shift
	20-40 km		20-30 km		30-40 km			[km]
Lidars								
Hohenp.	4	(30)	-1	(16)	8	(42)	24	-1.5
Table Mtn	4	(6)	0	(4)	8	(7)	5	0.0
Mauna Loa	4	(2)	1	(2)	7	(3)	3	0.5
Lauder	-10	(9)	-7	(8)	-13	(10)	13	-1.5
Sondes								
Uccle	0	(17)	0	(16)	0	(18)	29	-1.5
De Bilt	0	(16)	0	(14)	0	(20)	13	-1.5
Hohenp.	0	(15)	-1	(13)	1	(17)	21	-1.5
Payern	-2	(15)	0	(14)	-5	(17)	30	-1.5
Paramaribo	-27	11	-27	11	N/A		2	-4.0
Lauder	-3	(8)	-5	(7)	5	(12)	11	-1.5

Note: for lidars, averages 20 - 40 km
for sondes, averages 20 km - burst altitude

Table 2. IFE1.6 compared with lidar and ozone sondes. The average difference ('av.diff.') is taken over the altitude range (sondes up to burst altitude) and over all coincidences.

Location	av.diff (StDev)[%]						Nr.	shift
	20-40 km		20-30 km		30-40 km			[km]
Lidars								
Hohenp.	2	(30)	-8	(20)	10	(36)	32	-1.5
Table Mtn	0	(16)	-2	(20)	2	(11)	8	-1.0
Mauna Loa	-2	(9)	-6	(7)	2	(10)	4	-1.5
Lauder	-7	(11)	-4	(10)	-9	(11)	16	-1.5
Sondes								
Alomar	7	(12)	1	(13)	17	(10)	6	-1.5
Ny Ålesund	6	(9)	3	(9)	10	(11)	12	-1.5
De Bilt	-9	(22)	-18	(22)	4	(21)	18	-1.5
Hohenp.	1	(12)	-5	(14)	10	(10)	32	-1.5
Payern	-1	(15)	-5	(16)	5	(14)	46	-1.5
Paramaribo	-3	(7)	-3	(7)	N/A		3	-4.0
Lauder	-2	(10)	-4	(10)	N/A		15	-1.5

Note: for sondes, averages up to burst altitude

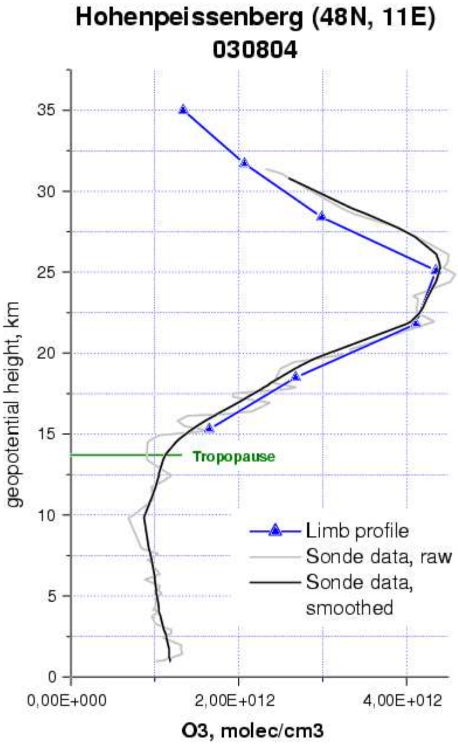

Figure 3. Comparison of IFE1.6 and sonde data over Hohenpeissenberg.

Fig. 10 for the lidar in Mauna Loa. The shifts mentioned were applied to all SCIAMACHY data at a given location, the size of the shifts was judged by eye to yield the best average comparisons. Especially for the De Bilt location, the shift should instead have varied on a day-to-day basis, and results presented for De Bilt are therefore quite arbitrary. Note that the differences in Tables 1 and 2 have been determined after the mentioned altitude shifts have been applied to the SCIAMACHY profiles. All results are individual comparisons - per state only one IFE1.6 ozone profile is retrieved.

Especially in the Paramaribo case (only 2 states of four almost identical SCIAMACHY profiles each) the OL2.1 results compare poorly with ozone sondes. Although it concerns only two (OL2.1) or three independent states, it is interesting to note that the IFE1.6 ozone profiles for these two dates (bottom panel of Fig. 4) compare much better to the same ozone sondes than their OL2.1 counterparts (Top panels of Fig. 4), which are clearly much lower in ozone.

