VERIFICATION OF SCIAMACHY LEVEL 1 AND 2 NEAR-IR NADIR DATA PRODUCTS BY WFM–DOAS ANALYSIS

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ABSTRACT

Initial results are presented concerning the verification of operational SCIAMACHY near–infrared (NIR) Level 1 nadir radiance spectra and corresponding Level 2 near–realtime (NRT) BIAS data products such as CH_4, CO, and H_2O total column amounts. The focus of this study is channel 8 (2265–2380 nm). The verification approach used here is based on applying an independent retrieval method (WFM–DOAS) to the Level 1 data followed by a comparison of the retrieved trace gas columns with the corresponding operational BIAS products. The analyses is based on orbits being part of the "verification orbits data sets" made available by ESA/ESTEC for initial operational data products verification purposes. They reflect state–of–the–art operational processing of SCIAMACHY data. Verification data VERSION 1 were made available end of August 2002. VERSION 2 data have been distributed on 25 November, 2002. The spectral absorption features of the strong NIR absorbers CH_4, H_2O, and CO_2 are clearly visible in these spectra. The accuracy of these spectra, however, does not seem to be good enough to enable a high quality quantitative retrieval and to identify the weak absorbers CO and N_2O. The corresponding NRT BIAS products (CH_4, CO, H_2O, N_2O) cannot be considered scientifically useful at present. They suffer significantly from the quality of the spectra (e.g., from residual dark signal calibration errors and dead/bad pixels not rejected by pixel mask) and probably also from Level 1–2 processing problems. In comparison, the accuracy of the WFM–DOAS derived columns is significantly higher. In order to improve the dark signal correction special nadir states ("nadir/dark–states") have been executed on November 24, 2002. They provide quasi real–time (within approx. 1 minute) dark signal measurements. An initial investigation using these measurements is also presented.

1 INTRODUCTION

Vertical column densities of important atmospheric trace gases (CH_4, CO, CO_2, H_2O, and N_2O) can be derived from the SCIAMACHY near–infrared (NIR) nadir measurements. Operational data products are derived with the BIAS (Basic Infrared Absorption Spectroscopy) retrieval algorithm [1]. A number of scientific institutions are working on scientific algorithms in order to generate scientific data products. Scientific data products have the potential for higher accuray and precision needed for important scientific applications, e.g., to better constrain surface sources and sinks of greenhouse gases. For such an application the accuracy of the retrieved CH_4 and CO_2 columns has to be on the order of a few percent or better for a single measurement.

Scientific data products can also be used to verify the operational data products. This is the focus of this study using the WFM–DOAS algorithm [2,3,4]. WFM–DOAS (Weighting Function Modified Differential Optical Absorption Spectroscopy) is a modified DOAS algorithm mainly being developed for the retrieval of trace gas vertical column densities from SCIAMACHY and GOME/ERS-2 nadir radiance and solar irradiance spectra. An overview about the spectral fitting windows used for this study is given in Tab. 1. Both BIAS and WFM–DOAS use Level 1 spectra, generated by operational Level 0–1 processing [5], as input. WFM–DOAS has also been applied to Level 0 data in this study (nadir/dark–states analysis).

Table 1: BIAS and WFM-DOAS spectral fitting windows.

ID	Channel	Spectral region [nm]	Main vertical column fit parameters
WFM_DOAS_0	6	1558.0–1594.0	CO_2
WFM_DOAS_1	8	2281.7–2284.6	CH_4
WFM_DOAS_2	8	2360.0–2368.7	CO (driver), CH_4, H_2O
BIAS_1	8	2269.0–2275.0	N_2O (driver), CH_4, H_2O
BIAS_2	8	2360.0–2366.0	CO (driver), CH_4, H_2O

The orbits analysed in this study are: VERSION 1: orbits 2337 and 2338 from August 11, 2002, covering parts of Europe and Africa. VERSION 2: orbit 2509 from August 23, 2002, which has a similar coverage as orbit 2337. Combined nadir/dark–states: orbit 3840, November 24, 2002 (coverage similar as 2509).

Channel 8 (and also channel 7) shows a significant decrease of transmission with time probably due to a growing ice layer on the detector. Beginning of August 2002 the transmission was brought back to its maximum value due a special decontamination procedure. On August 11 the channel 8 transmission (as compared to its maximum value) was approx. 0.9 and on August 23 approx. 0.7. For orbit 3840 the transmission was also close to its maximum value due to a previous decontamination. A high transmission is important as the channel 8 (and 7) signal to noise performance is roughly proportional to transmission. The channel 8 dark signal is dominated by thermal emission of the optical bench. Especially at the end of channel 8 (i.e., towards longer wavelength) the dark signal is much higher than the signal originating from atmospheric photons. Therefore, a small error in dark signal correction may result in a large radiance error. All data analysed in this study correspond to nearly maximum channel 8 transmission, i.e., the transmission loss issue is not specifically addressed here.

2 DESCRIPTION OF WFM–DOAS RETRIEVAL ALGORITHM

WFM–DOAS is based on linear least–squares fitting a linearized radiative transfer model plus a low–order polynomial to the logarithm of the ratio of a measured nadir radiance and solar irradiance spectrum [2,3,4]. The main difference with respect to standard DOAS is that the WFM–DOAS reference spectra are derivatives of the radiance rather than trace gas absorption cross–sections. The fit parameters are the desired vertical columns directly, i.e., there is no explicit airmass factor conversion. For reasons of computational speed the WFM–DOAS reference spectra have been pre-computed. The error on the retrieved columns introduced by this (very fast) look-up table approach has been estimated to about a few percent using simulated measurements [4].

