

VERIFICATION OF CO, CH₄, AND CO₂ RETRIEVED TOTAL COLUMNS FROM THE SCIAMACHY NEAR-INFRARED CHANNELS

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ABSTRACT

The first results from the retrieval of methane (CH₄), carbon monoxide (CO), and carbon dioxide (CO₂) total columns from the SCIAMACHY instrument are now available. Although the columns retrieved by the operational BIAS product do not yet show physically consistent variations, the first results from in-house scientific algorithms look promising. The verification and validation work has just started. The actual quality of the measurements will be established during the coming 1-2 years by comparison with other satellite measurements and with measurements from ground-based stations.

1. INTRODUCTION

With the launch of the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) instrument onboard the ENVISAT satellite on 1 March 2002, the global distribution of CO, CH₄, H₂O, N₂O, and CO₂ is being measured for the first time by a medium-resolution grating spectrometer in the near-infrared (NIR) region between 1000 and 2380 nm. The aim of this paper is to verify the official retrieved NIR nadir tracer columns delivered by ESA. In order to determine the quality of these nadir total columns, the concentrations were compared to simulations by a chemical transport model and to scientific in-house retrieval products. This work is part of the SCIAMACHY Processors Calibration and Verification Plan (SPCVP) algorithm verification. The columns are also being validated within the AO 241 project "Validation of CO and METHane SCIAMACHY data products" (COMETH). Three methods are used; i) comparison with the results from independent retrieval algorithms developed at the SRON-National Institute for Space Research, ii) comparison with calculations by a chemical transport model, iii) comparison with products from another satellite instrument (MOPITT onboard EOS-TERRA). The technique of data assimilation will be used for the comparison of non-co-located satellite measurements. These methods allow for the identification of errors in the measured and modeled data. The comparison of the SCIAMACHY data with calculations by the chemical transport model TM3 is carried out in cooperation with the Institute for Marine and Atmospheric Research Utrecht (IMAU), and the comparison with the Canadian/American MOPITT instrument is done in cooperation with the National Center for Atmospheric Research (NCAR). The data assimilation will be carried out in cooperation with the Royal Netherlands Meteorological Institute (KNMI). An overview of the validation techniques is given in [1].

The SCIAMACHY instrument is stable and all instrument modes are functional and working well. The wavelength calibration is stable and the on-board calibration sources, the channel 1-6 dark currents, the analog offsets, and the throughput are as expected. The only anomaly is ice buildup in the NIR channels 7 and 8. The influence of the ice is relatively smooth and no spectral features are introduced. The main effect is a reduced signal-to-noise ratio. This anomaly has strongly influenced the retrieval from channel 7 and 8. The quality of the retrieved products from these channels will be limited until the influence of the ice on the transmission and the dark current signal has been fully characterized. In this paper, however, we show that retrievals done by our retrieval algorithms show promising results. This gives us the confidence that we will be able to retrieve the NIR trace gases with an acceptable accuracy when the detectors are fully calibrated and characterized. This work is now ongoing.

2. THE RETRIEVAL ALGORITHMS

The operational SCIAMACHY retrieval algorithm for channel 8 is the Basic near-Infrared Absorption Spectroscopy (BIAS) [2]. This technique uses a least square fitting of differences between a calculated and the modeled spectrum for

selected micro windows (see table 1). In the near-real-time (NRT) product look-up tables are used for determining the slant-path factors and line-by-line computed cross sections. The use of micro windows could lead to a higher sensitivity to dead and noisy pixels but it is foreseen to use information from the instrument model to correct for this.

Two retrieval algorithms have been developed at SRON for the retrieval of atmospheric trace gases from the SCIAMACHY NIR region. The first algorithm uses an iterative maximum likelihood method (hereafter called IMLM) for determining the atmospheric tracer concentrations from the radiance measurements. A modeled spectrum is then fitted to the measured spectrum in an iterative way. The calculation of the modeled spectrum starts with the calculation of optical depths deduced from a priori atmospheric profiles of the absorbing gases H₂O, CH₄, CO, and N₂O, temperature and pressure (US standard atmosphere). From these optical depths the earth radiance is calculated in a forward model, which is then transformed by a simplified instrument model to represent the radiation detected by the instrument detectors. Limits of the sensitivity of the retrieved CO and CH₄ concentrations due to detector noise was described by [3]. The paper showed that retrieved concentration of CH₄ has a precision of 1%, and that the lower limit for the precision of CO is down to 10% in most cases. This precision does not include model errors due to imperfect knowledge of the molecular spectrum, clouds, the omission of molecular scattering, etc., and it furthermore depends strongly on the surface albedo, latitude, and the total column amount of the trace gasses. In this paper a micro window was used for retrieving the CH₄, CO and H₂O column (see table 1), and the solar spectrum was taken from MODTRAN. Furthermore, the correct wavelength calibration and an additional mask to remove badly behaving pixels were used. Other adjustments of the retrieval due to the ice-growth are explained in chapter 4.