4. VALIDATION WITH FTIR AT KIRUNA

Comparisons of OL2.1 with groundbased FTIR at Kiruna were made. The collocation criteria were within 500 km on the same day. 16 coincidences were found between July - Dec 2002. Average results are shown in Fig. 5.

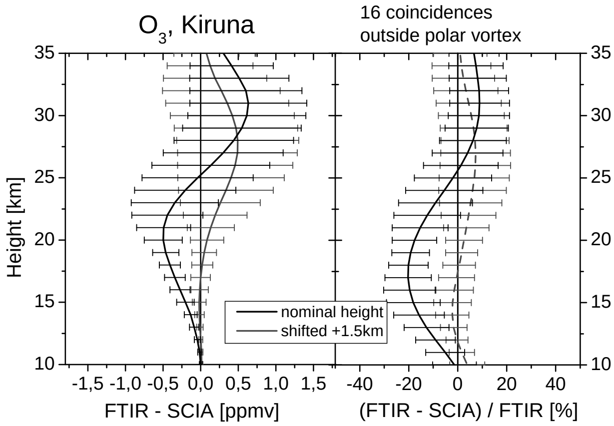

Figure 5. Relative differences averaged for all coincidences outside the polar vortex (16) of OL2.1 with the FTIR measurements at Kiruna (July - Dec 2002). Grey lines denote results if SCIAMACHY profiles were shifted upwards by 1.5 km, this significantly improves the results.

5. VALIDATION WITH MICROWAVE

At both Lauder and Mauna Loa, groundbased microwave instruments are operational within the Network for the Detection of Stratospheric Change (NDSC). In Fig. 6 we present a comparison between 17 SCIAMACHY OL2.1 profiles and microwave coincident profiles over Lauder.

In Figs. 7, to 10 we present coincidences with multiple correlative instruments (lidar, microwave, and for Lauder also ozone sondes), for both the OL2.1 and the IFE1.6 profiles.

Only very few SCIAMACHY measurements were collocated with multiple ground-based instruments, and in fact the Lauder location was the only one where coincidences with microwave, lidar, as well as ozone sondes were found for the OL2.1 validation reference set (3 coincidences).

Collocation criteria were that correlative measurements were within 24 hours, 2.5° latitude, and 12° longitude from the SCIA state. Plots are shown in mixing ratio as well as number density units. The latter were calculated by converting mixing ratios using temperature and pressure profiles from analyses. Straight interpolation was used to get all the data on the same grid when doing the intercomparisons. Evidently, the lidar and microwave profiles compare very well to OL2.1 over Mauna Loa. At this location, there is no altitude shift needed for the three coincidences presented. In contrast with the conclusion for the OL2.1 data, at Mauna Loa, results for IFE1.6 comparisons improve significantly when a 1.5