3 WFM–DOAS AS APPLIED TO LEVEL 1 DATA (VERSION 1)

From the WFM–DOAS analysis of VERSION 1 channel 8 nadir spectra the following conclusions can be drawn [3,4]: The fit residuals are large, especially for low albedo scenes (e.g., over ocean) and at the end of channel 8 (CO window), i.e., for low radiance levels. The retrieved columns are significantly underestimated in many cases (and sometimes over water even negative). The amplitudes of the fit residuum are different for different ground pixels but the spectral behaviour is similar. This could be explained by residual dark signal calibration errors. In order to deal with this a “Correction Function” has been determined and included in the fit, resulting in significantly better fits and more accurate columns [4]. A “Correction Function” has been included for all results shown in this section.

Figures 1–6 show examples of WFM–DOAS fits and preliminary maps of column amounts of CH_4, CO and CO_2. The cloud mask (grey pixels) has been generated using PMD 1 measurements (Fig. 7). The total columns of the well mixed gases CH_4 and CO_2 should be highly correlated with Earth surface topography ($\sim$ -10%/kilometer; Fig. 8). In Fig. 2 and 6 the Atlas mountains in north-west Africa are clearly visible in the retrieved CH_4 and CO_2 column fields. Column variability due to, e.g., inter–hemispheric gradients, surface pressure variations and surface sources and sinks, is generally smaller (1–10% or below). A detailed validation has not yet been performed. As shown in Fig. 3, the fit residual of about 5% exceeds the rather weak (approx. 2%) absorption signal of CO. The CO fit error is typically around 80% (best values are approx. 30%). The retrieved CO columns are shown in Fig. 4. Especially because of the very low quality of the CO fits it is presently not clear if the “red areas” shown in Fig. 4 are correlated with enhanced CO levels due to, e.g., biomass burning in Africa.

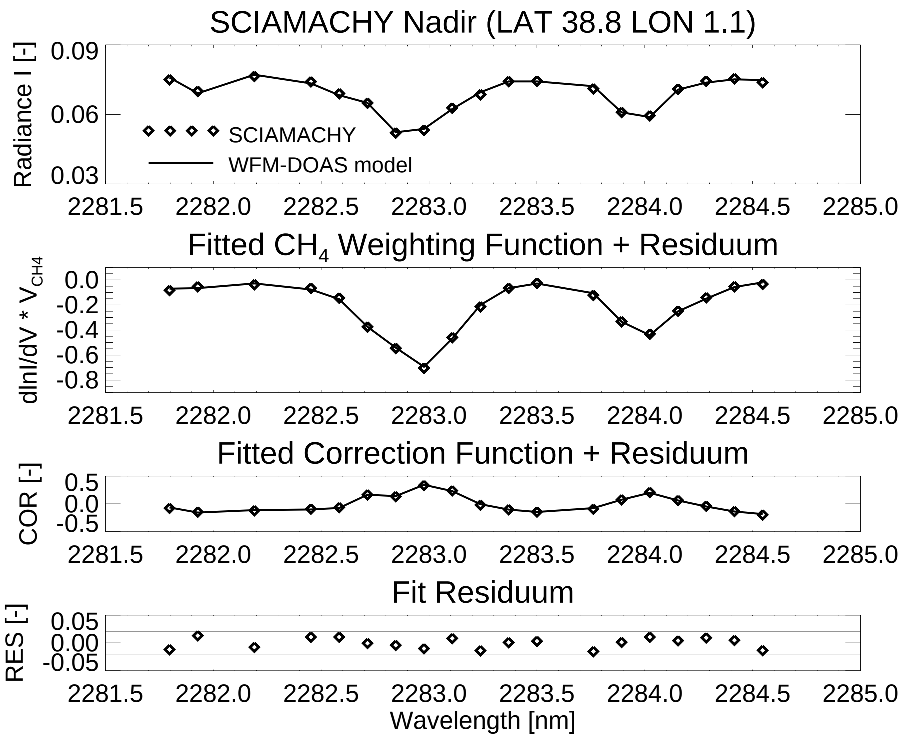

Figure 1: Example of a WFM–DOAS fit as applied to a channel 8 nadir measurement over the Mediterranean Sea (fitting window: WFM_DOAS_1). The retrieved methane column is 4.27x10^{19} molec./cm^2 ± 6% (without correction function: 1.15x10^{19} molec./cm^2 ±22%).

