VALIDATION OF SCIAMACHY SCIENTIFIC RETRIEVALS OF CO, CH_4, N_2O, AND NO_2 BY FTIR AT THE GROUND TRUTHING STATION ZUGSPITZE

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ABSTRACT

Solar FTIR measurements at the Permanent Ground Truthing Station Zugspitze (47 °N, 11 °E), Germany are used to validate ENVISAT/SCIAMACHY Scientific Data Products retrieved at the University of Bremen, i.e., the infrared WFM-DOAS ver. 0.4 total column products of CO, CH_4, N_2O, and the scientific DOAS NO_2 column product (ver. UB1.0). For WFM-DOAS, only relative changes due to the annual cycle are investigated, since these column retrievals include empirical scaling factors. To obtain a statistically significant fit to the CO annual cycle (≈10 % amplitude) out of the scatter of the SCIAMACHY WFM-DOAS data (available data cover Jan-Oct 2003), all pixels within a radius of at least 1000-2000 km around Zugspitze had to be averaged for each day. The weaker (2.5 % amplitude) annual cycles of CH_4 and N_2O could not be retrieved from SCIAMACHY data, even using averages of all pixels within a full latitudinal band of ±2000 km north/south relative to the Zugspitze around the globe. Validating one full year of UB1.0 NO_2 total column data (Jul 2003 – Jun 2003) a perfect agreement of the annual cycle to the ground FTIR data has been found, after removing obvious enhancements due to pollution episodes not captured by the high altitude (2964 m asl.) Zugspitze FTIR. After this correction, the SCIAMACHY UB1.0 columns of NO_2 are 16 % below the Zugspitze FTIR columns on average.

1 INTRODUCTION

The Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (SCIAMACHY) is a space borne UV/visible spectrometer onboard ENVISAT launched in 2002. In this paper we focus on the validation of scientific total column products for the species CO, CH_4, N_2O (WFM-DOAS, ver.0.4), [1,2]), and NO_2 (DOAS UB1.0, [3]) retrieved at the University of Bremen. These scientific products play a key role for the users community since there have still no operational products been established for CO, CH_4, and N_2O, and, for NO_2, there is an operational NRT product available, but this still shows significant problems in reproducing the actual annual cycle, as shown in our accompanying paper [4].

A first validation study has been performed for the WFM-DOAS (WFMD) CO retrievals by comparing with data of the MOPITT (Measurements Of Pollution In The Troposphere) satellite instrument. A highly consistent behavior relative to MOPITT had been found in the capability to detect highly elevated CO columns, e.g., a plume from biomass burning [1,2]. In this paper we want to promote the validation of CO (and CH_4, N_2O) by comparing the WFMD retrievals to the ground correlative solar FTIR data of the clean air site Zugspitze. The question to be addressed, therefore, is whether the WFMD retrievals can reflect the natural variability above the clean air site Zugspitze, which is dominated by the annual cycle for these species.

For the scientific NO_2 UB1.0 product a first validation study has been performed using the Bremen ground-based DOAS measurements network (BREDOM) showing a good overall consistency, with a low bias of unknown origin [3]. We add here a validation study with the ground-based solar FTIR technique since it is completely different from the (ground-based) DOAS retrieval technique in the UV/vis domain, thus helping to validate the satellite retrieval algorithm in a fully independent manner.

2 THE CORRELATIVE GROUND DATA SET FROM ZUGSPITZE SOLAR FTIR

Validation is performed using the correlative ground data that are being recorded by the NDSC Primary Status solar FTIR instrument at the Zugspitze (2964 m asl.) continuously. The Zugspitze FTIR instrument and retrieval set up has been described in detail elsewhere [5,6]. Briefly, a high-resolution Bruker IFS 120 HR Fourier Transform Spectrometer is operated with a actively controlled solar tracker, and liquid-nitrogen cooled MCT and InSb detectors. For the CO column retrievals (which are integrated profile retrievals in fact), the instrument is operated with a maximum optical path difference (OPD) of either 125 cm or 250 cm for the combined retrievals in 3 micro-windows, i.e., 2057.7850 - 2057.9100 cm^{-1}, 2069.6150 - 2069.7100 cm^{-1}, and 2157.3300 - 2159.1500 cm^{-1}. Methane retrievals are performed either in the 2835.550 - 2835.850 cm^{-1} micro-window using a 175-cm OPD, or in the 1201.800 - 1202.650 cm^{-1} micro-window using a 250-cm OPD. For the N_2O retrievals the 2439.200 - 2440.000cm^{-1} micro-window is used with an OPD of