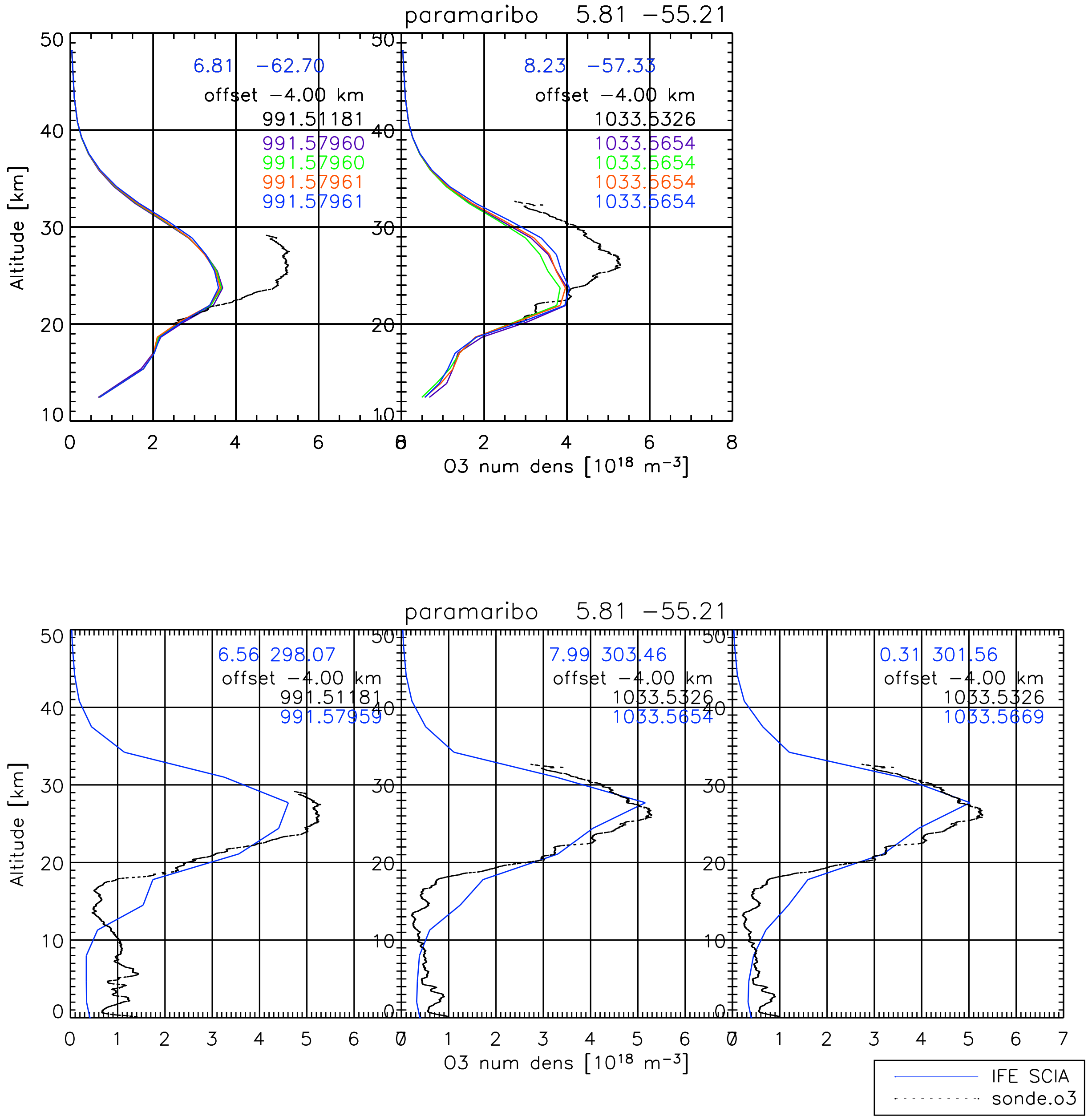

Figure 4. Top panel: Paramaribo OL2.1 data compared with ozone sondes. Four SCIAMACHY profiles (different colours) per state. Bottom panel: Paramaribo IFE1.6 data compared with ozone sondes. One SCIAMACHY profile (blue) per state.

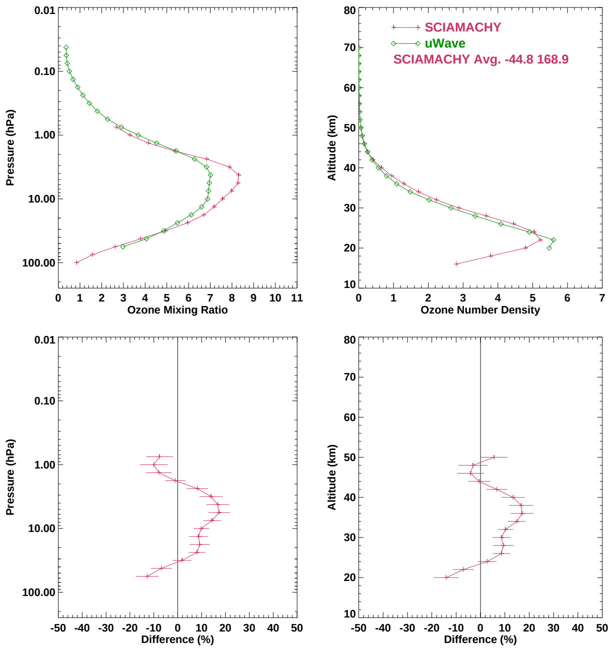

Figure 6. OL2.1 compared with microwave data over Lauder, New Zealand (45° S, 170° E). Average over 17 coincidences. Results are given in units of mixing ratio (left panels) and number density (right panels). Relative differences are (SCIAMACHY-microwave)/mean in %.

