VALIDATION OF SCIAMACHY OZONE COLUMN DENSITIES AND PROFILES USING GROUND-BASED FTIR AND MILLIMETER WAVE MEASUREMENTS

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ABSTRACT

Ground-based FTIR and millimeter wave measurements of the Institute of Meteorology and Climate Research (IMK), Forschungszentrum Karlsruhe, and the Swedish Institute of Space Physics (IRF) are used for validation of SCIAMACHY ozone measurements. FTIR and millimeter wave measurements used for this study were routinely carried out between 2002 and 2004 at IRF at Kiruna, Sweden. In addition IMK carried out millimeter wave measurements on Mount Zugspitze in the Alps in 2003.

SCIAMACHY level 2 NRT-products of 2002 are only validated by FTIR data since millimeter wave observations started in late 2002 when SCIAMACHY data were unavailable. For the years 2003 and early 2004 total ozone column abundances retrieved with the TOSOMI algorithm of the Royal Netherlands Meteorological Institute (Koninklijk Nederlands Meteorologisch Instituut, KNMI) are validated by the FTIR and microwave measurements. Finally, ozone limb profiles between July and November 2002 taken from the current SCIA Level 2 Off-Line masterset are validated by the FTIR measurements at Kiruna.

1. INTRODUCTION

Ground-based FTIR and millimeter wave measurements of the Institute of Meteorology and Climate Research (Institut für Meteorologie und Klimaforschung, IMK, `www.fzk.de/imk/asf`), Forschungszentrum Karlsruhe, and the Swedish Institute of Space Physics (Institutet för rymdfysik, IRF, `www.irf.se/`) are used for validation of SCIAMACHY ozone measurements (AOID 191). The observations at IRF at Kiruna (67.8°N, 20.4°E, 420 m a.s.l.) are routinely carried out using a Bruker 120 HR FTIR spectrometer and the new microwave radiometer KIMRA. The NDSC complemetary site Kiruna is well suited for ground-based measurements due to its low tropospheric water vapour content for long periods in the year. Furthermore, this site is situated inside as well as outside the polar vortex in the course of the winter which enables the study of ozone loss and mixing processes. Polar night at this site is quite short so FTIR measurements are normally interrupted for less than two months.

In 2003 the ground-based millimeter wave radiometer MIRA2 of IMK was operated at the alpine Environmental Research Station Schneefernerhaus (Umwelt Forschungsstation Schneefernerhaus, UFS, `www.schneefernerhaus.de`) on Mount Zugspitze (47.4°N, 11°E, 2650 m a.s.l.). This high altitude site was chosen due to its low tropospheric water vapour content and its good accessibility by cable car and rack railway.

2. EXPERIMENTAL

2.1 FTIR

The FTIR measurements at Kiruna are performed using a Bruker IFS 120 HR. This instrument has a spectral resolution of about 0.003 cm^{-1}. Two detectors (MCT and InSb) and the NDSC optical filter set covering the spectral range 700-5000 cm-1 are used to increase the signal to noise ratio. The recorded solar absorption spectra are coadded up to 10 min. Further details about this instrument are given in [1].

2.2 Microwave radiometry

MIRA2 (*Mi*crowave *Ra*diometer) was developed by IMK and covers the frequency range 268-281 GHz. The bandwidth is 1.3 GHz and the specral resolution about 1.2 MHz. A detailed description of this radiometer system is given in [2].

The new KIMRA (*Ki*runa *M*icrowave *Ra*diometer) instrument was jointly developed by IMK and IRF. This radiometer system covers the frequency range 192-228 GHz and has otherwise a similar setup as the MIRA2 instrument.