Because this algorithm only allows a scaling and not variation in the vertical trace-gas profile shape, a second and more detailed retrieval algorithm was developed based on Philips-Tikhonov-Twomey regularization (hereafter PTTR retrieval). This algorithm allows the vertical profiles to vary when fitting the measured and modeled spectra. It is therefore slower than the maximum likelihood method. The comparison of the two algorithms will help the understanding of the strengths and limitations of both algorithms under different atmospheric conditions. The quality of both algorithms will be established by validating the results by comparison with other independent measurements and model results.

The radiative transfer model for the PTTR retrieval is the same as the one used by IMLM. The approach is to fit the four vertical absorbing gas-profiles, an albedo factor in the form of a linear polynomial, and a baseline term in the form of a second linear polynomial. The retrieved profiles are then integrated in order to obtain total columns. Tropospheric inhomogeneities are represented by an altitude level discretization of about 20 levels. Pressure and temperature profile information is taken from the MSIS90 climatology [4]. There is no need for *a priori* information other than pressure and temperature profiles, since there appear to be approximately 10 degrees of freedom for signal in the modeled spectrum.

Table 1. Retrieval algorithm spectral fitting windows

Algorithm	Channel	Spectral region (nm)	Main fitting parameters
BIAS_1	8	2269.0-2275.0	N ₂ O (driver), CH ₄ , H ₂ O
BIAS_2	8	2360.0-2366.0	CO (driver), CH ₄ , H ₂ O
IMLM	8	2354.0-2371.0	CO (driver), CH ₄ , H ₂ O
PTTR retrieval	8	Discontiguous pixels throughout, excluding 2326-2334 nm	CO, CH ₄ , H ₂ O, N ₂ O

3. VERIFICATION OF THE BIAS PRODUCTS

3.1 The channel 8 calibration and data availability

The unanticipated ice deposition on the channel 7 and 8 detectors makes it necessary to calibrate the channel 8 radiances more frequently than was first anticipated, taking into account the reduction of the dark current signal with time. The operational processor at ESA was initially built to update the dark current signal in the annotation dataset once per month, but because the ice-layer reduces the transmission with up to a few percent per day (directly after each decontamination) an update of the dark current signal must be done at least once per orbit. Since October 2002 the dark current has been measured in the eclipse of every orbit, but these measurements are not included in the operational L0-1 processor at the time of writing. Because the dark signal measurement reported in the L1b files used by the ESA L1-2 processor can be up to one month old, the retrieved columns in the operational L2 product are not expected to be correct. Other changes to the on-ground calibration also had to be implemented in the L1b calibration annotation dataset; during the commissioning phase the SPCVP verification team found that the dead-and-bad pixel mask needed to be updated and that the wavelength calibration was wrongly implemented for the second half of channel 8. This is currently being updated in the key data used by the operational processor. The L2 data provided by ESA on CDROM and on the validation ftp site before December 16 2002 (when software version 4.0 was implemented) do not contain these updates and are thus frequently orders of magnitude too high, and the orbital column variations do not reflect the

real variation of the trace gas columns. Therefore a special verification dataset was made available to the SPCVP verification team on November 25 2002. The dataset contains the two orbits 2509 and 2510 where the dark signal was taken from a calibration orbit five orbits prior to 2509, and the updated dead-and-bad pixel mask and correct channel 8 wavelength calibration were used. The expected decrease in the dark signal during these 5 orbits was ~ 15 BU/s. Thus it was expected that the L2 NIR columns from these two orbits should be of the right order of magnitude and show physically consistent variations due to the above mentioned updates.

3.2 The BIAS total columns

The BIAS total columns from the verification orbits 2509 and 2510 (software version 4.0) for CH_4 (from two fitting windows), CO, and PMD measurements are shown in Fig. 1. The CH_4 concentrations from fitting window 1 are off by orders of magnitude (natural variation: $2 - 4 \times 10^{19}$ molec/cm²), and the values from the second window are of the right order of magnitude but the concentrations are largely negative. The CO columns are also off by orders of magnitude (natural variation: $1-4 \times 10^{18}$ molec/cm²) and they seem to be anti-correlated with the CH_4 columns. The reason for the still poor performance of the BIAS products may be related to still unresolved calibration features, possible unmasked badly-behaving (noisy) pixels within the BIAS fitting windows, and/or bugs in the L1-2 processor.