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125 cm. For the NO_2 retrievals the 2914.51-2914.86 cm^{-1} micro-window is used with an OPD of 175 cm. The accuracies/precisions for total vertical column retrievals from ground-based high resolution solar absorption FTIR measurements are understood and well characterized. The actual numbers depend somewhat on changing geophysical parameters like the actual solar zenith angle. Typical numbers agreed upon within the NDSC infrared community for accuracies/precisions of single column retrievals are 7 %/4 % for CO [7,8], 6 %/2.5 % for N_2O [5,9], 5 %/3 % for CH_4 [10], and 11 %/6 % for NO_2 [11].

3 VALIDATION OF THE SCIENTIFIC WFMD SCIAMACHY COLUMN PRODUCTS OF CO, CH_4, AND N_2O

3.1 Validation approach for WFMD data

The retrieval of WFMD ver. 0.4 total column products of CO, CH_4, and N_2O [1,2] includes empirical column scaling factors (e.g., WFMD CO is scaled to MOPITT values with a scaling factor of 0.5; for N_2O the scaling factor is 0.66, and no scaling is used only for CH_4). Therefore, validation of absolute column values on overall average is not of interest. Rather, validation focus is put in our study on relative accuracy, i.e., investigating whether the atmospheric variabilities above the Zugspitze, which are dominated by the annual cycle for these species, can be retrieved from the SCIAMACHY data.

Individual WFMD retrievals in the near-infrared spectral domain are showing a significant scatter. This is because the small spectral signals are only slightly above the noise level, and because of the occurrence of systematic spectral residuals which are not understood yet [1,2]. Therefore, our validation approach is investigating to what extent the quality of SCIAMACHY data allows to reproduce the true variability of CO, N_2O and CH_4 columns which is mainly dominated by the annual cycle above the Zugspitze, in a statistically significant manner. For this purpose, the annual cycle found by the Zugspitze FTIR column measurements is compared to the available time series of SCIAMACHY WFMD columns (data for ≈30 days in the time span Jan - Oct 2003) using daily mean pixel averages within a stepwise increased selection radius around the Zugspitze ground site. The goal is to thereby stepwise reduce the scatter of the daily means by statistically averaging over increasing ensembles of pixels.

One might argue that also polluted regions may be more and more included into the ensemble while increasing the selection radius, and that could potentially be compensating the statistical effect of reducing the scatter of the daily means. However, this effect is obviously weaker than the reduction of scatter by the statistical effect of increasing the averaging ensemble, as our test in Section 3.2 below is proving (Table 1). Furthermore, we are looking in this study for the annual cycle, and in our recent study on total column and in situ series of CO [12], it has been found, that the annual cycles of CO observed at a variety of stations within the northern hemisphere, are comparable at all stations as to phase and amplitude (≈10 % amplitude, slightly lower for stations located within the free troposphere). This means, that increasing the selection radius for calculating daily means does not disturb the goal of obtaining a well defined annual cycle, but helps to reduce the scatter (see above).

Another issue of the validation approach is how to reduce the impact of varying ground altitudes of the different satellite pixels that are averaged on one hand, and, the different altitude of the Zugspitze mountain site on the other hand. We solve this problem in a 3-steps approach: i) All individual SCIAMACHY WFMD column values are normalized to coincident dry air column values which are also available from WFMD retrievals (via O_2 columns). The resulting quantity is the so-called “dry air column averaged mixing ratio”. This quantity does not depend on the average pixel ground level altitude, assuming a constant mixing ratio with altitude. This is a reasonable assumption for the range of mean pixel altitudes encountered around the Zugspitze (≈ 0.7 km – 2 km asl.). ii) To make the dry air column averaged mixing ratios of SCIAMACHY (unit ppmv) comparable to the FTIR column abundances above the Zugspitze (unit $1/cm^2$), both data sets are then normalized to their overall average, and these (dimensionless) *anomalies* are used for validation/intercomparison purposes. iii) Finally, all individual Zugspitze columns are normalized to daily mean local pressure. This is for consistency reasons, in order to make the Zugspitze ground data also independent from the actual pressure level, as the SCIAMACHY data are due to their normalization to the dry air column, see point i).