3. DATA ANALYSIS

3.1 FTIR

The FTIR spectra are analyzed using the radiative transfer code KOPRA (*K*arlsruher *O*ptimized *P*recise *R*adiative-transfer *A*lgorithm) [3] and the retrieval code PROFFIT (*Prof*ile *Fit*) [4] using Phillipps-Tikhonov approach. PROFFIT allows a simultaneous retrieval of several gases in several microwindows (MW). In the case of O_3 two MWs are used: 782.56 - 782.86 cm^{-1} and 788.85 - 789.37 cm^{-1}. The vertical resolution is obtained by considering the pressure broadening of absorption lines and is about 8 km in the vertical range from 10 to 35 km. The uncertainty in the resulting column abundances is less than 5%.

3.2 Microwave Radiometry

The data analysis of MIRA2 and KIMRA is performed at IMK using the Karlsruhe Millimeterwave Forward Model [5]. The Optimal Estimation Method is used for profile retrieval taking advantage of the pressure broadening of the spectral lines. The vertical resolution of the ozone profiles is at best 8 km in the vertical range from 17 to 55 km. The uncertainty in the resulting ozone column abundances is 25 DU - 50 DU, the upper limit is reached in summer.

4. LEVEL 2 NRT-PRODUCTS

For validation of the SCIAMACHY level 2 5.01 NRT-products of 2002 only FTIR data were used since millimeter wave observations at Kiruna started in late 2002 when SCIAMACHY data were unavailable. A distance of 500 km and measurements taken on the same day in each case were chosen as coincidence criterion.

Figure 1 shows the comparison between FTIR and the SCIAMACHY level 2 NRT ozone columns. All SCIAMACHY columns are lower than the FTIR ozone column abundances (upper panel), the mean deviation is -26.5 +/- 13.9 DU or -8.2 +/- 3.8 % (lower panel). Both datasets show a good correlation (Figure 2), the correlation coefficient amounts to 0.89.

5. OZONE COLUMN ABUNDANCES USING THE TOSOMI ALGORITHM OF KNMI

For the years 2003 and early 2004 ozone column amounts retrieved with the TOSOMI algorithm of the Royal Netherlands Meteorological Institute (Koninklijk Nederlands Meteorologisch Instituut, KNMI, `www.knmi.nl`) were used for validation. This algorithm has been developed by KNMI to retrieve ozone column densities from ozone monitoring instruments using the DOAS method [6] and has successfully applied to GOME data [7]. For the comparisons shown here a coincidence criterion of 600 km distance and measurements taken on the same day in each case were chosen.

The resulting ozone columns agree well with the FTIR columns (upper panel of Figure 3), the mean deviation is -12.3 +/- 16.7 DU or -3.7 +/- 4.5 % (lower panel of Figure 3). The correlation in this case is even better than for the level 2 NRT-products, the correlation coefficient amounts to 0.95 (Figure 4).

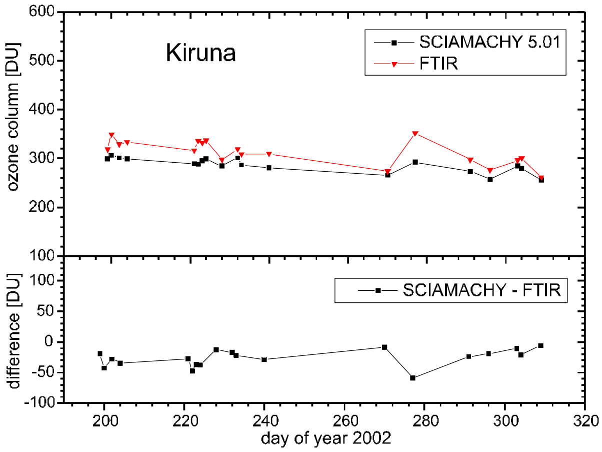

Fig. 1. Comparison of SCIAMACHY level 2 5.01 NRT ozone columns and FTIR measurements at Kiruna (upper panel). The difference between both datasets is shown in the lower panel.