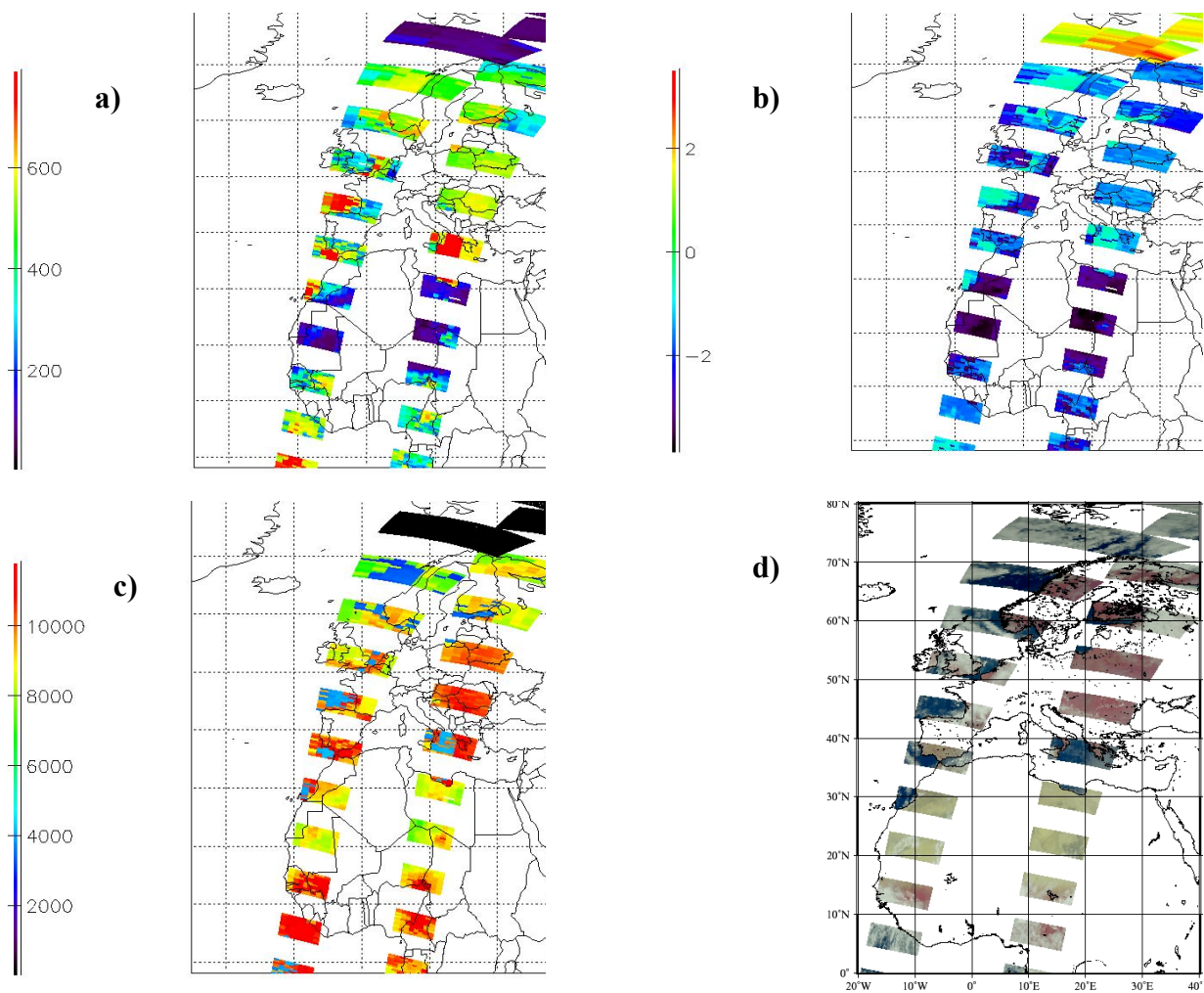


Fig. 1. (a) BIAS retrieved CH_4 (10^{19} molec/cm²) total columns from micro window 1, (b) BIAS retrieved CH_4 (10^{19} molec/cm²) total columns from micro window 2, (c) BIAS retrieved CO (10^{18} molec/cm²) total columns, (d) RGB translated PMD image showing clouds (white), sea (blue), vegetation (red), and sand (yellow).

4. VERIFICATION OF THE SCIENTIFIC CH₄ NADIR COLUMNS

Only 4 verification orbits have been retrieved by the SRON scientific retrieval algorithms (orbits 2337-2338 (August 11 2002), and 2509-2510 (August 23 2002)) because of the problems with the characterization of the level of the dark current signal in channel 8. The first results from the IMLM retrieved CH₄ total columns are shown in Fig. 2 (orbits 2337-2338) together with information about surface elevation and cloud coverage.