3.2 Validation results for WFMD CO

Fig. 1 shows the available SCIAMACHY WFMD CO/O_2 column anomaly data (covering 33 days in 2003); each SCIAMACHY point is the average of all pixels from one day within a 2000-km radius around the Zugspitze, with the cloud flagged pixels removed. Note, that we did not restrict WFMD data selection to any maximum threshold in the individual retrieval errors reported, since we did not find any significant reduction of the scatter of daily means by testing such a restriction (errors below 100 %) for N_2O. In Fig. 1 it can be seen, that there are 4 obvious outliers in the SCIAMACHY data. These have ad hoc been removed for Fig. 2 (retrieval error for strongest outlier is 20 %). Zugspitze FTIR daily mean column anomalies are shown in the same plot. A 3rd order polynomial fit to the FTIR data nicely shows the CO annual cycle with a ≈10 % amplitude.

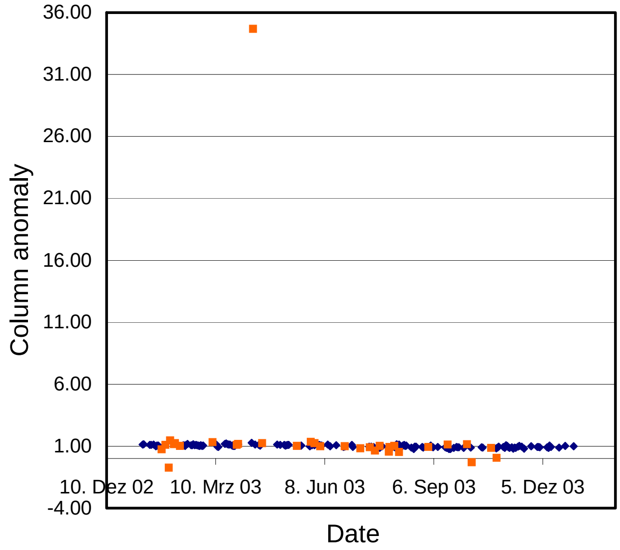

Fig. 1. Orange points: SCIAMACHY WFMD v0.4 CO/O_2 column anomaly: average of all pixels within a 2000-km radius around Zugspitze for daily overpass; cloud flagged pixels removed. Blue points: Zugspitze FTIR CO column anomaly: daily means of pressure corrected columns.

To investigate whether information on this annual cycle can also be retrieved from SCIAMACHY data in a statistically significant manner, a linear fit to both SCIAMACHY and FTIR data is performed, see Fig. 3.

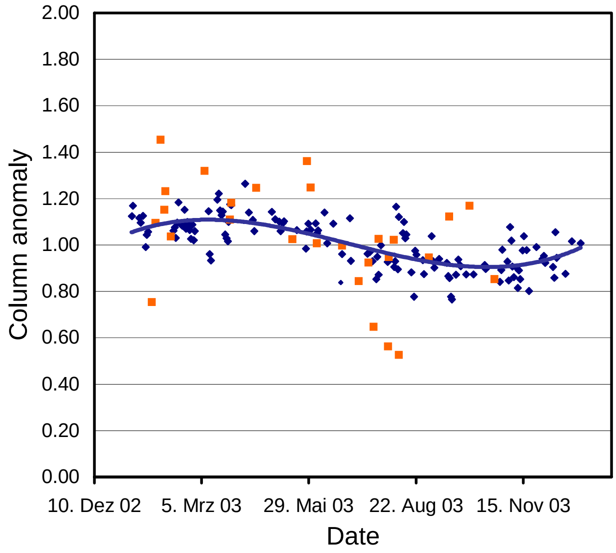

Fig. 2. Same CO data as in Fig. 1, however, 4 outliers of SCIAMACHY data removed. Blue line: 3rd order polynomial fit to the FTIR data.