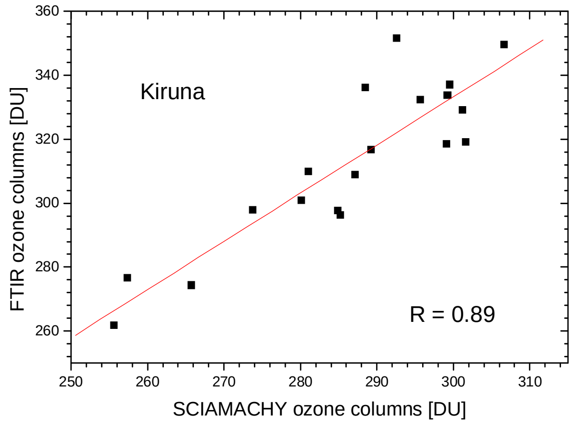

Fig. 2. Ozone columns as measured by FTIR at Kiruna plotted over SCIAMACHY level 2 NRT ozone columns.

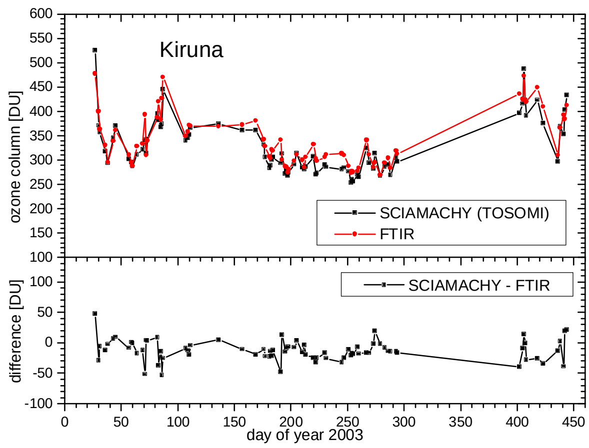

Fig. 3. SCIAMACHY ozone columns retrieved with the TOSOMI algorithm of KNMI in comparison with FTIR measurements at Kiruna.

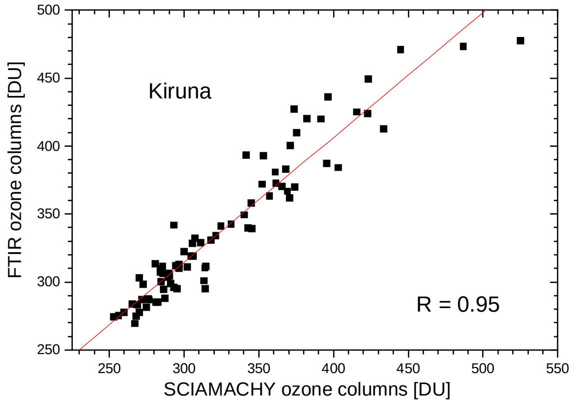

Fig. 4. Ozone columns as measured by FTIR at Kiruna plotted over SCIAMACHY ozone columns using the TOSOMY algorithm.

The ozone columns of the millimeter wave measurements cannot be compared directly with the SCIAMACHY total columns since the millimeter wave radiometer is not sensitive in the troposphere. Therefore only stratospheric ozone columns above 10 km of the radiometer measurements were compared with SCIAMACHY total columns resulting in an offset between both datasets due to the missing lower part of the ozone column in the microwave measurements.

But besides this offset both time series of ozone over Kiruna show the same seasonal variation in 2003 (upper panel of Figure 5) resulting in a mean difference of 81.2 ± 29.9 DU (lower panel of Figure 5). Both datasets show also a good correlation, the correlation coefficient is 0.82 (Figure 6).

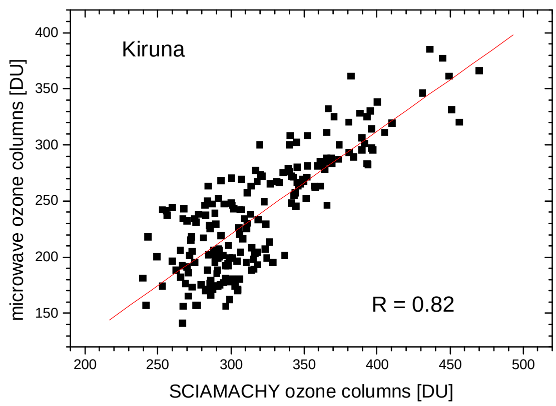

Fig. 6. Ozone columns as measured by microwave radiometry at Kiruna plotted over SCIAMACHY ozone columns using the TOSOMY algorithm.