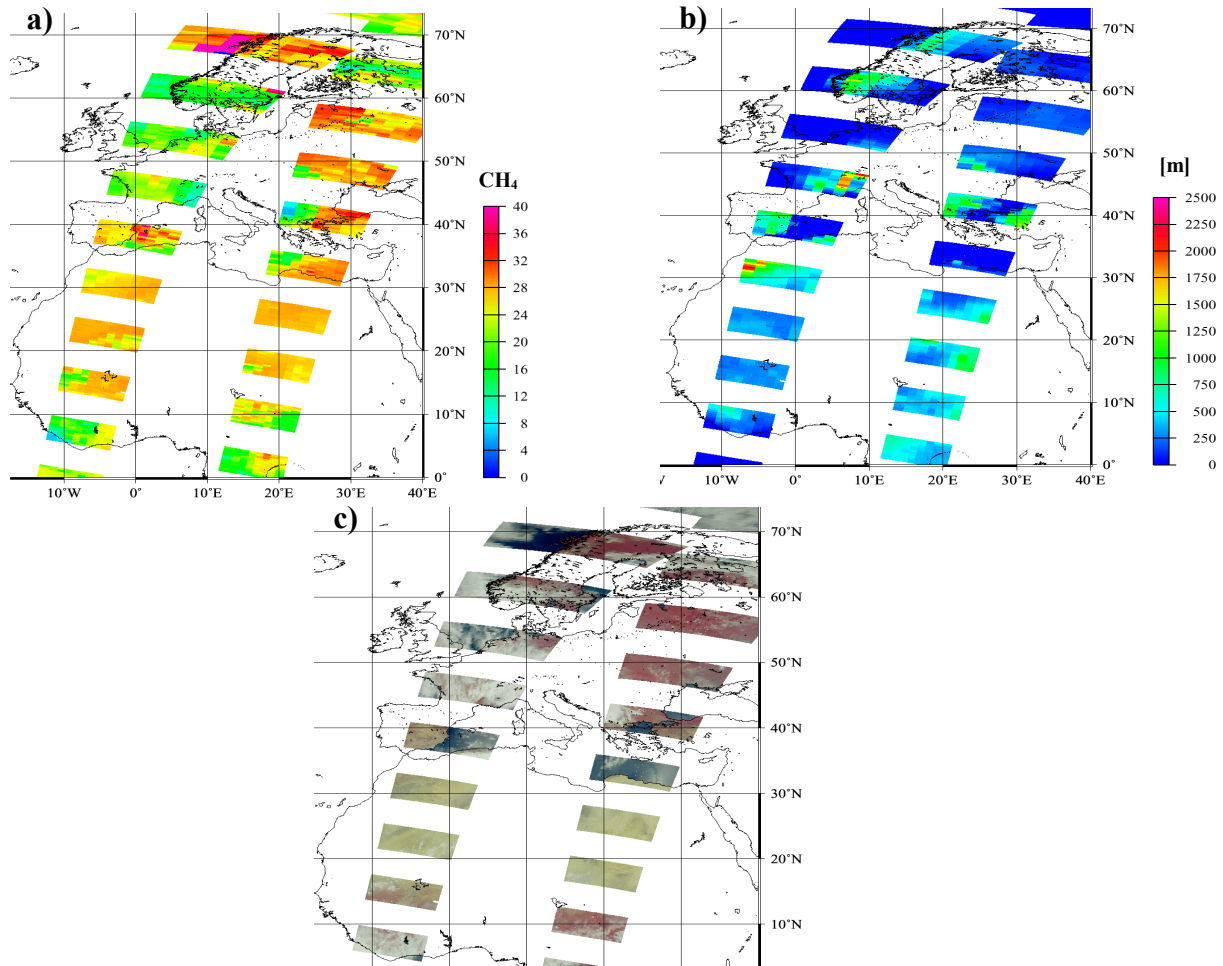


Fig. 2. (a) CH₄ total columns (10^{18} molec/cm²) orbits 2337 and 2338 August 11 2002 preliminary calibrated spectra, (b) topography (meters above sea level) averaged over the SCIAMACHY pixels (source: Data Announcement 88-MGG-02, Digital relief of the Surface of the Earth. NOAA, Boulder (CO), U.S.A.), (c) reflectivities in an RGB color scale indicating clouds (white), sea (blue), vegetation (red), sand (yellow), deduced from the SCIAMACHY polarization measurement devices (PMDs) in the visible wavelength region.

The L1b files for these two orbits contained dark current measurements that were a few weeks old. Dark current measurements taken during each orbit over the South Pole (in the eclipse) were therefore used by IMLM to apply the correct dark current signal corrections to the spectra. Furthermore, the slit-width in the instrument model had to be increased with a factor of 1.8, which may correspond to a loss of spectral resolution introduced by the ice layer on the detectors. The methane columns in Fig. 2 vary in a physically consistent way with the cloud cover and the surface elevation. For example; over the north-western part of Turkey the methane columns are decreasing with the increasing surface elevation. The same can be seen over the Moroccan Atlas Mountains. Over Macedonia, that is covered by clouds, the CH₄ columns are also very low because the satellite can only see the part of the atmosphere that is above the clouds. A factor introducing uncertainties in the retrieval is the low surface albedo over sea in the near-infrared region. For example over the sea outside of Northern Norway (Lofoten) where the albedo (transmission) was found to be extremely low (not shown here), erroneously high CH₄ columns were retrieved. The corresponding retrieval error was also large.