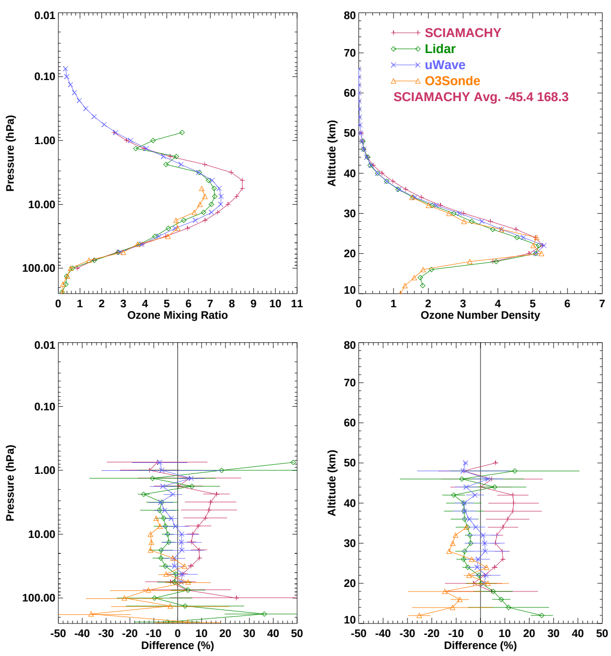

Figure 7. OL2.1 compared with microwave, lidar, and sonde data over Lauder. Average over 3 coincidences. Results are given in units of mixing ratio (left panels) and number density (right panels). Relative differences are (instrument-mean)/mean in %.

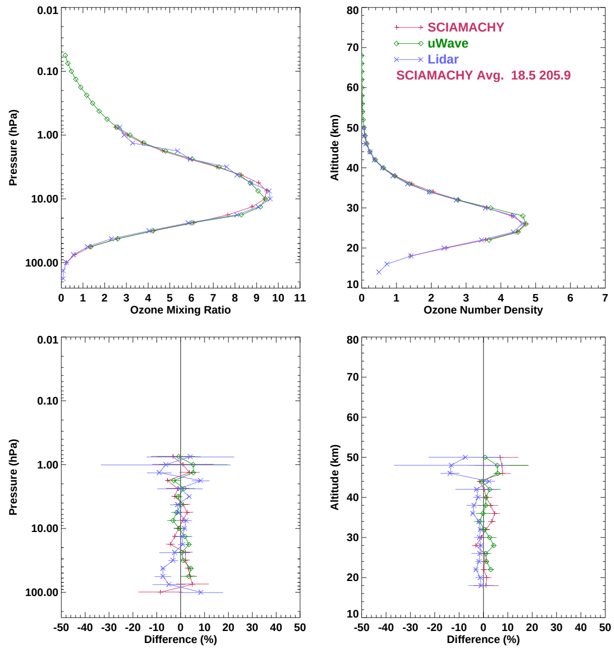

Figure 8. OL2.1 compared with microwave and lidar at Mauna Loa. Average over 3 coincidences. Results are given in units of mixing ratio (left panels) and number density (right panels). Relative differences are (instrument-mean)/mean in %.

km altitude shift is applied. This may be due to different subsetting, as many more coincidences were found with IFE than with OL data.

6. VALIDATION OF IFE1.6 WITH AIRBORNE LIDAR

During two field campaigns (in September 2002 and February/March 2003) the stratospheric ozone lidar experiment (OLEX) was deployed on board the DLR Falcon research aircraft with the goal to measure ozone profiles at various geophysical locations from low to high latitudes (4°S-79°N) at different seasons. Currently, 16 coincidences from 8 orbits ranging from 67°N to 4°S can be compared with IFE1.6. The results are shown in Fig. 11. For these profiles the coincidence with the respective SCIAMACHY limb scans was not worse than 6 h and 1000 km, respectively, and in general much better. The IFE1.6 profiles were shifted downwards by 1.5 km. Considering the possible uncertainty in the altitude retrieval of 3 km, all profiles agree within this margin.

7. VALIDATION WITH SAGE II AND HALOE

Comparisons of OL2.1 with SAGE II version 6.2 and HALOE version 19 were made. The collocation criteria were 1000 km, 12 hours in both cases.