The comparison between the microwave measurements on Mount Zugspitze and the SCIAMACHY ozone columns is shown in the upper panel of Figure 7. The mean difference to the SCIAMACHY column abundances amounts to 50.1 ± 34.1 DU (lower panel of Figure 7). The mean difference is lower than that of the Kiruna measurements probably because of the higher altitude of the measurement site on Mount Zugspitze, the standard deviation is in the same order for both time series. The correlation between the two Zugspitze datasets is much worse than that of the Kiruna datasets. The reason is that the overall variation of the ozone column over Mount Zugspitze during this time span was much smaller than the seasonal variation over Kiruna. This results in a larger impact of the scatter in the plot of the microwave data over the SCIAMACHY data and the worse correlation coefficient of only 0.5 (Figure 8).

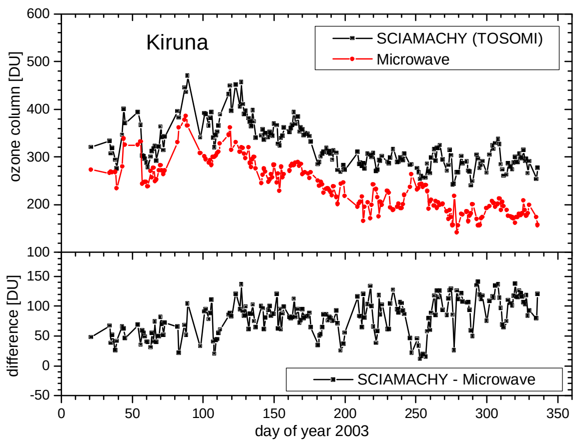

Fig. 5. SCIAMACHY total ozone columns retrieved using the TOSOMI algorithm of KNMI in comparison with stratospheric ozone columns as measured by microwave radiometry at Kiruna.

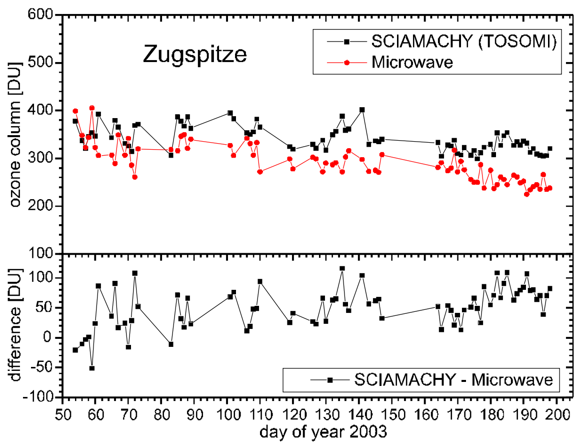

Fig. 7. SCIAMACHY total ozone columns retrieved using the TOSOMI algorithm of KNMI in comparison with stratospheric ozone columns as measured by microwave radiometry on Mount Zugspitze.

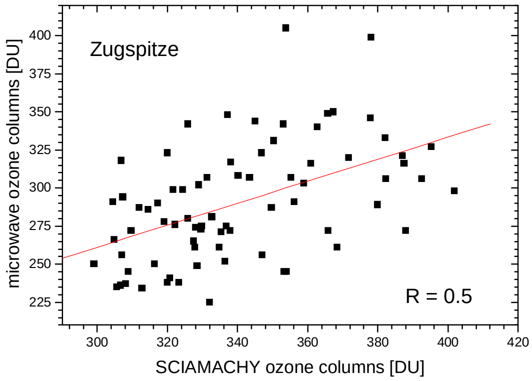

Fig. 8. Ozone columns as measured by microwave radiometry on Mount Zugspitze plotted over SCIAMACHY ozone columns using the TOSOMY algorithm.