In Fig. 3 the correlation of the methane columns and their errors with the surface elevation and albedo for cloudy and non-cloudy cases are shown. The clear relation between the column amount and the surface elevation is visible in Fig. 3b where the data have been masked for clouds using a simple algorithm based on the SCIAMACHY PMD measurements from channels 2-4. This relation shows that the variations in the methane columns are physically consistent. A spread in the methane column values is found for elevations lower than $\sim 500\text{m}$ which is when the boundary layer is included in the column. Whether the spread in the values below 500m reflects boundary layer pollution or whether the variation is more affected by low surface albedos (shown by the increase in the errorbars) needs to be looked into in more detail. The few outliers around the surface elevation of 1000m (located at the Ukrainian/Rumanian border) might represent pixels that were wrongly defined as cloud-free in our relatively simple cloud algorithm.

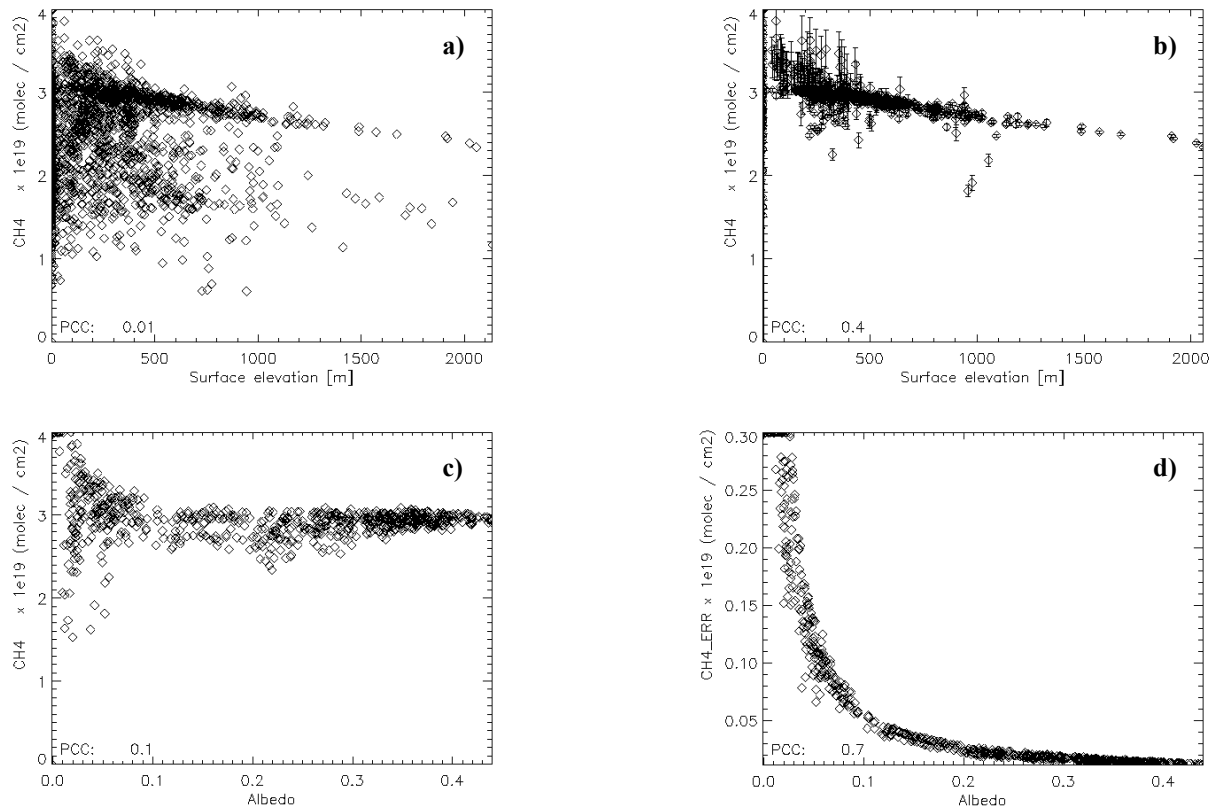


Fig. 3. (a) IMLM retrieved CH₄ total columns (10^{19} molec/cm²) v.s. surface elevation, (b) as in (a) but only for the cloud-free scenes and including the column errors based on instrument noise only, (c) IMLM retrieved CH₄ total columns (10^{19} molec/cm²) v.s. calculated albedo (based on the transmission level), (d) IMLM retrieved CH₄ total column errors (10^{19} molec/cm²) based on instrument noise only v.s. calculated albedo (based on the transmission level). PCC: pearson correlation coefficient.

A very encouraging result is the clear independence of the methane columns with the surface albedo as shown in Fig. 3c. An exception is low albedos (below 10%) where the determination of the column amount gets influenced by the instrument noise as is also shown in Fig. 2d. The CH₄ column error is calculated in this study from noise considerations only.