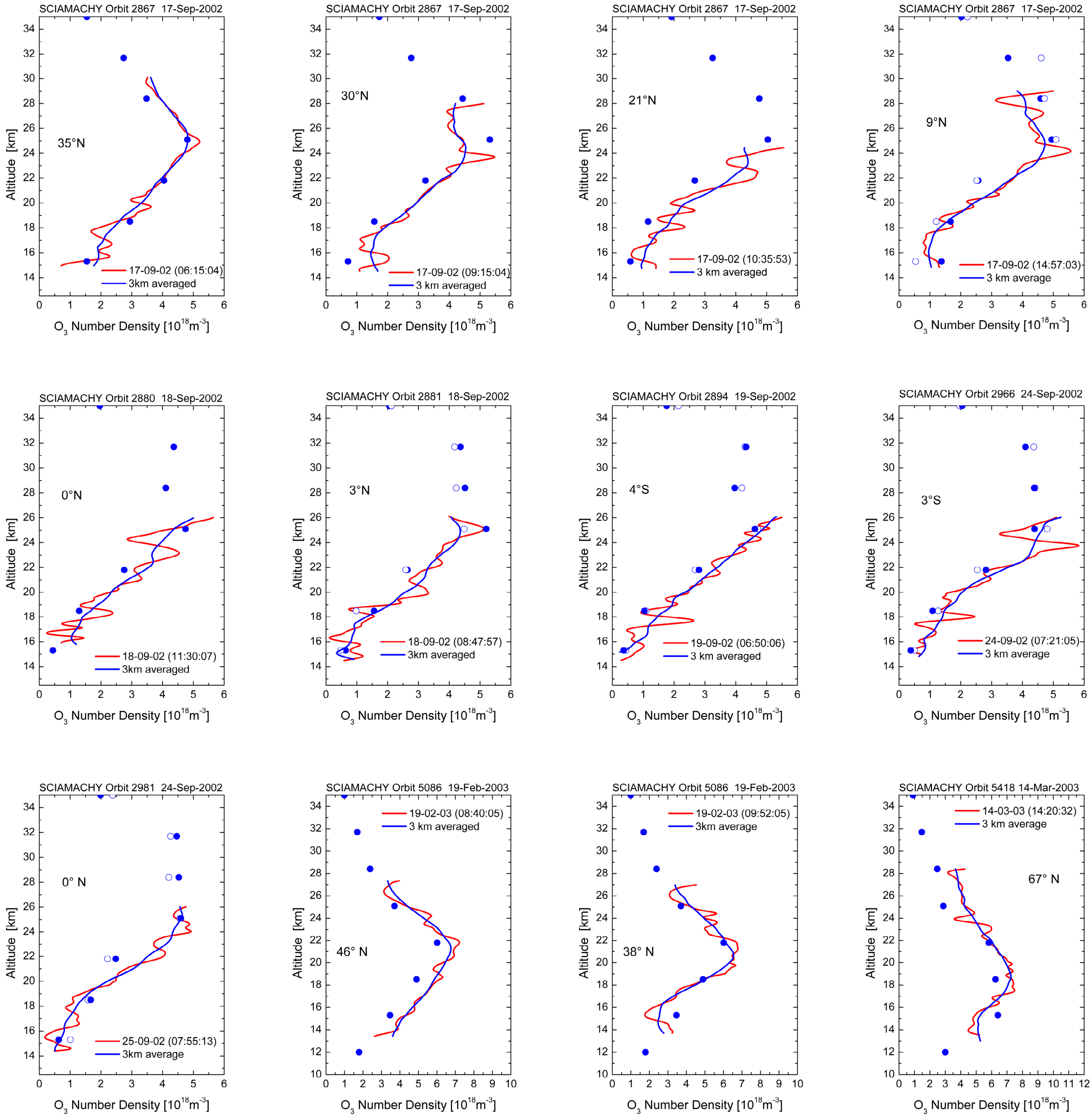

Figure 11. Comparison of IFE1.6 (blue circles) and OLEX lidar ozone profile (red lines) at various latitudes from the Tropics to the Arctic. The blue lines are the OLEX results averaged to give a similar resolution as the SCIAMACHY retrieval (3 km). In those cases where one OLEX profile can be compared with two adjacent limb scans the northerly and southerly state are depicted by closed and open cricles, respectively.

