RETRIEVAL OF TRACE GAS VERTICAL COLUMNS FROM SCIAMACHY/ENVISAT NEAR-INFRARED NADIR SPECTRA: FIRST PRELIMINARY RESULTS

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ABSTRACT

The European environmental satellite ENVISAT was successfully launched on 1st of March 2002. The UV/visible/near-infrared grating spectrometer SCIAMACHY is part of ENVISAT's atmospheric science payload. SCIAMACHY observes the atmosphere in nadir, limb, and solar and lunar occultation viewing geometries with moderate spectral resolution (0.2-1.5 nm). At the University of Bremen a modified DOAS algorithm (WFM-DOAS) is being developed primarily for the retrieval of CH_4, CO, CO_2, H_2O, N_2O, and O_2 total column amounts from ratios of SCIAMACHY nadir radiance and solar irradiance spectra in the near-infrared and visible spectral regions. First preliminary results concerning this activity are presented. SCIAMACHY is currently (Sept. 2002) in its commissioning phase and only preliminary, i.e., not yet fully calibrated, Level 1 data products are available, generated mainly for initial Level 0 to 1 processing verification purposes. A method aimed at improving the retrieval in case of systematic artifacts resulting from, e.g., residual calibration errors, is presented. This study focuses on methane vertical column retrieval using channel 8 (2260–2385 nm). One of the major scientific objectives of the SCIAMACHY methane measurements is to derive information on methane (surface) sources and sinks. Such an application requires a relative radiometric accuracy close to the signal–to–noise performance of the instrument (S/N $\sim$ 50–100 in channel 8 for albedo 0.1 and solar zenith angle 60°) and an accurate and fast retrieval algorithm. This study presents first steps undertaken to reach this ambitious goal, focusing on the retrieval algorithm.

INTRODUCTION

WFM–DOAS (Weighting Function Modified Differential Optical Absorption Spectroscopy) is a modified DOAS algorithm (Buchwitz et al., 2000a) mainly being developed for the retrieval of trace gas vertical column densities from SCIAMACHY (Bovensmann et al., 1999) and GOME/ERS-2 (Burrows et al., 1999) nadir radiance and solar irradiance spectra. The term vertical column density (or simply vertical column) refers to the vertically integrated concentration profile of a given trace gas (unit: number of molecules per area). Initial results concerning the application of this algorithm to preliminary SCIAMACHY Level 1c nadir spectra (Slijkhuis, 2000) are presented. WFM–DOAS is independent of the official ESA/DLR ENVISAT operational Level 1 to 2 algorithms and Level 2 data products which are not discussed here. Analysis of simulated SCIAMACHY nadir measurements indicates, as shown by Buchwitz et al. (2000a), that the retrieval precision (defined as measurement error due to instrument noise) is about 1% for CH_4, H_2O, and CO_2, and about 10% for the weak absorbers CO and N_2O. In order to obtain a retrieval accuracy close to these values, systematic retrieval errors resulting from, e.g., residual calibration errors or retrieval algorithm limitations, need to be minimized as much as possible. This study focuses on orbit 2338 (11-Aug-2002) covering parts of central Europe and western Africa.

DESCRIPTION OF THE WFM–DOAS RETRIEVAL ALGORITHM

WFM–DOAS is based on fitting a linearized radiative transfer model I_i^{mod} plus a low–order polynomial P_i to the logarithm of the ratio of a measured nadir radiance and solar irradiance spectrum, i.e., observed sun-normalized radiance I_i^{obs}. Index i refers to the center wavelength λ_i of (linear diode array) detector pixel number i. Provided there exists an appropriate spectral fitting window, I_i^{obs} depends on the true but unknown vertical columns of the trace gases of interest (components of vector $\mathbf{V}^t$). The WFM–DOAS equation can be written as follows:

$$\left\| \ln I_i^{obs}(\mathbf{V}^t) - \left[\ln I_i^{mod}(\bar{\mathbf{V}}) + \sum_{j=1}^{J} \frac{\partial \ln I_i^{mod}}{\partial V_j} \bigg|_{\bar{V}_j} \times (\hat{\underline{V}}_j - \bar{V}_j) + P_i(\underline{a_m}) \right] \right\|^2 = \|RES_i\|^2 \rightarrow min. \quad (1)$$