6. OZONE LIMB PROFILES OF THE SCIA LEVEL 2 OFF-LINE MASTERSET

Ozone limb profiles between July and November 2002 taken from the current SCIA Level 2 Off-Line masterset were compared with the FTIR measurements at Kiruna. A distance of 500 km and measurements taken on the same day in each case were chosen as coincidence criterion for the validations shown here.

The comparison of the profiles of 18 July is shown in the left hand panel of Figure 9. A quite poor agreement between the original profiles is found. For better comparability the SCIAMACHY profile was smoothed to the FTIR vertical resolution by performing a forward calculation using the SCIAMACHY profile and inverting the resulting spectrum using the same parameters as for the original FTIR retrieval. The smoothed SCIAMACHY profile is also shown in Figure 9, but the agreement is not improved. The difference between the FTIR profile and the smoothed SCIAMACHY profile is shown in the right hand panel of Figure 9. The difference cannot be explained alone by the uncertainties of the FTIR measurement which are also shown in this plot.
The results of all 16 coincident measurements between July and November 2002 are summarized in Figure 10. All SCIAMACHY profiles used for this comparison were smoothed to FTIR vertical resolution. The left hand side of the figure shows the absolute and the right hand side the relative difference. The mean differences are quite large (up to 20%), but a shift of the SCIAMACHY profiles of +1.5 km reduces the discrepancies significantly. The mean relative difference is now smaller than 10% for all altitude levels between 10 and 35 km and no systematic bias can be found.

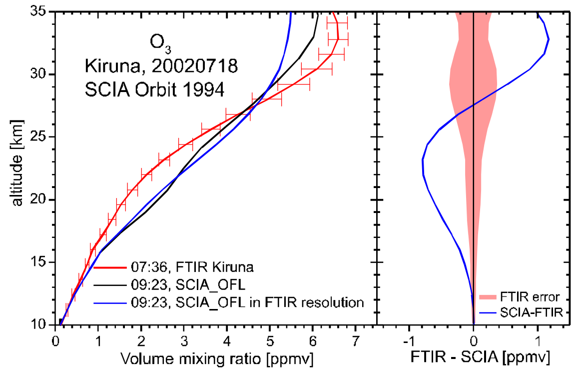

Fig. 9. SCIAMACHY limb profile of 18 July 2002 over Kiruna compared to the corresponding FTIR profile (left hand side). The difference between the FTIR and SCIAMACHY profile is shown on the right hand side.

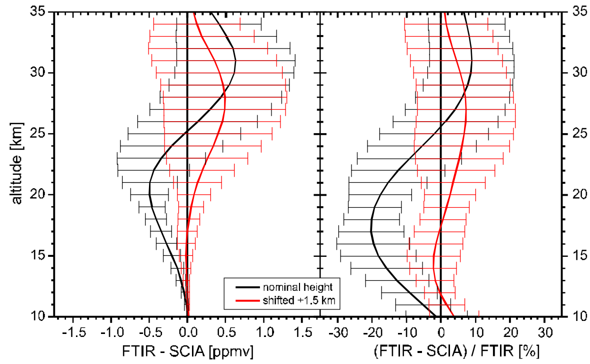

Fig. 10. Mean absolute (left hand side) and relative (right hand side) difference of 16 coincident measurements (black). The mean difference is significantly reduced if the SCIAMACHY profiles are shifted by +1.5 km (red).

7. CONCLUSIONS

Ground-based FTIR and microwave measurements at Kiruna, Sweden, and on Mount Zugspitze, Germany, were used for validation of SCIAMACHY total ozone column abundances and ozone profiles. The comparison with FTIR column densities measured at Kiruna showed that the SCIAMACHY level 2 NRT total ozone columns are on average 8.2 +/- 3.8 % lower than the FTIR columns. Both datasets show a good correlation, the correlation coefficient is 0.89.