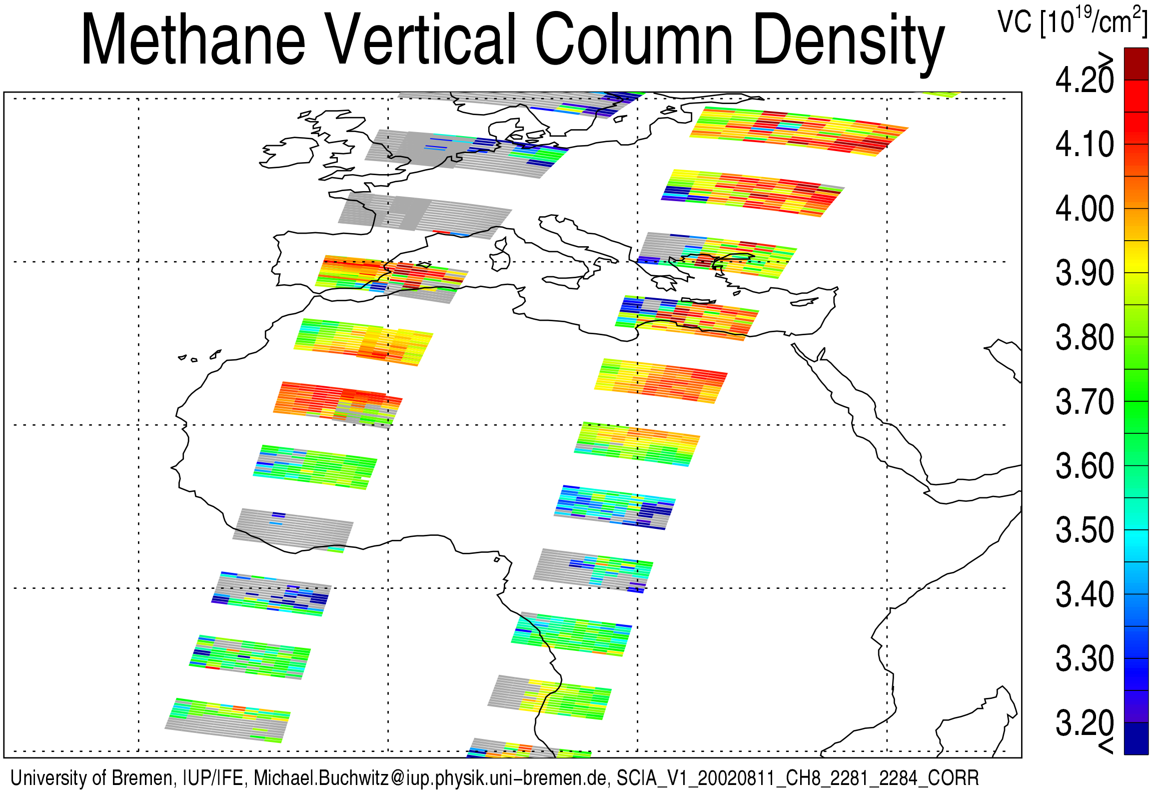

Figure 2: Preliminary methane columns as derived with WFM–DOAS. Expected structures in the column field resulting from surface topography are clearly visible (e.g., Atlas mountains). Example fit: Fig. 1.

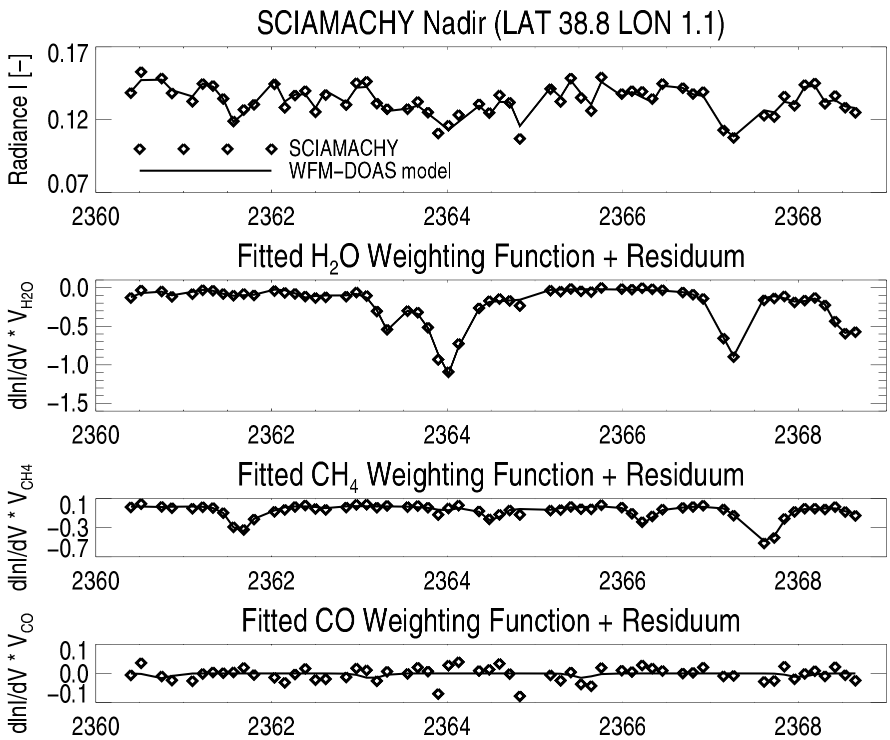

Figure 3: Example of a WFM–DOAS fit as applied to a channel 8 nadir measurement over the Mediterranean Sea (fitting window: WFM_DOAS_2). The retrieved CO column is 1.28x10^{18} molec./cm^2 ±134% (without correction function the column was negative).