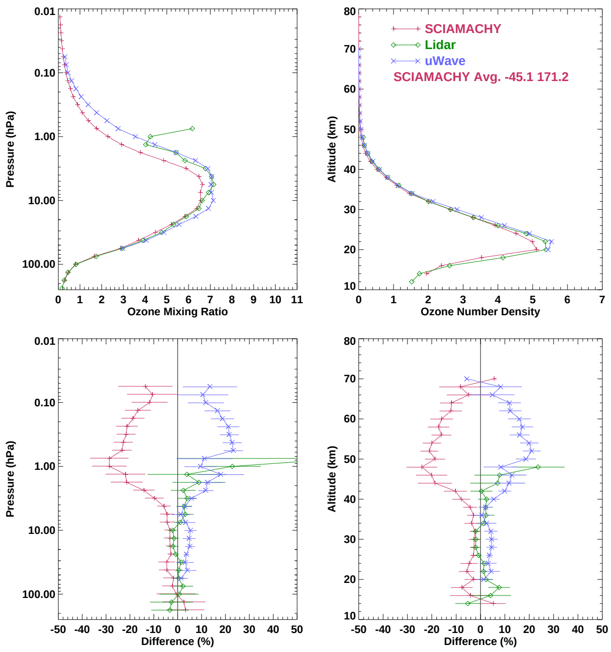

Figure 9. IFE1.6 compared with microwave and lidar at Lauder. Average over 12 coincidences. IFE1.6 data were shifted downward by 1.5 km. Results are given in units of mixing ratio (left panels) and number density (right panels). Relative differences are (instrument-mean)/mean in %. Note that no conclusions can be drawn above 45 km, because the SCIAMACHY signal above 45 km is too low for the retrieval to work, and the SCIAMACHY profile will show only a-priori values.

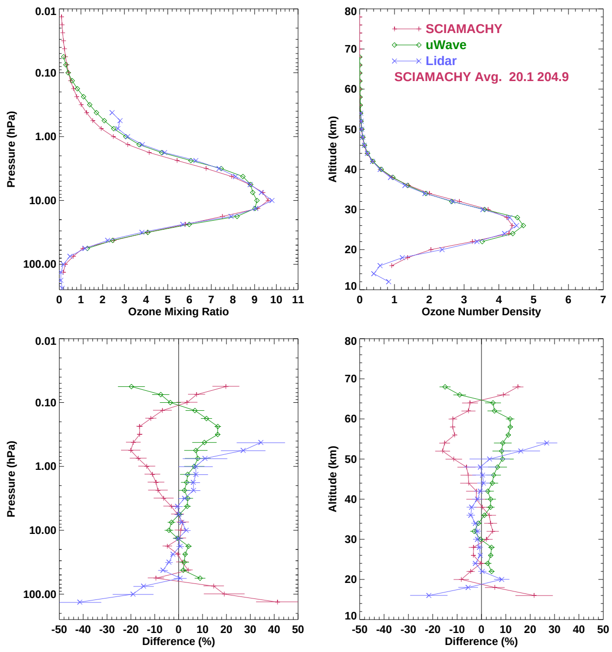

Figure 10. IFE1.6 compared with microwave and lidar at Mauna Loa. Average over 21 coincidences. IFE1.6 data were shifted downward by 1.5 km. Results are given in units of mixing ratio (left panels) and number density (right panels). Relative differences are (instrument-mean)/mean in %. Note that no conclusions can be drawn above 45 km, because the SCIAMACHY signal above 45 km is too low for the retrieval to work, and the SCIAMACHY profile will show only a-priori values..

Comparisons with HALOE: 51 collocations with validation reference set were found. Of these, 8 were within different air masses (judged by analysis with UKMO Potential Vorticity data at 475 K) and have been discarded. Geographically, the collocation distribution is highly biased towards NH high latitudes: Between 60°N and 90°N 24 collocations were found, between 30°N and 60°N there were 12, only 1 collocation was found in the tropics, and 5 on southern latitudes. The accuracy of HALOE version 19 profiles is 20% from 15–30 km, 6% from 30–60 km. Averaged results of the comparison in volume mixing ratio (vmr) between HALOE and OL2.1 are shown in Fig. 12. Comparisons with SAGE II: 56 collocations with validation reference set were found. Of these, 12 were within different air masses and have been discarded. Again, the geographic distribution of collocations is highly biased: between 60°N and 90°N 26 collocations were found, between 30°N and 60°N there were 11, 1 collocation was found in the tropics, and 5 on southern latitudes. The accuracy of SAGE II ozone profiles between 10 and 50 km is 10%. Averaged results of SAGE II-OL2.1 comparisons in vmr are shown in Fig. 13