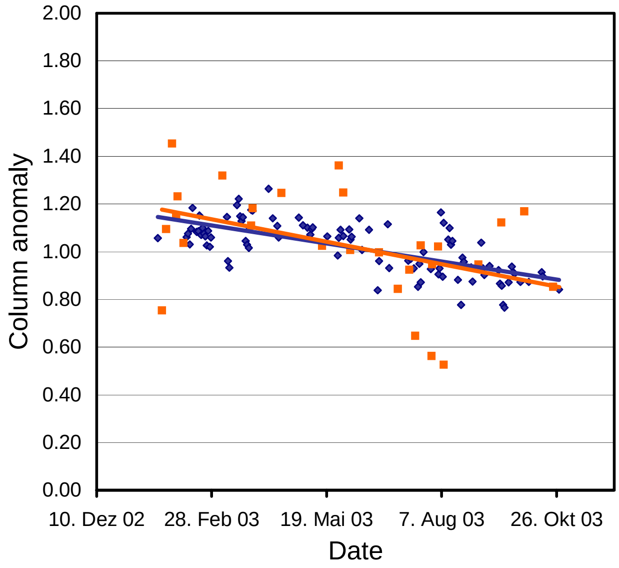

Fig. 3. Same CO data as Fig. 2, but the plotted time span of FTIR data is reduced to match the time span of available SCIAMACHY WFMD data. Solid lines: Linear fits. See Table 1 for the fit parameters.

It can bee seen from Fig. 3, that the slope of the linear fits of both data sets agree quite well. Table 1 shows the fitting errors for the slopes of these linear fits for both FTIR and SCIAMACHY data sets. It can be seen, that also for SCIAMACHY data the fitting error of the slope is significantly smaller than the value of the slope itself and the regression coefficient is reasonably good (R= -0.7). This means that the obtained negative slope, which is due to the annual cycle, can be retrieved in a statistically significant manner, from SCIAMACHY WFMD data for the considered selection radius of SCIAMACHY pixels of 2000 km around the Zugspitze.

Table 1. Slope, slope error, and regression coefficient R from the linear fit to the "FTIR" data, and to the SCIAMACHY CO data for a 2000-km pixel-selection radius around the Zugspitze ("SCIA 2000") as shown in Fig. 3. "SCIA 1000" means a 1000-km selection radius, and "SCIA 1000_cl" is with cloud flagged pixels included.

	Slope	Slope error	R
FTIR	-9.5E-4	±9.8E-5	-0.70
SCIA 2000	-1.2E-3	±4.9E-4	-0.43
SCIA 1000	-6.4E-4	±5.9E-4	-0.21
SCIA_cl 1000	-4.4E-4	±4.3E-4	-0.18

The question to be addressed now is, what the minimum selection radius is, in order to obtain the negative slope in a statistically significant manner. Table 1 shows the fitting errors and R for a reduced selection radius of 1000 km. Now, the fitting error of the slope is comparable to the absolute value of the slope. I.e., the negative slope, being a signature of the CO annual cycle, can no longer be retrieved in a statistically significant manner from the SCIAMACHY data for a 1000-km selection radius. So our finding is, that a minimum selection radius of 1000 – 2000 km around Zugspitze is necessary, in order to retrieve the negative slope due to the CO annual cycle in a statistically significant manner from WFMD SCIAMACHY data.

Finally, we investigate, whether the information content in the SCIAMACHY data as to the annual cycle could be increased by including cloud flagged pixels also into the daily average. This question arises, since the cloud clearing algorithm applied is rather conservative [1,2]. Table 1 shows the result for the case of a 1000-km selection radius. In fact, including cloud flagged pixels does essentially not change the fit quality (slope error and R). This confirms that the cloud clearing algorithm is rather conservative.