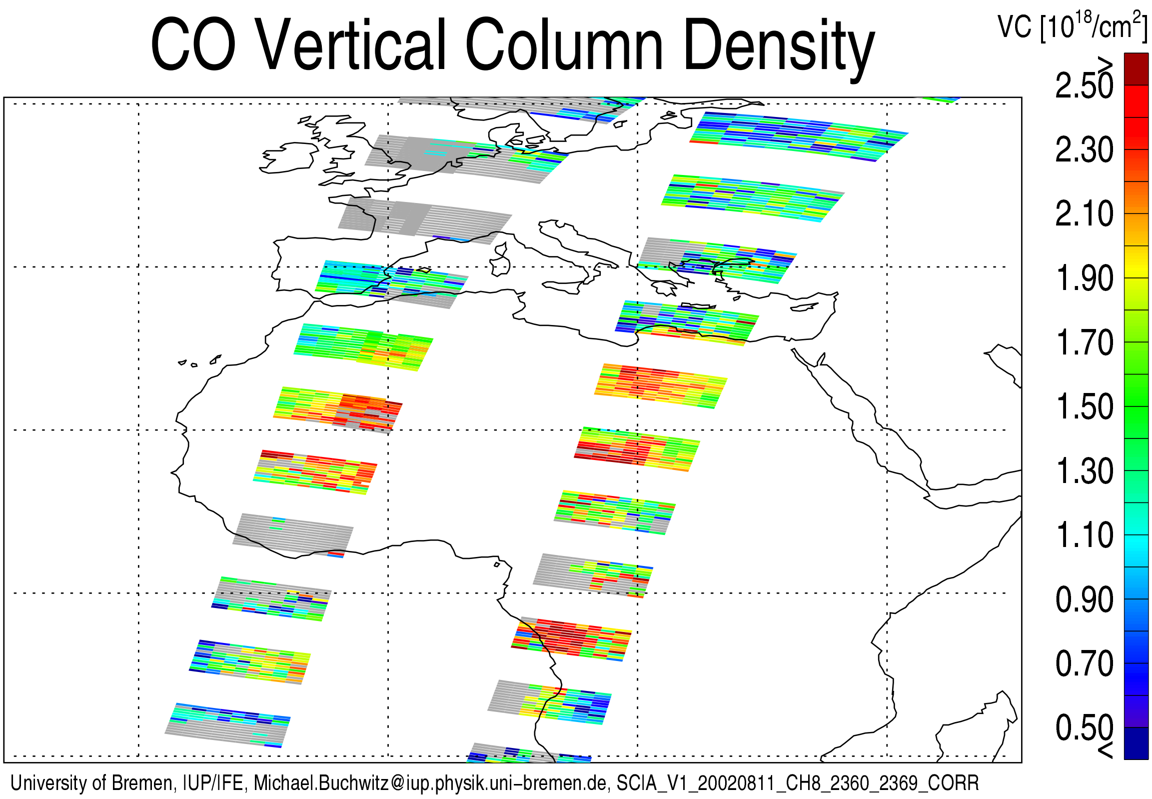

Figure 4: Preliminary CO columns as derived with WFM–DOAS. The fit errors are typically 80% (best values ∼30%). Example fit: Fig. 3.

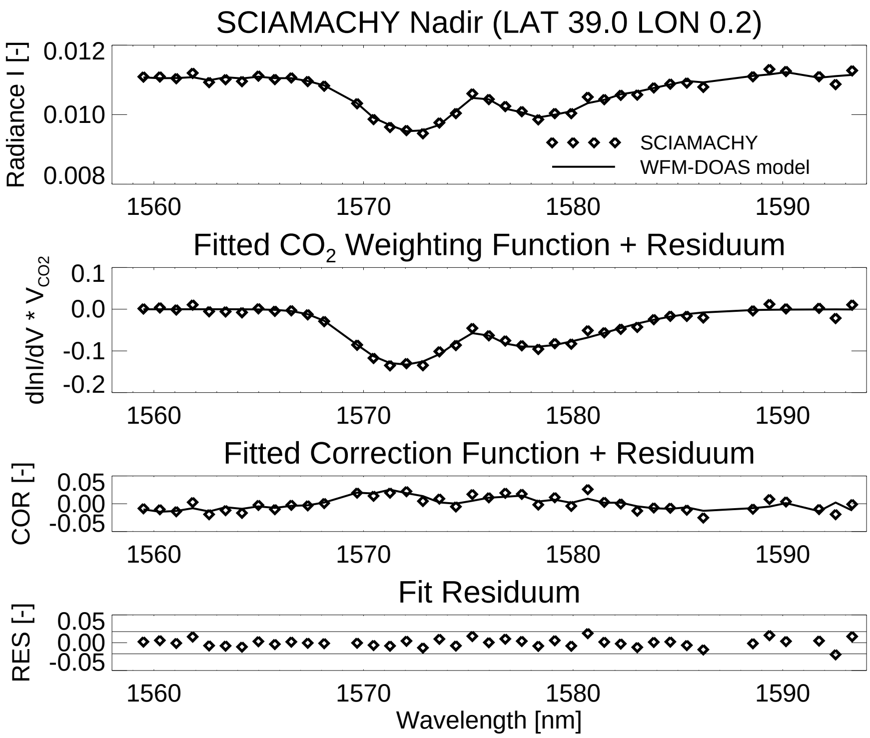

Figure 5: Example of a WFM–DOAS fit as applied to a channel 6 nadir measurement over the Mediterranean Sea (fitting window: WFM_DOAS_0). The retrieved CO_2 column is 8.90x10^{21} molec./cm^2 ±7% (without correction function: 7.08x10^{21} molec./cm^2 ±7%).