The retrieved methane column at sea level is $3.1 \cdot 10^{19}$ molec/cm² (where a straight line extrapolated back to zero in Fig. 3b would cross the y-axis) may be compared with the TM3 simulated columns (Fig. 4) over the northern-hemisphere oceans ($\sim 3.8 \cdot 10^{19}$ molec/cm²). The retrieved columns are found to be $\sim 18\%$ too low. This TM3 model-run has itself not been fully validated, and the modeled CH₄ total columns might be a few percent too high. Still, the retrieved CH₄ columns are clearly too low. This bias could be caused by the preliminarily calibrated measured spectra, or by the fact that the solar spectrum information in this early retrieval version is taken from a model and not from the SCIAMACHY solar measurements. We expect to get better columns when the instrument is better characterized.

At the moment we cannot say whether the measurements are sensitive to variations in CH₄ sources and sinks. That can only be seen when normalizing the columns to the surface pressure. Furthermore, we need much more data than the four orbits that are available right now to show statistically significant results.

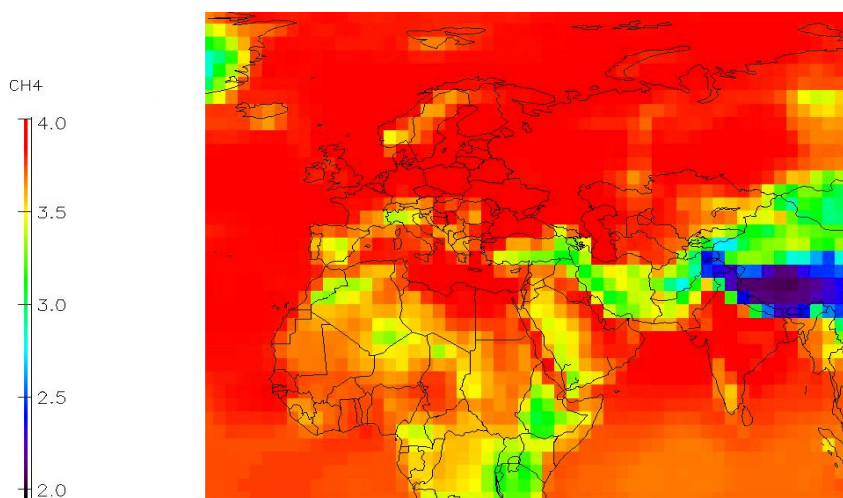


Fig. 4. TM3 modeled CH₄ total columns (10^{19} molec/cm²) (clouds not considered), horizontal resolution of $2.5^{\circ} \times 2.5^{\circ}$. ECMWF data were used as input to the chemical transport model.

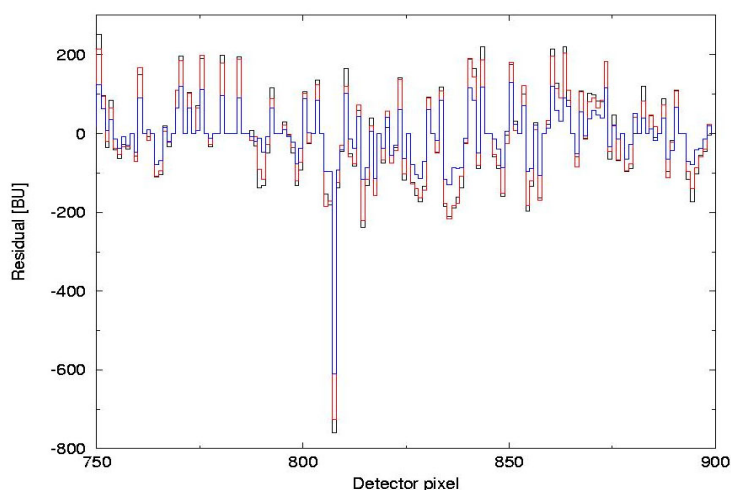


Fig. 5. Residuals between the measured and a modeled spectrum for different albedos. Black and red curves: residuals during high albedo cases (desert). Blue curve: residuals during a low albedo case (boulders).

The CO signal (1-2% of the signal) is still below the systematic residuals (10-20% of the measurement), giving erroneously low or 0 column values in the retrieval. The pattern of the residuals is illustrated in Fig. 5. The systematic residuals are suspected to be caused by non-characterized pixel-to-pixel gain variations with respect to the on-ground calibration. Another possibility is imperfections in the forward model, although spectral uncertainties of even as much as 20% in line intensity would not give residuals of more than a few percent and the effects of neglecting scattering are not expected to have this spectral shape. In Fig. 5 the solar spectrum is taken from MODTRAN but the same residuals are found when the measure solar spectrum was used. Thus the origin of these systematic residuals are at the moment under investigation.