3.3 Validation results for WFMD CH_4 and N_2O

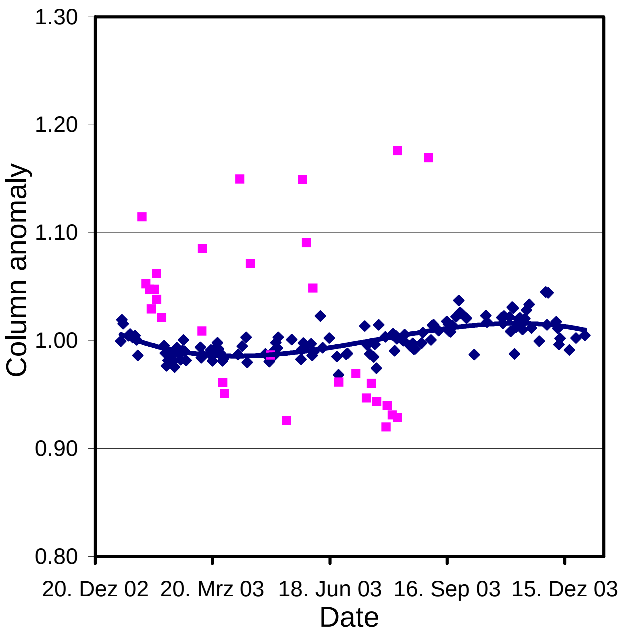

Fig. 4. Pink points: SCIAMACHY WFMD v0.4 CH_4/O_2 column anomaly: average of all pixels within a full latitudinal band of ±2000-km north/south relative to the Zugspitze for daily overpass; cloud flagged pixels removed. Blue points: Zugspitze FTIR CO column anomaly: daily means of pressure corrected columns.

Figs. 4 and 5 show that the annual cycles of total CH_4 and N_2O monitored by the Zugspitze FTIR show a ≈2.5 % amplitude. The scientific WFMD of both CH_4 and N_2O are not able to reflect this annual cycle in a statistically siginificant manner due to high scatter, even if all pixels within a full latitudinal band of +/-2000 km north/south of Zugspitze are averaged for each day, see Figs. 4 and 5.

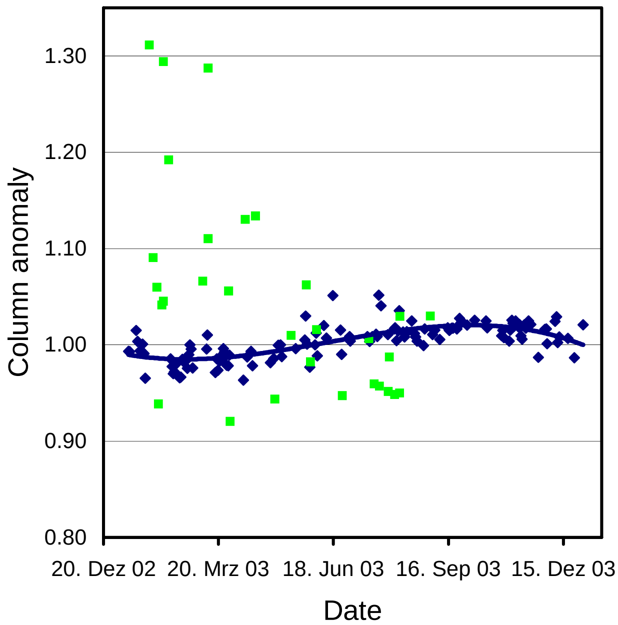

Fig. 5. Green points: SCIAMACHY WFMD v0.4 N_2O/O_2 column anomaly: average of all pixels within a full latitudinal band of ±2000-km north/south relative to the Zugspitze for daily overpass; cloud flagged pixels removed. Blue points: Zugspitze FTIR CO column anomaly: daily means of pressure corrected columns.

4 VALIDATION OF THE SCIENTIFIC DOAS UB1.0 SCIAMACHY NO_2 COLUMN PRODUCT

4.1 Validation approach

Contrary to the WFMD retrievals considered in Section 3, the scientific UB1.0 NO_2 retrievals do not include an empirical scaling factor. Therefore, we are considering absolute column values in the following.

Validating NO_2, the possible effect of tropospheric pollution has to be taken into account, that can occasionally significantly enhance the total columns by up to orders of magnitude, depending on the site properties like its altitude and its horizontal distance to pollution sources. The alpine high-altitude site Zugspitze (2964 m asl.) is within the free troposphere for more than 60 % of the year. Therefore, the Zugspitze FTIR ground measurements are impacted much less often by tropospheric pollution than the SCIAMACHY pixels selected for this study within a radius of 200 km around the Zugspitze. This is since the average pixel ground heights (≈ 0.7 km – 2 km asl.) are significantly lower than the Zugspitze altitude. Thus we made the ad hoc decision to eliminate SCIAMACHY column values which are obviously exceeding the average values of the days before and after by a factor of >1.5.