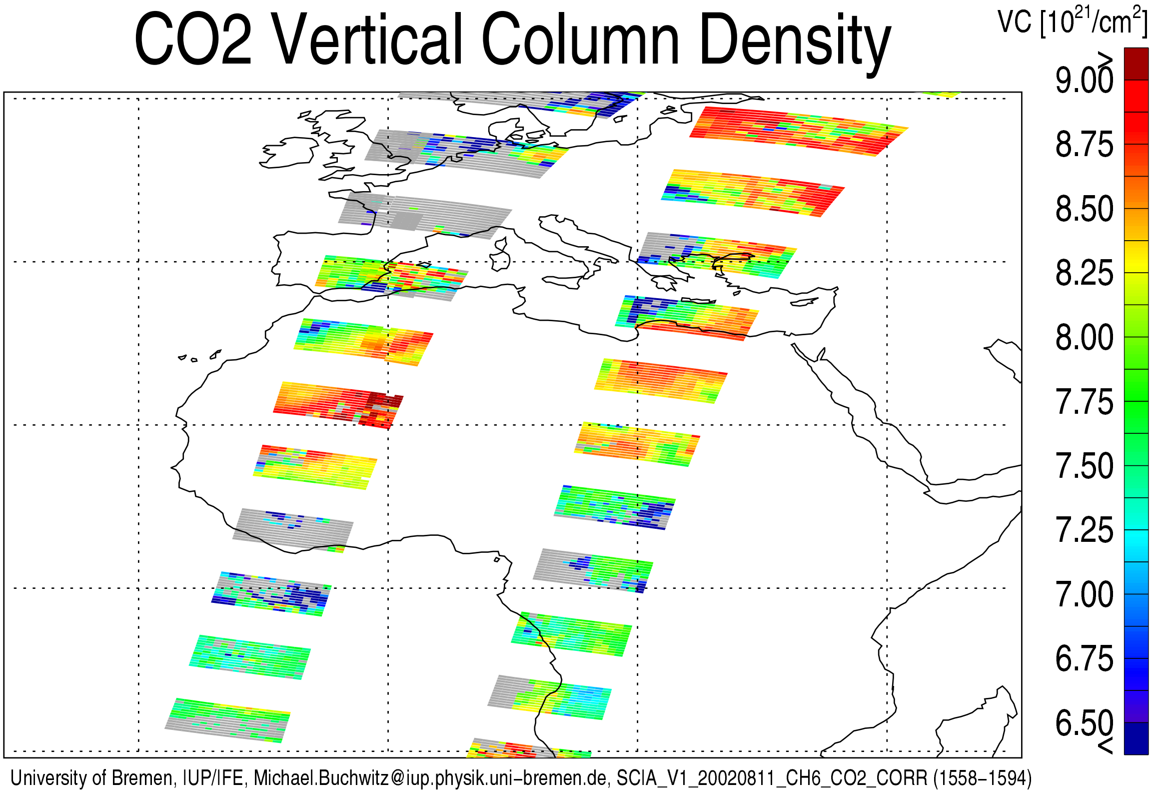

Figure 6: Preliminary CO_2 columns as derived with WFM–DOAS. Expected structures in the column field resulting from surface topography are clearly visible. Example fit: Fig. 5.

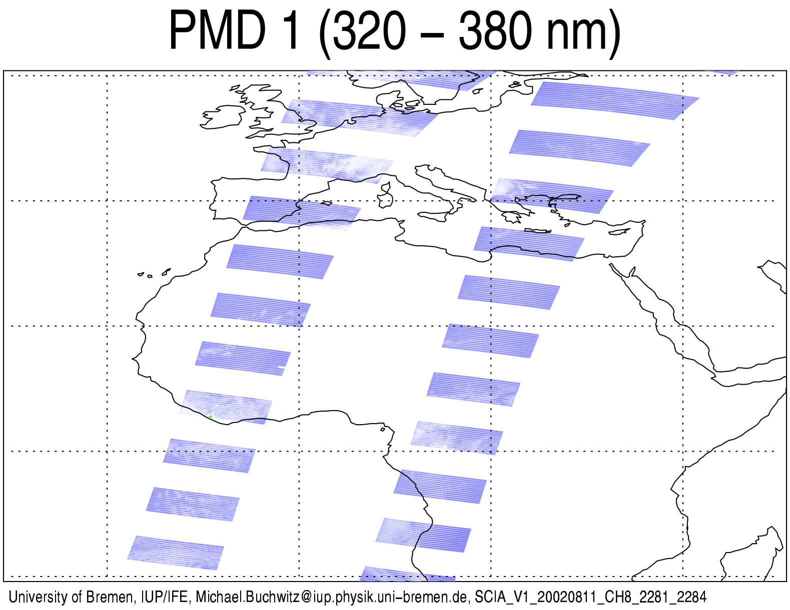

Figure 7: Broadband signal of SCIAMACHY's UV Polarisation Measurement Device (PMD) used for cloud detection.

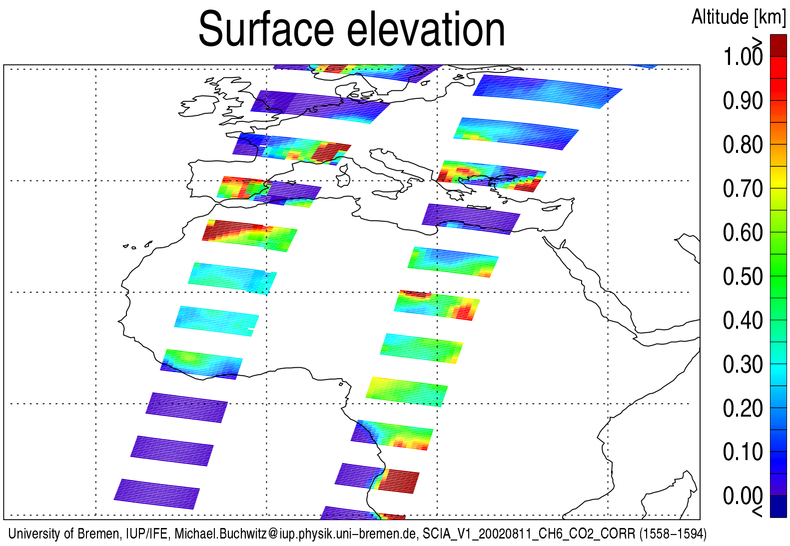

Figure 8: Average Earth surface elevation for orbits 2338 (left) and 2337.