A derivative, or weighting function, with respect to a vertical column refers to the change of the radiance due to a change (scaling) of a pre-selected trace gas vertical profile. To simplify the notation, the dependence of the radiance on other important parameters (e.g., temperature profile or albedo) has been omitted in Eq. (1). In the following the term in square brackets is called the WFM–DOAS model. The WFM–DOAS reference spectra are the logarithm of the sun–normalized radiance and its derivatives. They are computed with the radiative transfer model SCIATRAN (Buchwitz et al., 2000b) for assumed (e.g., climatological) "mean" columns $\bar{\mathbf{V}}$. The fit parameters (underlined in Eq. (1)) are the desired trace gas vertical columns $\hat{V}_j$ and the polynomial coefficients a_m. An additional fit parameter also used in this study is the temperature profile shift. The fit parameters are determined by minimizing (in least–squares sense) the difference between observation and WFM–DOAS model, i.e., fit residuum RES_i.

In order to avoid time consuming on-line radiative transfer simulations, a look-up table approach has been implemented. The reference spectra have been generated for cloud free conditions assuming a US Standard Atmosphere (CH_4 and CO_2 scaled to current concentrations), a tropospheric maritime and stratospheric background aerosol scenario, a surface albedo of 0.1, and direct nadir observation. The scan angle dependence is taken into account using a simple geometrical correction (Buchwitz et al., 2000a). The tabulated reference spectra depend on solar zenith angle ($0°$-$90°$ in steps of $5°$), surface elevation (0, 1, 2, 3 km) and water vapor column (scaling factors: 0.5, 1.0, 1.5, 2.0, 4.0). WFM–DOAS has been implemented as an iterative scheme, mainly to account for the high variability of atmospheric water vapor.

The (fast) look-up table approach introduces errors. Most of the CH_4 retrieval results presented in this study have been generated using a small fitting window (2281.7-2284.6 nm) in channel 8. The error introduced by the currently implemented look-up table has been estimated by applying the algorithm to simulated measurements. Table 1 summarizes the results. As can be seen, the error is below 1% in most cases.

APPLICATION OF WFM–DOAS

Water vapor vertical column retrieval using GOME data

Before the first SCIAMACHY data were available, WFM–DOAS was tested using GOME nadir spectra (Burrows et al., 1999). The first four channels of GOME and SCIAMACHY are nearly identical. The main difference is the spatial resolution, which is better for SCIAMACHY. WFM–DOAS has been applied to the 685–710 nm spectral region (channel 4) to retrieve water vapor total column amounts (see Fig. 1). In addition to H_2O, O_2 (to account for clouds) and temperature (to improve the accuracy of the retrieved H_2O columns) has been included in the fit. The GOME derived H_2O columns have been compared with the Daily Gridded Integrated Water Vapor data product routinely generated from SSM/I microwave measurements (Fig. 2). The comparison has been limited to cloud free scenes (GOME limitation) over water (SSM/I limitation). Good agreement has been found between GOME and SSM/I. However, the GOME derived columns are $\sim$15% too low compared to SSM/I. This is probably due to albedo effects (see Tab. 1) in combination with (now improved) spectroscopic data (Rothman et al., 1998).
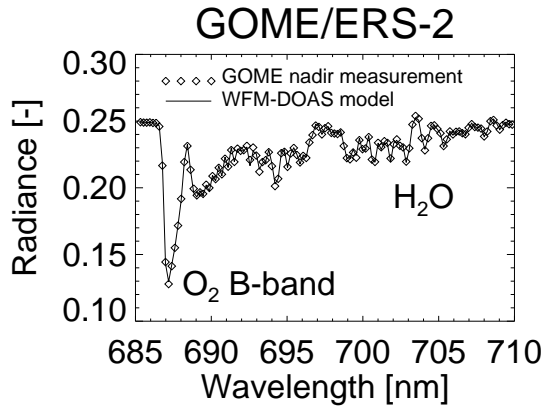
GOME/ERS-2