The first results from the IMLM retrieval of CO₂ from SCIAMACHY channel 6 are now available. The product has not yet been fully verified but the first comparison with cloud cover and surface elevation show that the columns vary in a physically consistent way (Fig. 6). The CO₂ columns are still somewhat albedo-dependent (not shown here), and the reason for this has to be looked into.

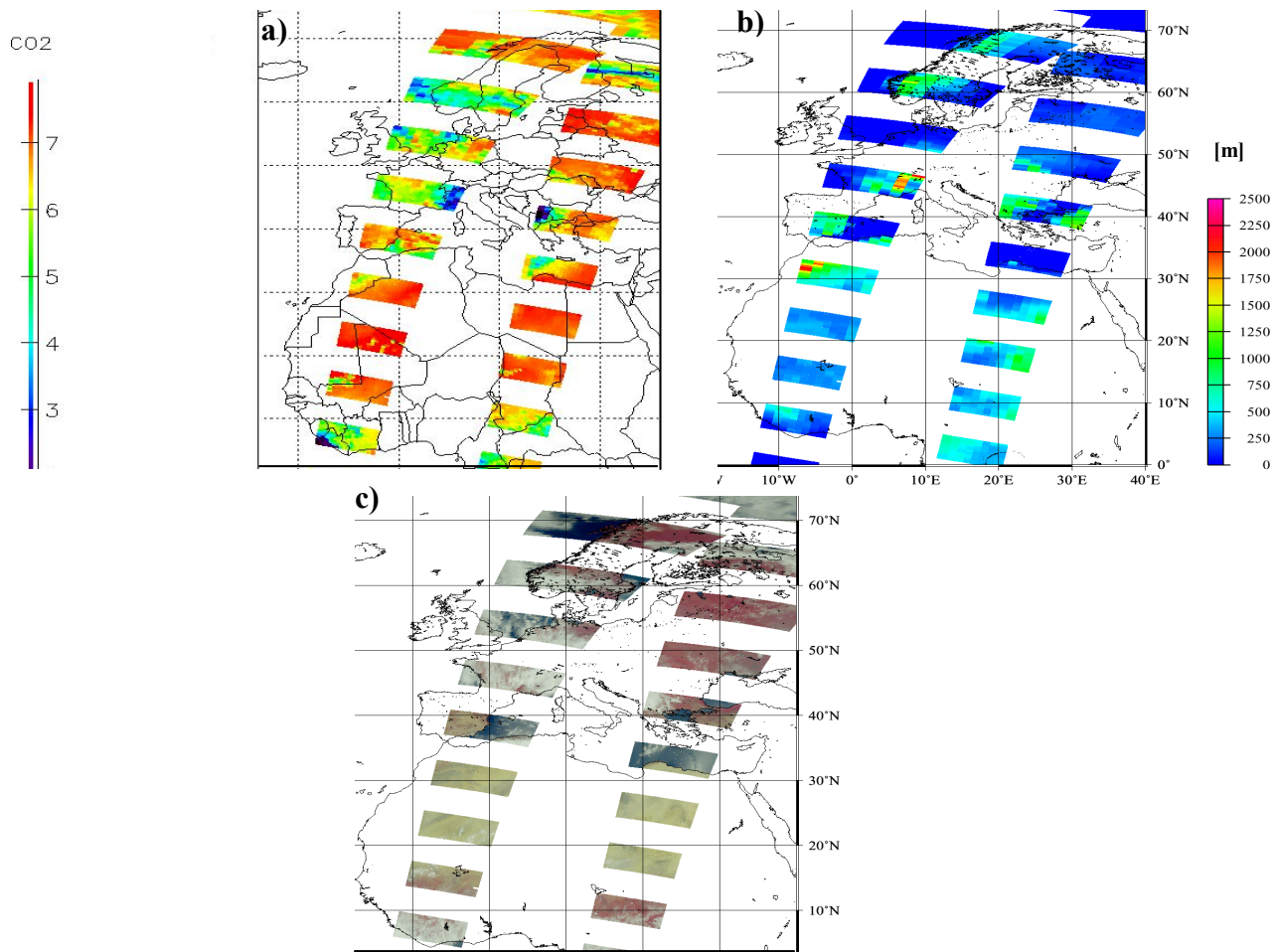


Fig. 6. (a) IMLM retrieved CO₂ total columns (10^{21} molec/cm²) for orbits 2337 and 2338 August 11 2002, (b) and (c) see caption Fig. 2.