4 WFM–DOAS BIAS COMPARISON

Figures 9–11 show a comparison of the WFM–DOAS derived columns with the corresponding BIAS derived columns (orbit 2338 from VERSION 1). The grey rectangles in the top and middle panels show the expected range of (climatological) columns. Ground pixels marked grey in the bottom panel are cloud contaminated ground pixels.

As can been seen, the BIAS columns are generally far outside the range of reasonable values (this is also true for the VERSION 2 data not shown here). Note that ground pixel numbers ∼600–1000, where the BIAS columns are closer to realistic columns, correspond to the Sahara region (high albedo) where the radiance levels are relatively high and the dark signal correction is not so critical as compared to low albedo scenes. The WFM–DOAS columns are generally within the range of reasonable values.

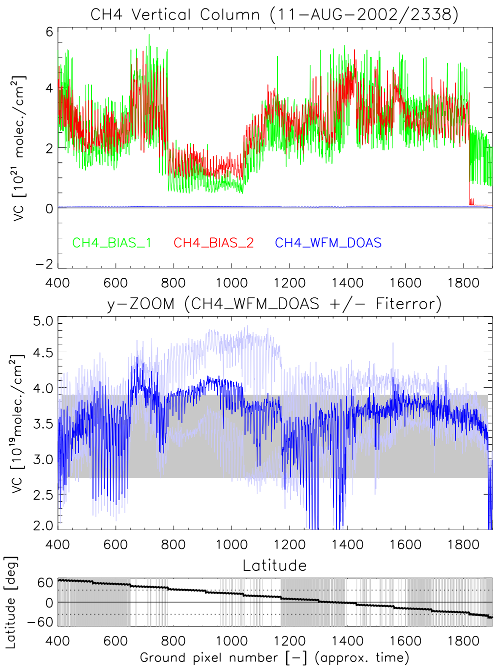

Fig. 9. BIAS - WFM–DOAS comparison: CH_4. WFM–DOAS fitting window: WFM_DOAS_1.

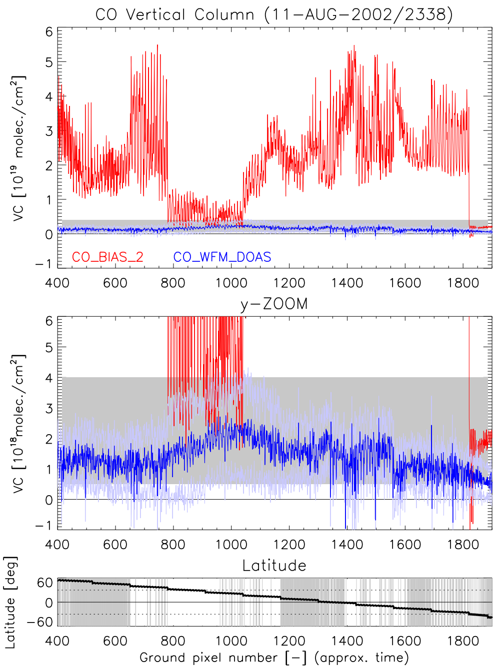

Fig. 10. BIAS - WFM–DOAS comparison: CO. WFM–DOAS fitting window: WFM_DOAS_2.

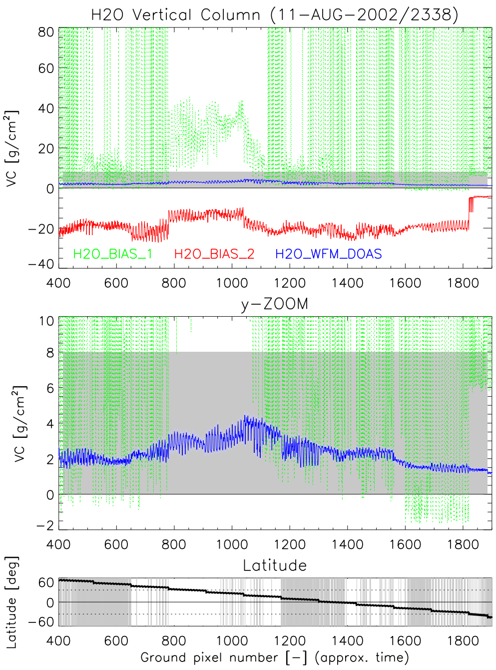

Fig. 11. BIAS - WFM–DOAS comparison: H_2O. Vertical column unit: g/cm^2. WFM–DOAS fitting window: WFM_DOAS_2 (optimized for CO retrieval, not for H_2O; WFM–DOAS H_2O as shown here is only a by-product with reduced quality).