4.2 Validation results for DOAS UB1.0 NO_2

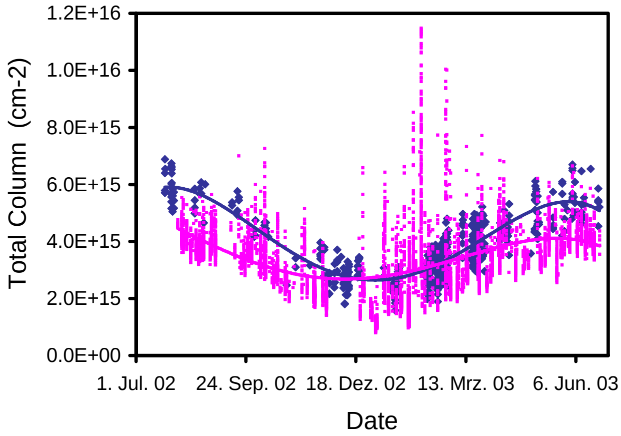

Fig. 6. FTIR columns of NO_2 from individual FTIR measurements with a 10-20 min integration (blue, solid line is a 4th order polynomial fit), versus scientific SCIAMACHY DOAS UB1.0 retrievals from a 200 km-selection radius around the Zugspitze (pink, solid line is a 4th order polynomial fit).

In Fig. 6 the direct comparison of NO_2 Zugspitze FTIR columns versus one full year of SCIAMACHY UB1.0 data is shown. For a 200-km selection radius around the Zugspitze, the average NO_2 columns ratio over the time span shown is: SCIAMACHY DOAS_UB1.0 / FTIR = 0.89.

Clearly the satellite data are partly impacted by pollution while the FTIR data show no obvious enhancements. This is due to lower average pixel altitudes compared to the Zugspitze (2964 m asl.).

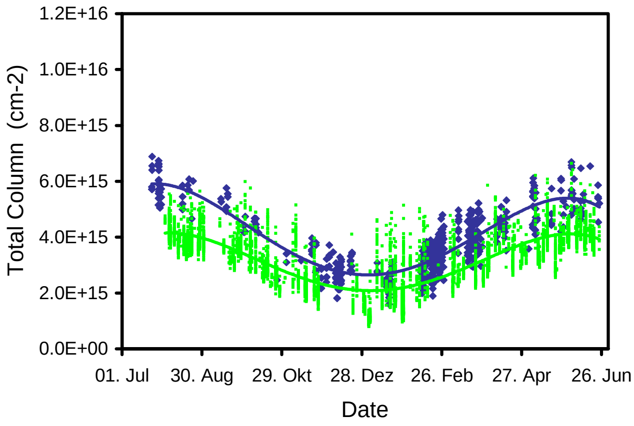

Fig. 7. FTIR NO_2 data as shown in Fig. 6 (blue), but pollution episodes removed from SCIAMACHY data (green).

Eliminating pollution episodes from the SCIAMACHY DOAS UB1.0 data is performed in Fig. 7. We performed a simple ad hoc exlcusion of columns exceeding the mean columns of the days before and after by more than a factor of 1.5. This results in a revised average NO_2 columns ratio over the time span shown of: SCIAMACHY DOAS_UB1.0 (w/o_pollution) / FTIR = 0.84. In other words, the SCIAMACHY UB1.0 columns of NO_2 are 16 % below the Zugspitze FTIR columns on average. The real underestimation of NO_2 columns by SCIAMACHY UB1.0 is even somewhat higher due to the altitude difference between the Zugspitze and the average ground altitudes of pixels around.

The effect of correcting (scaling) the SCIAMACHY columns by this factor of 1/0.84 is shown in Fig. 8. Obviously, the NO_2 annual cycle is perfectly monitored by the SCIAMACYH DOAS UB1.0 data, and it compares perfectly well to annual cycle found from the ground FTIR data.