Fig. 1. Example of a WFM-DOAS fit as applied to a GOME channel 4 nadir spectrum obtained over the Atlantic Ocean near Ireland.
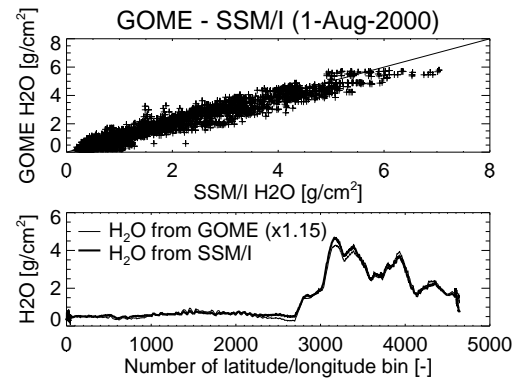

Fig. 2. Typical result of the comparison of GOME and SSM/I derived H_2O columns. The GOME derived columns have been enhanced by 15%. Bottom panel: same data but different representation (smoothed for better visibility).

Table 1. WFM-DOAS CH_4 vertical column retrieval error estimated using simulated measurements (solar zenith angle (SZA) 30°, except No. 6). Difference between error A and B: For B a temperature profile shift parameter is included in the fit.

No.	Investigated error source	True CH_4 [10^{19}mol./cm^2]	Retrieved CH_4 error A [%]	Retrieved CH_4 error B [%]
1	Simu. measurement $\simeq$ reference scenario (test of, e.g., wavelength interpolation)	3.65	0.0	0.0
2	Albedo 0.025	3.65	–0.7	–0.4
3	Albedo 0.05	3.65	–0.3	–0.1
4	Albedo 0.4	3.65	0.6	0.6
5	Line–of–sight scan angle correction	3.65	–1.0	–0.9
6	SZA interpolation (SZA=32.5°)	3.65	0.0	0.0
7	Surface elevation 0.75 km	3.33	–0.5	-1.0
8	No aerosol in atmosphere	3.65	–0.6	–0.6
9	Enhanced water vapor ($\times$ 1.8)	3.65	0.0	0.0
10	Reduced water vapor ($\times$ 0.6)	3.65	0.0	0.0
11	Tropical atmosphere	3.66	–4.5	1.0
12	Midlatitude summer atmosphere	3.51	–3.3	–0.5
13	Enhanced CH_4 in BL (1.75 $\rightarrow$ 2 ppmv)	3.74	0.2	–0.3

Application to SCIAMACHY channel 8

Typical results of WFM–DOAS as applied to SCIAMACHY spectra in the region 2281.7-2284.6 nm are shown in Figures 3 and 4 which refer to fits with and without including a correction spectrum (see below), respectively. WFM–DOAS (performed without any correction) revealed a clear correlation between the quality of the retrieval and the radiance level, which in turn is primarily determined by the surface reflectivity of the corresponding ground pixel: The higher the radiance (or reflectivity), the better the fit. Over sand (Sahara) the quality of the fit is best (reasonable albeit underestimated methane columns, relatively small fit residuals) but over water (Atlantic Ocean, Mediterranean Sea) significantly worse. However, the fit residuals are rather systematic, i.e., not dominated by noise. Non-optimal dark signal correction might explain the observed systematic artifacts. Especially in channel 8 the dark signal is high (mainly resulting from thermal emission of the optical bench) and a small error in dark signal correction can result in a relatively large (relative) radiance error, especially over low albedo scenes.

Based on this and related studies performed during the commissioning phase the need to improve the dark signal calibration - especially of the NIR channels - had been recognized. As a result, better in–orbit dark signal measurements have been performed since December 2002. Optimal use of these measurements requires modification

of Level 0–1 processing (Slijkhuis, 2000) followed by reprocessing (expected for 2003).