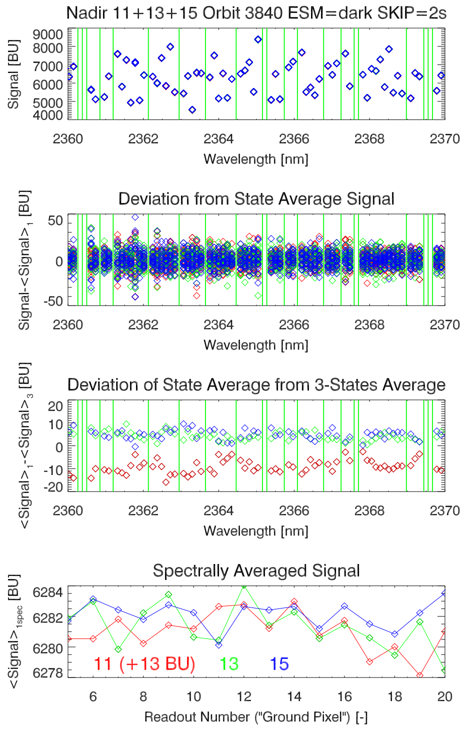

Fig. 12. Analyis of the "dark signal" of 3 nadir/dark–states (data set NDAS; states 11, 13, and 15; last 16 readouts for each state when scan mirror points inside instrument). The green vertical lines correspond to dead/bad pixels (excluded). Top panel: Overplot of the signals of the individual readouts. Second panel: as top panel but average signal subtracted. Third panel: average signal for each state (mean value over all 3 states subtracted).

5 ANALYSIS OF VERSION 2 DATA AND NADIR/DARK STATES

In this section VERSION 1 and 2 data and nadir/dark–states are analysed and compared. The analysis is restricted to the CO fitting window in channel 8 (WFM_DOAS_2) and three consecutive nadir states (one state over the Mediterranean Sea followed by two states over north Africa). In order to investigate a possible solution of the NIR dark signal correction problem mentioned above, special nadir/dark–states have been defined. They were executed on November 24, 2002. Here, during the last 10 seconds of each nadir state, the nadir scan mirror is rotated such that (ideally) no atmospheric light can enter the instrument. The basic idea is to have quasi real-time dark signal measurements. Figure 12 shows a first analysis of these measurements. From this figure it can be concluded that: (i) The variability (noise) of the (0.5 s) dark signal spectra (per state, i.e., within $\sim$1 minute) is less than about 30 BU (0.5% of 6000 BU). (ii) The difference between the average dark signals of the three states is approx. 25 BU (for each state the last 16 readouts have been averaged). External stray light seems to significantly contribute to this difference as concluded from the dark signal difference between states 13+15 (north Africa = high albedo scene) in comparison with state 11 (Mediterranean Sea = low albedo scene). The signal difference between state 11 and states 13+15 is $\sim$13 BU per 0.5 s (average over fitting window). (iii) The variability of the dark signal averaged over the fitting window is less than approx. 4 BU (per 0.5 s) within 8 seconds (last 16 readouts per state).

In order to assess the usefulness of these data for retrieval, four different sets of data have been analysed by WFM–DOAS (see Tab. 2). Each set consists of three consecutive nadir states as described above (state duration 65 s, 0.5 s integration time, 130 ground pixels per state; first state: ground pixel number 1–130 of Fig. 13; followed by two states with ground pixel numbers 131–390). The geolocation of the corresponding ground pixels of the data sets is not exactly identical but similar (they are exactly identical only for data sets V2_A and V2_D). All ground pixels correspond to (nearly) cloud free conditions (as concluded from the SCIAMACHY PMD measurements or - for orbit 3840 - from TOMS reflectivity). Data set V2_D has been included as the NDAS data are (also only) dark signal corrected Level 0 data (the nadir/dark–states are not included in the Level 1 files).
All four data sets have been identically processed by WFM–DOAS (a “Correction Function” has not been included). From Fig. 13 it can be concluded that for measurements over land the NDAS measurements (blue curves) enable the best retrieval: compared to VERSION 2 data (which are announced to reflect best current operational Level 0–1 processing, incl. dark signal correction) the RMS of the fit residuals are smaller and - also very important - the retrieved methane columns (although probably underestimated) show less of the strange scan angle synchronized variability visible in all the other data sets (one nadir scan corresponds to 10 nadir ground pixel: 8 forward pixel (pixel number 1–8, 11–18, .., 381–388) and 2 backward scan pixel (9–10, 19–20, ...)). Further study is needed to find out if and by how much NDAS-type measurements may help to improve the retrieval over water (no detailed optimization of the retrieval has been done so far). The (blue) NDAS curve shown in the bottom panel clearly shows how challenging this problem is: The rectangular bumps of the NDAS curve (pixel numbers 111–130, 241–260, and 371–390) correspond to the (uncorrected dark) signal obtained with the nadir mirror pointing inside the instrument. The y–values for ground pixel numbers less than 110 show the (dark signal corrected) nadir signal for measurements over water, the y–values corresponding to pixel number 110 show the (uncorrected) signal when the mirror points inside the instrument. The dark signal is approx. two orders of magnitudes larger than the nadir signal obtained over water. Note that not all data for V2_A have been processed because of (many irregularly appearing) negative radiance values in the Level 1 file (therefore the red line starts at approx. pixel number 100). Negative radiance values are also present in the other data sets (only exception: V1_A). From the close agreement of the (red) V2_A and the (green) V2_D curves it can be concluded that - at this stage - only the dark signal correction matters.

Table 2: Description of the four data sets mainly used for nadir/dark–states analysis.