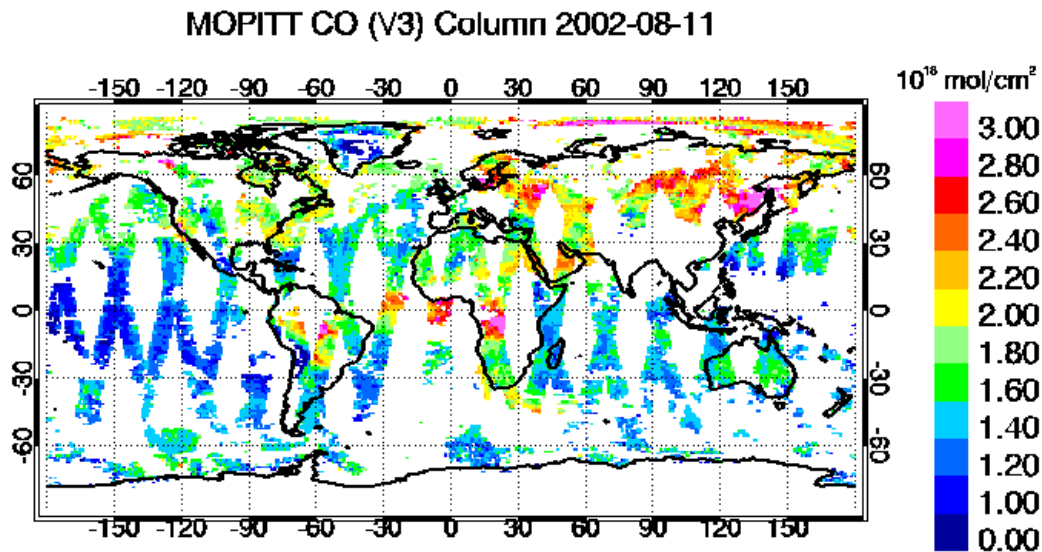
5. CO MEASUREMENTS BY THE MOPITT INSTRUMENT

The Measurements of Pollution In The Troposphere (MOPITT) instrument, which was launched onboard the EOS-TERRA satellite in December 1999, measures the spatial and temporal variation of CO and CH₄ (e.g. [5] and [6]). MOPITT is a gas correlation spectrometer measuring CO and CH₄ total column and CO vertical profile within the troposphere. The horizontal resolution is 22×22 km, and for CO the vertical resolution is 3-5 layers within the troposphere. The technique of gas correlation spectroscopy is described for example in [7].

The MOPITT level 2 data are validated at NCAR. The validation is done by comparing MOPITT measurements with measurements from airplane campaigns and ground-based stations. At the time of writing only the MOPITT CO measurements have been extensively validated. The MOPITT CH₄ product is not yet available due to noise problems in the data. Comparisons of MOPITT CO profiles with routine aircraft measurements from the CMDL network showed that the average bias of the MOPITT profiles is less than 20 ppbv ([8]). On individual days the difference can, however, reach up to 50 ppbv in the lower troposphere. The MOPITT CO total columns are derived by integrating the retrieved profiles. A comparison of MOPITT 3-day averaged total columns with measurements by ground-based Fourier-transform InfraRed (FTIR) spectrometers at 6 stations showed that the total column mean biases are less than 10%, depending amongst others on geographical location and the time of the measurement (L. Emmons, personal communications 2002). In May 2001 one of the two MOPITT-coolers stopped working, reducing the number of infrared channels available for profile retrievals from 4 to 2. It is expected that comparable vertical resolution will be achieved for this data as for the first year of data.

The MOPITT data are publicly accessible via the NASA Langley Atmospheric Sciences Data Center. An example of MOPITT CO total column measurements is given in Fig. 7. In the figure, the interhemispheric CO gradient is visible.

Furthermore, the August forest fires near Moscow and transport of CO from forest fires in Africa across the Atlantic Ocean can be seen.



Gridded at 1x1deg from MOP02-20020811-L2V5.6.2.beta.hdf (apriori fraction < 50%)

Fig. 7. MOPITT CO total columns (10^{18} molec/cm²) from August 11 2002. The figure was obtained from the NCAR MOPITT homepage, quick-look images of gridded CO data from retrieval version 3 (source: <http://www.eos.ucar.edu/mopitt/data/plots/mapsv3.html>).

6. CONCLUSIONS

The SCIAMACHY CH₄ and CO total columns currently retrieved by the operational BIAS algorithm are not correct. The reason may be related to still unresolved calibration features, possible unmasked badly-behaving (noisy) pixels within the BIAS fitting windows, and/or bugs in the L1-2 processor. Scientific algorithms have been developed for the retrieval of CO and CH₄ from SCIAMACHY. The first results for the CH₄ columns look promising. The horizontal variations in the column amounts were found to be physically consistent and albedo independent, but the column amounts are systematically too low (~18%). There are several possible reasons for this systematic bias; the measured spectra from channel 8 are still not fully calibrated/characterized in the L1b data or there might be errors/inaccuracies in the forward model. The CO signal is still below the systematic residuals and it is therefore not yet possible to retrieve CO with a high enough accuracy. It is anticipated that it will be possible to retrieve CO when the L1b calibration data are improved. The first attempt to retrieve CO₂ shows that the columns vary consistently with surface elevation and cloud cover. The column amounts seem still to be somewhat albedo dependent. The reason for this has to be further investigated.

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