In order to deal with the spectral artifacts present in the test spectra available for this study, a correction scheme has been developed. It is based on an estimation of the spectral behavior of the systematic measurement error using a small number of nadir pixels. The resulting "correction spectrum" has been included in the fit, leading to an additional term (including fit parameter) in Eq. (1). The correction spectrum consists of basically two terms. One term is the fit residuum RES_i^k determined for ground pixel k by applying a WFM–DOAS fit without any correction. This term is orthogonal to the subspace of measurement space spanned by the weighting functions. The second term lies in weighting function space and is estimated using pre-defined columns $V_j^{\hat{t}}$ appropriate for the time and location of the measurement (here: reasonable guess). $V_j^{\hat{t}}$ can be – but does not need to be – identical with $\bar{V}_j$ (see Eq. (1)). The correction spectrum (see also Fig. 3) is defined as follows (i refers to wavelength):

$$COR_i \;=\; \left\langle COR_i^k \right\rangle_{k=1,K} \;=\; \left\langle RES_i^k \;+\; \sum_{j=1}^{J} \left. \frac{\partial \ln I_i^{mod}}{\partial V_j} \right|_{\bar{V}_j} \times (\hat{V}_j^k - V_j^{\hat{t}}) \right\rangle_{k=1,K} \tag{2}$$

The averaging symbol $<>$ refers to averaging K corrections functions COR_i^k determined individually for K ground pixels. Here $K=8$ consecutive ground pixels over the Atlantic Ocean at approx. 15°S latitude have been chosen. A WFM–DOAS retrieval (without any correction) has been applied to each of the K ground pixels resulting in K fit parameter values $\hat{V}_j^k$ for each of the J trace gases considered simultaneously in the fit (here $J=3$: CH_4 (main absorber), H_2O and N_2O (weak)). Including this correction spectrum significantly improves the quality of the fit, resulting in smaller fit residuals and more accurate columns (compare Figures 3 and 4), basically for all ground pixels along the orbit (Fig. 5), but especially over water. Note that the correction spectrum potentially not only accounts for measurement errors but might also help, at least to a certain extent, to correct for algorithm inaccuracies, e.g., interpolation errors, convolution errors (slit function uncertainties) or errors of the spectroscopic data.

Cloud contaminated ground pixels have been identified using sub-pixel (approx. 30×7 km^2) Polarization Measurement Device (PMD) measurements. SCIAMACHYs UV PMD has been selected because of its high sensitivity to scattering by (not too low) clouds in combination with its relatively low sensitivity to other parameters (albedo, gas absorption). A simple threshold algorithm has been used for this study to generate a cloud mask.

Figure 7 shows an other example of a WFM–DOAS fit. Here a fitting window in the CO absorption region of channel 8 has been selected. The spectral absorption features of CH_4 and H_2O have clearly been identified. The fit residuum, however, exceeds the rather weak ($\sim$2%) absorption signal of CO. It is expected that an improved radiometric calibration and/or further retrieval algorithm refinements will result in better fits.

SCIAMACHY CHANNEL 6 AND 7: CO$_2$

SCIAMACHY channels 6 and 7 cover absorption bands of CO_2. Fig. 8 shows SCIAMACHY sun-normalized radiance spectra in spectral regions mainly foreseen for CO_2 total column retrieval. The CO_2 absorption features are clearly visible in the SCIAMACHY spectra. One of the main scientific objectives of the SCIAMACHY CO_2 total column measurements is to constrain CO_2 surface sources and sinks (as for CH_4) in order to improve our current knowledge of the carbon cycle. The requirements on data and algorithms for this task are probably even higher than for methane.