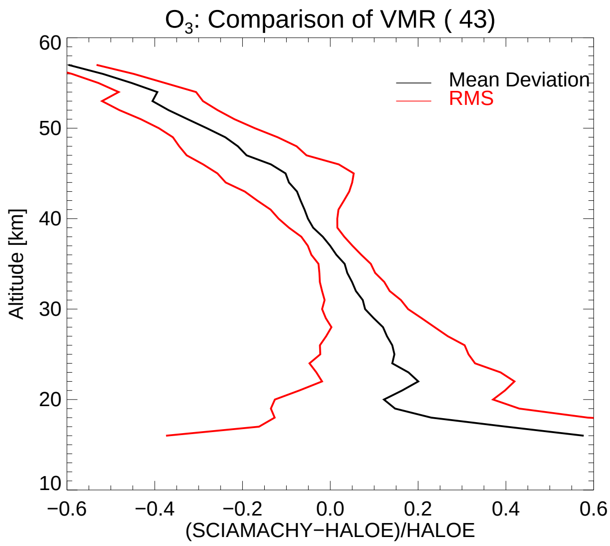

Figure 12. Average relative difference (black) and rms values (red) between OL2.1 and HALOE profiles.

Comparisons of OL2.1 to both HALOE and SAGE II profiles, are in many cases influenced by the altitude shifts due to ENVISAT pointing problems. OL2.1 profiles are reasonable between about 22 to 57 km, with a positive bias of up to 20% to HALOE and 15% to SAGE II and an rms of about 20%.

HALOE results were also compared with IFE1.6. The collocation criteria were 500 km and the same day. Note that the time span considered here was March 2003, in which the pointing problem is less than during the second half of 2002. The relative differences are shown in Fig. 14. IFE1.6 profiles are between about 20 to 41 km within 8 to 13% and an rms of about 10 to 20%.

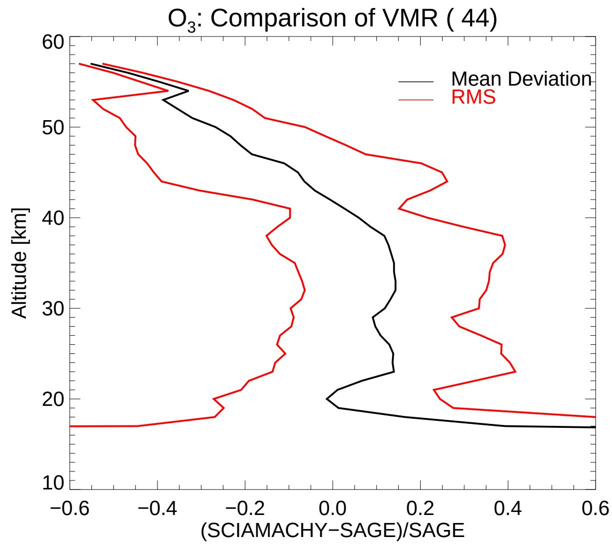

Figure 13. Average relative difference (black) and rms values (red) between OL2.1 and SAGE II profiles.

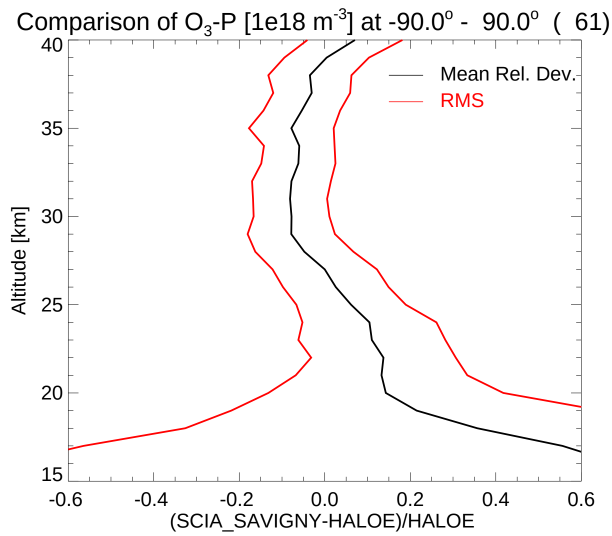

Figure 14. Average relative difference (black) and rms values (red) between IFE1.6 and HALOE profiles.

8. VALIDATION OF OL2.1 COMPARED WITH SBUV/2

SBUV/2 (flown on NOAA-16) ozone profiles were compared to OL2.1. The accuracy of SBUV/2 ozone profiles is expected to be up to 10%. Comparison results were averaged in 20° latitude bands, but do not appear to depend much on latitude. Results for two latitude bands in the Northern Hemisphere are shown in Fig. 15.