The scatter of both data sets is comparable (Fig. 8). However, we point out that the scatter is of different origin for the FITR data set (scatter dominated by the diurnal cycle plus diurnal variability), and the SCIAMACHY data (scatter dominated by the columns variability and the differing ground altitudes of the columns considered within the 200-km selection radius around the Zugspitze), respectively. So we only draw the conclusion, that the scatter of the SCIAMACHY UB1.0 NO_2 is within a reasonable range.

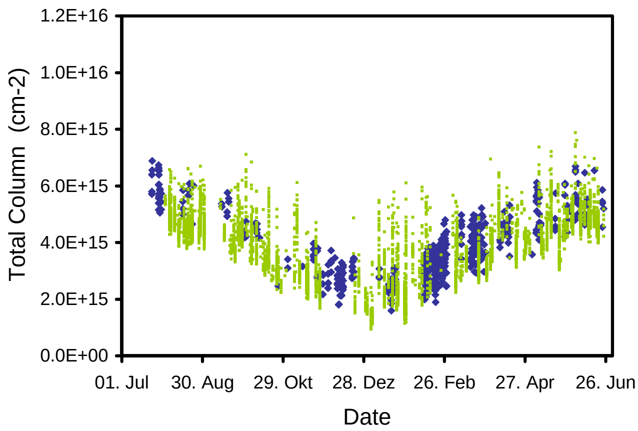

Fig. 8. As Fig. 7, but SCIAMACHY columns (green) scaled by a factor of 1/0.84.

5 CONCLUSION

Solar FTIR measurements at the Permanent Ground Truthing Station Zugspitze (47 N, 11 E), Germany were used to validate ENVISAT/SCIAMACHY Scientific Data Products retrieved at the University of Bremen, i.e., the infrared WFM-DOAS ver. 0.4 total column products of CO, CH_4, N_2O, and the scientific DOAS NO_2 column product (ver. UB1.0).

The infrared WFMD column retrievals include empirical scaling factors, therefore it is no issue to validate their overall absolute accuracy. Rather, focus was put on validating relative accuracy, i.e., investigating to what extent the quality of SCIAMACHY data (precision limited by spectral noise and systematic spectral residuals) allows to reproduce the actual variability of CO, CH_4, and N_2O columns, which is mainly dominated by the annual cycle, in a statistically significant manner. For this purpose, the annual cycle found by the Zugspitze FTIR column measurements is compared to the available time series of SCIAMACHY WFMD columns (i.e., Jan - Oct 2003) using daily mean pixel averages calculated from a stepwise increased selection radius around the Zugspitze. The resulting trade off was investigated between thereby reducing the scatter in SCIAMACHY data by improving the statistics and introducing additional variabilities from emission sources. It was demonstrated that an increasing selection radius helps in reducing the scatter of CO. As a result it was found that, in order to obtain a statistically significant fit to the CO annual cycle (≈10 % amplitude) from SCIA WFMD data, all pixels within a radius of at least 1000-2000 km around Zugspitze had to be averaged for each day.

The weaker (2.5 % amplitude) annual cycles of CH_4 and N_2O could not be retrieved from SCIAMACHY data, even using averages of all pixels within a full latitudinal band of ±2000 km north/south relative to the Zugspitze around the globe.

In order to reduce the impact of varying ground altitudes of the different satellite pixels used for intercomparison, SCIAMACHY WFMD columns have been normalized to dry air columns. These have additionally been normalized to their overall average, and these anomalies then been compared to the ground FTIR column anomalies, to make both satellite and ground data sets comparable.

Validating one full year of UB1.0 NO_2 data (Jul 2003 – Jun 2003) a perfect agreement of the annual cycle to the ground FTIR data has been found, after removing obvious enhancements due to pollution episodes not captured by the high altitude (2964 m asl.) Zugspitze FTIR. This is surprising, since the operational NO_2 data product from the validation reference set provided by ESA in early 2004 (data available for July – Dec 2003) is showing a significant problem by underestimating the annual cycle, as discussed in our accompanying paper [4].

After removing pollution episodes, the SCIAMACHY UB1.0 columns of NO_2 are 16 % below the Zugspitze FTIR columns on average. The real underestimation of NO_2 columns by SCIAMACHY UB1.0 is somewhat higher due to the altitude difference between the Zugspitze and the average ground altitudes of pixels around.

6 ACKNOWLEDGMENTS

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