OUTLOOK

Recently ESA has made available a limited number of orbits with an improved dark signal calibration (still not yet fully calibrated, e.g., with respect to polarization correction, in–orbit pixel–to–pixel gain correction and wavelength calibration). These spectra are currently being analyzed by WFM–DOAS without including any correction functions. Preliminary results have been presented by Buchwitz et al. at the EGS–AGU–EUG Joint Assembly, Nice, France, 6-11 April 2003. An electronic version of the poster can be downloaded from the University of Bremen WFM–DOAS web page `http://www.iup.physik.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/`. The improved spectra enable the retrieval of reasonable methane and CO_2 columns (retrieved from SCIAMACHY channel
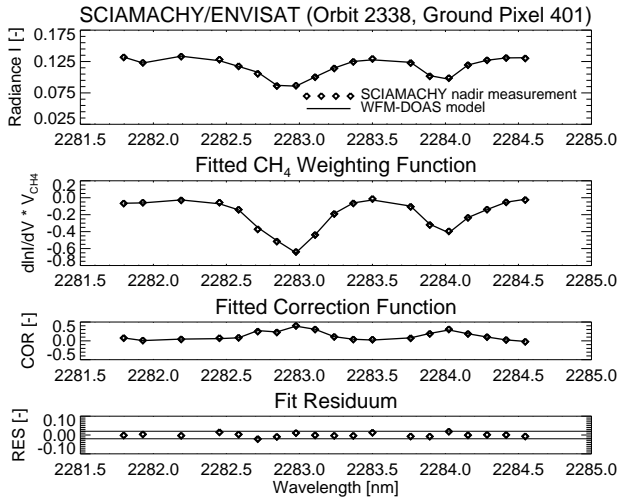
6) without any correction function.

Fig. 3. Example of a WFM-DOAS fit as applied to a SCIAMACHY channel 8 nadir measurement over the Mediterranean Sea. The agreement between measurement and WFM–DOAS model is within 2% as can be seen in the bottom panel. The squares in the second panel denote the CH_4 fit residuum, defined as fitted CH_4 weighting function (= derivative times fit parameter) plus fit residuum. The retrieved methane column is 3.76×10^{19} molec./cm$^2 \pm 6\%$ (fit error estimated from residuum).
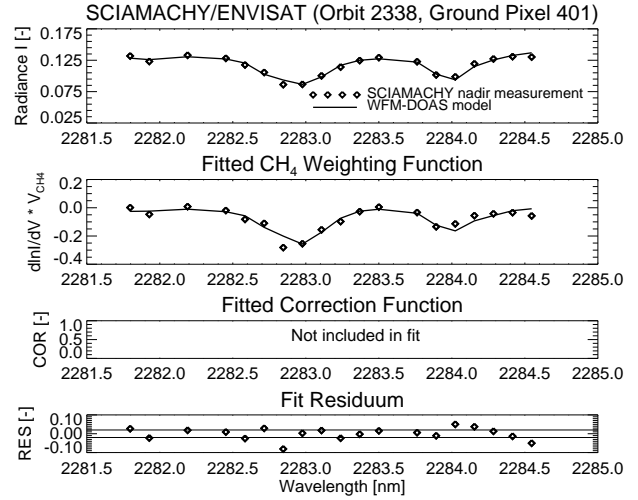
Fig. 4. As Figure 3. but without including the correction spectrum in the fit. The retrieved methane column is 1.49×10^{19} molec./cm$^2 \pm 14\%$ (clearly underestimated).
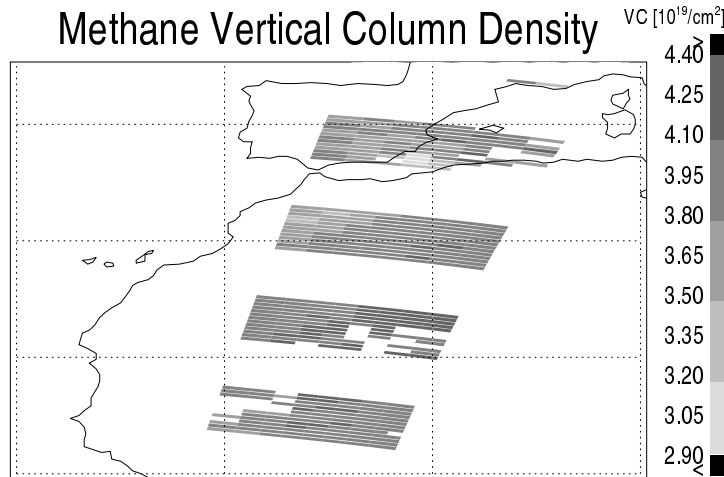
Fig. 5. Methane vertical columns retrieved from orbit 2338 (11 August 2002). The spatial resolution is approx. 30×120 km^2. The columns retrieved for cloud contaminated ground pixels (see Fig. 6) are not shown. Clearly visible are the expected relatively low methane columns over the Atlas mountains resulting from decreasing surface pressure (i.e., air mass) with increasing ground altitude.