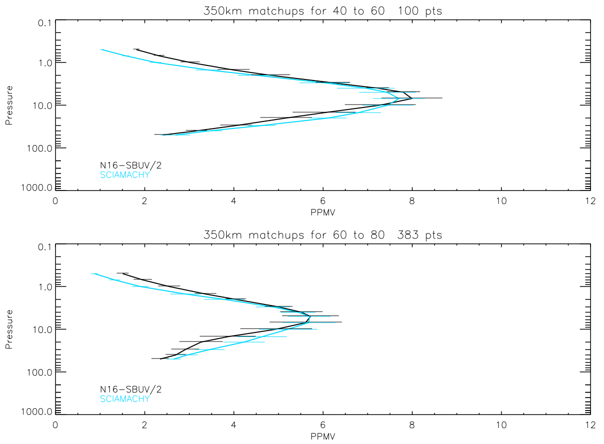

Figure 15. Average OL2.1 and SBUV/2 profiles in two Northern Hemisphere latitude bands.

9. VALIDATION OF IFE1.6 WITH SAGE III

SAGE III and IFE1.6 were compared, and averaged over northern and southern hemisphere. No altitude correction at all was performed. All measurements are before 2004. Collocation criteria were latitude within 3°, longitude within 10°, same day measurements.

The results have been averaged over all measurements in the Northern (Fig. 16) and Southern Hemisphere (Fig. 17).

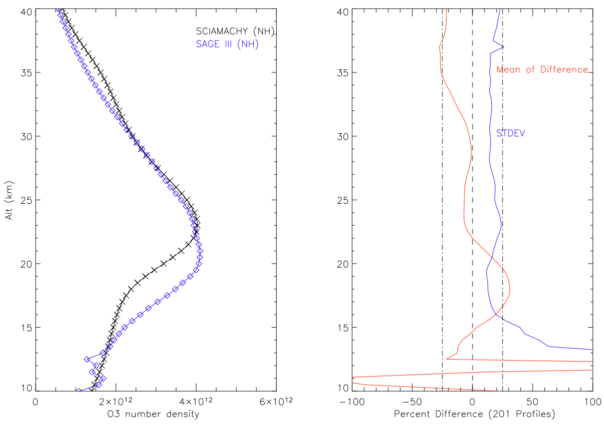

Figure 16. Average IFE1.6 and SAGE III profiles (left panel) and relative differences (right panel) for 201 Northern Hemisphere coincidences.

10. CONCLUSIONS

A qualitative first validation of the OL2.1 and IFE1.6 SCIAMACHY ozone profiles shows good results. Comparisons of a selected set of SCIAMACHY ozone profiles (both OL2.1 and IFE1.6) with groundbased and ozone sonde data show average differences between 20 and 40 km of 0-10%, depending on the location. Individual differences can be much larger (RMS values between 10 and 40%, depending on location). Comparisons with satellite data show a positive bias of 15% to 20% at 22 to 57 km for OL2.1 and an agreement within 10% (to HALOE) and 20% (to SAGE III) at 20 to 40 km for IFE1.6. All conclusions are preliminary at this stage, since due to the small data set, and the pointing problems that translate into altitude shifts that vary in time and with location, comparison results cannot be made consistent. Even if different subsetting of data (e.g., changes in collocation criteria) takes place, results vary significantly. This is not unexpected when rms values on the relative differences are high.

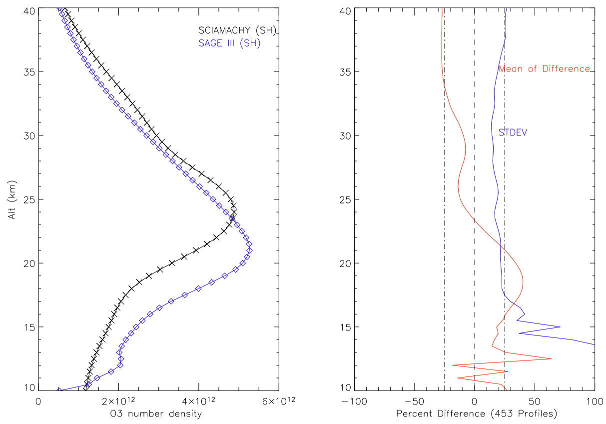

Figure 17. As Fig. 16, but for Southern Hemisphere (453 coincidences)

For future thorough validation, we will need a much larger dataset, and a dataset generated with accurate pointing, as otherwise the profiles cannot be really validated and not be used for quantitative scientific applications. For that validation effort, the climatologies used in the retrievals should also be validated. In addition, averaging kernels should be taken into account. Also the impact of the a priori on the retrieved profiles should be quantified. This applies to both the operational and the non-operational product.

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