The comparison of the FTIR total ozone columns with SCIAMACHY total ozone columns derived using the TOSOMI algorithm of KNMI resulted in an even better agreement: the SCIAMACHY columns are on average 3.7 +/- 4.5 % lower than the FTIR columns and the correlation coefficient amounts to 0.95.

Since the used microwave radiometers at Kiruna and on Mount Zugspitze are not sensitive in the troposphere only stratospheric ozone columns were used for the comparison with SCIAMACHY total ozone columns of 2003 derived with the TOSOMI algorithm. This results in an offset and a larger scatter in the mean difference. The mean difference of the Kiruna measurements to SCIAMACHY ozone columns is 81.2 ± 29.9 DU and both datasets show the same seasonal variation and a good correlation. The correlation coefficient amounts to 0.82. For the Zugspitze measurements the mean difference amounts to 50.1 ± 34.1 DU. The offset in this case is smaller probably due to the high altitude of the measurement site, but the standard deviation is nearly the same as for the Kiruna measurements. Since the seasonal variation of the Zugspitze measurements is smaller than that of the Kiruna measurements, the impact of the scatter is larger resulting in a rather poor correlation coefficient of 0.5.

The comparison of ozone limb profiles of the SCIA level 2 off-line masterset with the FTIR measurements at Kiruna revealed that the SCIAMACHY profiles have to be shifted by +1.5 km to get a good agreement. The mean difference between the smoothed and shifted SCIAMACHY profiles and the FTIR measurements are then smaller than 10 % for all altitude levels between 10 and 35 km.

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REFERENCES

1. Th. Blumenstock, H. Fischer, A. Friedle, F. Hase, and P. Thomas, Column amounts of $ClONO_2$, HCl, HNO_3, and HF from ground-based FTIR measurements made near Kiruna, Sweden, in late winter 1994, *Journal of Atmospheric Chemistry*, 26, pp. 311-321, March 1997.
2. H. Berg, R. Krupa, G. Hochschild, G. Kopp, and M. Kuntz, Millimeter wave radiometer with adjustable internal calibration load for high resolution measurements of stratospheric constituents, *Proceedings of 2nd ESA Workshop on Millimetre Wave Technology and Applications: Antennas, Circuits and Systems*; pp. 372-377; Espoo, May 1998.
3. G.P. Stiller, M. Hoepfner, M. Kuntz, T. von Clarmann, G. Echle, H. Fischer, B. Funke, N. Glatthor, F. Hase, H. Kemnitzer, and S. Zorn, The Karlsruhe optimized and precise radiative transfer algorithm. Part I: requirements, justification, and model error estimation, *Optical Remote Sensing of the Atmosphere and Clouds*, J. Wang, B. Wu, T. Ogawa, Z. Guan, (eds.), Proceedings of SPIE Vol. 3501, 257-268, 1998.
4. Hase, F., J.W. Hannigan, M.T. Coffey, A. Goldman, M. Höpfner, N.B. Jones, C.P. Rinsland, S.W. Wood: Intercomparison of retrieval codes used for the analysis of high-resolution, ground-based FTIR measurements, *Journal of Quantitative Spectroscopy & Radiative Transfer*, 87, 25–52, 2004.
5. G. Kopp, The Karlsruhe Millimeterwave Forward Model, *Atmospheric Millimeter and Sub-Millimeter Wave Radiative Transfer Modeling II*, Logos Verlag Berlin, 2001, ISBN 3-89722-585-9, ISSN 1615-6862
6. Veefkind, J. P., and J. F. de Haan, Chapter 3 – DOAS Total O3 Algorithm, *OMI Algorithm Theoretical Basis Document, Volume II: OMI Ozone Products, ATBD-OMI-02*, P. K. Bhartia (editor), 2002.
7. Valks, P., J. P. Veefkind, J. F. de Haan, and R. van Oss, TOGOMI Algorithm Theoretical Baseline Document, *TOGOMI/KNMI/ATBD/001, Issue 1.2*, 01/11/2003.