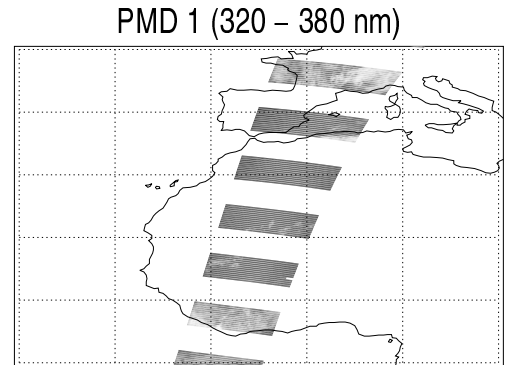
Fig. 6. Broadband signal of PMD 1 used for generating the cloud mask for Fig. 5 (using a threshold determined by visual inspection). Low signal corresponds to dark-grey, high signal to light-grey (mainly clouds). Clearly visible are the cloud structures in the lower and upper part of the PMD image.
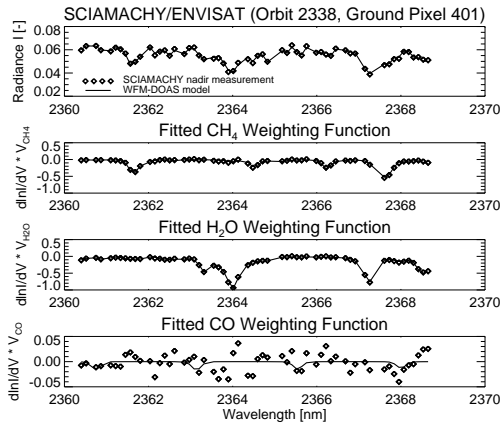
Fig. 7. Example of a WFM-DOAS fit as applied to a SCIAMACHY nadir measurement over the Mediterranean Sea for a spectral fitting window in the second half of channel 8.
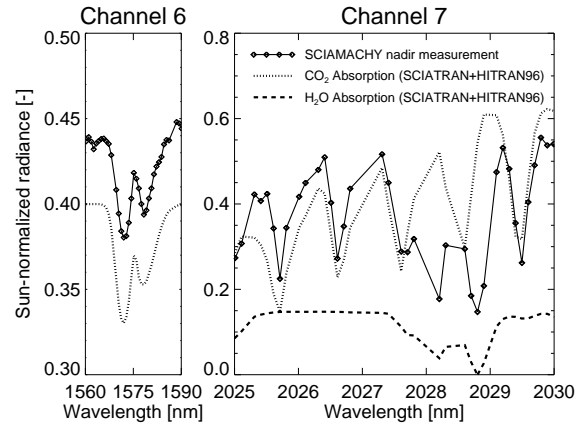

Fig. 8. SCIAMACHY nadir spectra showing spectral regions in channel 6 and channel 7 to be used for CO_2 retrieval. The dotted and dashed lines show the absorption features of CO_2 and H_2O (vertically shifted and scaled).

CONCLUSIONS

First preliminary results have been presented concerning the WFM–DOAS retrieval of total column amounts of important atmospheric trace gases from SCIAMACHY (and GOME) near-infrared nadir measurements. In this study only initial - not fully calibrated - test data have been analysed (one orbit). Nevertheless, the absorption features of CH_4, H_2O, and CO_2 have been clearly identified in the SCIAMACHY nadir spectra. The fit residuals are currently significantly larger than instrument noise. In order to deal with the rather systematic spectral artifacts present in the analysed spectra, a correction spectrum has been determined (using nadir pixels of one nadir scan in the southern hemisphere) and included in the fit, resulting in significantly better fits and more accurate columns (all along the orbit). More studies, an improved calibration, and algorithm refinements are needed to enable accurate retrievals of CH_4, H_2O, CO_2, CO and N_2O columns.

ACKNOWLEDGEMENTS

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