ID	Data set description	Orbit
V1_A	VERSION 1, Level 1c, fully calibrated (except polarisation)	2337 (11-Aug-2002)
V2_A	VERSION 2, Level 1c, fully calibrated (except polarisation)	2509 (23-Aug-2002)
V2_D	VERSION 2, Level 1c, dark signal correction only (-cal 1,5)	2509 (23-Aug-2002)
NDAS	Level 0, dark signal from same nadir state (last 10 seconds)	3840 (24-Nov-2002)

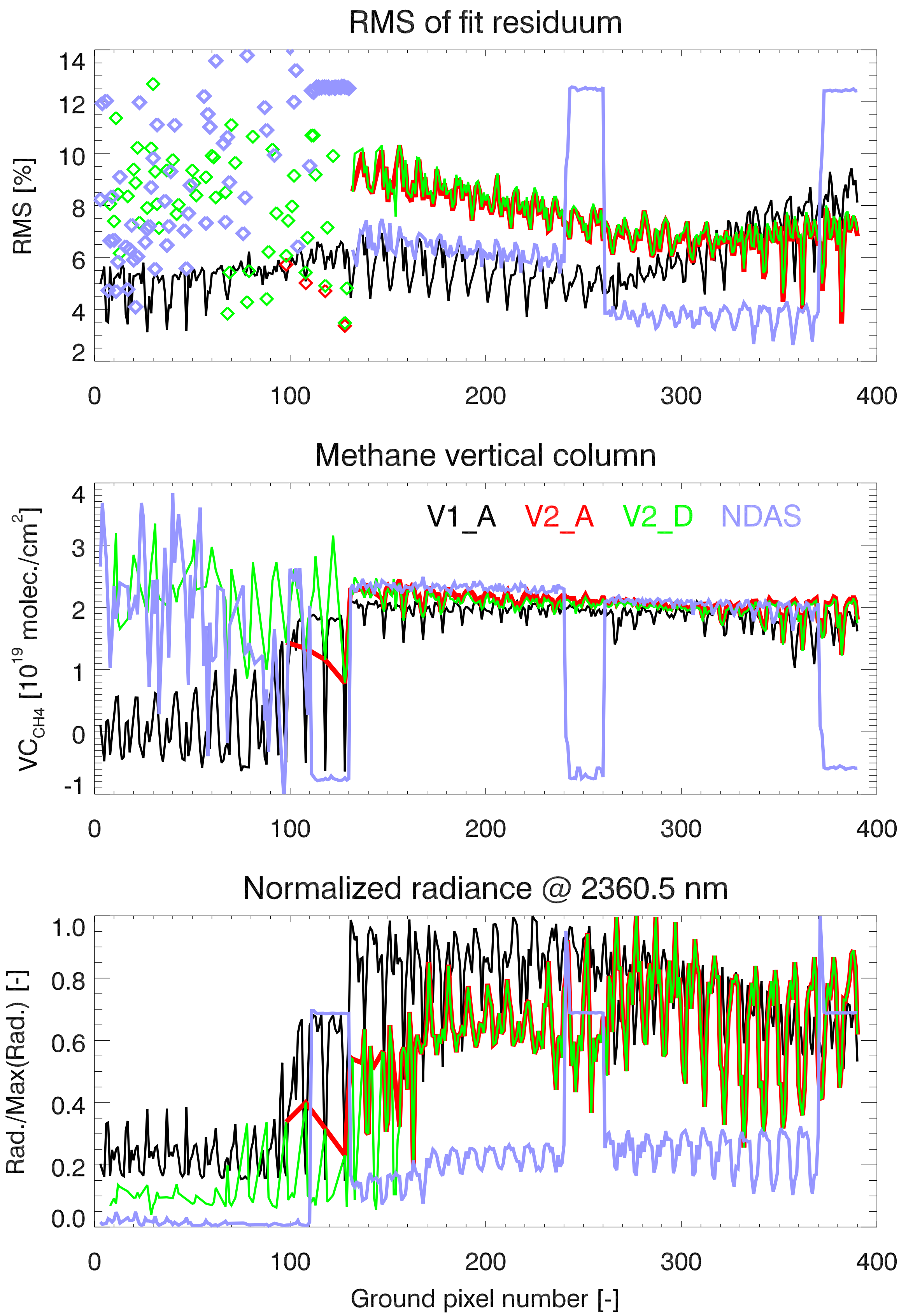

Figure 13: WFM–DOAS analysis of the four data sets described in Tab. 2. See section 5. for a detailed discussion.

6 CONCLUSIONS

Initial SCIAMACHY Level 1 and NRT Level 2 data products made available for verification purposes have been investigated in this study (VERSION 1 and 2 data sets). By applying WFM–DOAS to VERSION 1 data it was found that the fit residuals are dominated by systematic (rather stable) spectral features, not by instrument noise. Based on this finding a "Correction Function" has been determined and included in WFM–DOAS resulting in better fits and resonable trace gas columns. Concerning VERSION 2 Level 1 spectra only the important region of the CO band in channel 8 has been investigated so far: Here, in contrast to VERSION 1 data, the spectra over water (e.g., Mediterranean Sea) suffer from many negative radiance values in the Level 1 file. The wavelength calibration, however, has been improved with respect to VERSION 1 ("0.3 nm shift" issue [3]). This study suggests that the radiometric calibration of the NIR channels needs to be significantly improved to enable the retrieval of accurate vertical column amounts of, e.g., CH_4 and CO. The main problem seems to be the dark signal correction. The corresponding VERSION 1 and VERSION 2 CH_4, H_2O, N_2O, and CO operational NRT BIAS vertical column data products strongly deviate from climatological values. They cannot be considered scientifically useful at present. In comparison, the accuracy of the WFM–DOAS derived columns is shown to be significantly higher. First steps have been undertaken in analysing the special nadir/dark–states executed on November 24, 2002. First results indicate that these states enable a better dark signal correction, resulting in significantly better spectra and more accurate trace gas columns (at least over land, for measurements over water more studies are needed).

7 REFERENCES

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