CH_4 AND CO TOTAL COLUMNS FROM SCIAMACHY: COMPARISONS WITH TM3 AND MOPITT

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ABSTRACT

The methane (CH_4) and carbonmonoxide (CO) total columns retrieved from SCIAMACHY's near-infrared channel 8 have been compared to measurements from the MOPITT satellite instrument, and with model calculations by the chemistry transport model TM3. Since the operational products for these species still deviate from the expected levels by orders of magnitude, results from independent scientific algorithms are presented here. The total columns from each of these scientific algorithms are similar, but significant differences still remain. First results show that both monthly averaged and daily data show good agreement with TM3 model calculations and measurements from the MOPITT satellite.

Key words: SCIAMACHY; CH_4; CO;.

1. INTRODUCTION

The SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) which was launched on board the ENVISAT satellite on March 1 2002, has allowed, for the first time, to measure the global distributions of methane (CH_4) and carbonmonoxide (CO) down to the Earth's surface. These gases play an important role in tropospheric chemistry and possible climate change. Therefore, a good knowledge of the global distributions of these gases is a prerequisite to fully understand their role in atmospheric chemistry.

Global distributions of CO are also measured by the MOPITT instrument on board the EOS-TERRA satellite in the thermal infrared (e.g. [1],[2]). Methane has been measured earlier by both the Interferometric Monitoring of Greenhouse Gases (IMG) instrument on board the ADEOS satellite ([3]) and MOPITT in the infrared. Up till now, MOPITT has been unsuccessfull in retrieving CH_4 total columns from their data. Ground-based measurements of CO and CH_4 total columns are available from a number of ground stations, but a significant fraction of these are at elevated locations. Since most of the CO and CH_4 resides in the lower parts of the atmosphere, these stations only measure the total column directly above the station, whereas the larger spatial coverage of a SCIAMACHY ground pixel will mostly also include contributions from lower altitudes to the measured total column ([4]).

The retrievals of CO and CH_4 from SCIAMACHY's near-infrared channels have proven more complex than anticipated, due to the presence of an unexpected ice layer on the detectors. However, its effects have been reduced by applying dedicated in-flight decontamination procedures and additional in-flight calibration measurements, as well as improvements to the calibration.

The CO and CH_4 total columns retrieved from SCIAMACHY are currently in the process of being comprehensively validated through intercomparisons of independent scientific retrieval algorithms, and comparisons to ground-based measurements, chemical transport model calculations, and satellite measurements. The different validation techniques are described in [5]. This validation is part of the AO 241 project "Validation of CO and METHane SCIAMACHY data products" (COMETH) and of the EU project "EnVisat for Environmental Regulation of GREENhouse gases" (EVERGREEN). This paper reports on the current status of the comparison of CO and CH_4 total columns with calculations by the TM3 model and CO measurements from the MOPITT instrument. Comparisons with ground-based measurements are reported in [4].

2. THE RETRIEVAL ALGORITHMS

The near-infrared nadir spectra measured by SCIAMACHY's channel 8 (2265 to 2380 nm) enable the retrieval of CH_4 and CO total columns. The retrieval within this wavelength range is hampered by the growth of an ice layer on the detector. This ice layer leads to losses in transmission of up to ∼70% (see http://www.sron.nl/∼SCIA_CAL/SCIACALtransmission.html). The consequences are threefold:

- The signal-to-noise ratio of the spectra is reduced. This loss in transmission is partially compensated by heating the detector every 3–6 months, evaporating the ice layer. However, the decreasing of the

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transmission behaves differently after each of these decontamination periods.

- The dark signal decreases and must therefore be measured every orbit, which is done since October 2002.
- Scattering in the ice layer gives rise to extended wings in the slit function. The latter can give rise to errors in the retrieved columns of up to $\sim$25% for SCIAMACHY channel 8 spectra observed $\sim$4 weeks after the decontamination.

In addition to the problems due to the ice growth on the detector, the dark signal also varies within an orbit, leading to total columns that are too high for latitudes above $\sim 30^{o}$ North.

The operational calibration and retrieval algorithm, Basic near-Infrared Absorption Spectroscopy (BIAS) do not include a correction for these issues and therefore the operational CH_4 and CO products still deviate from the expected levels by orders of magnitude. For this reason, only results from scientific algorithms have been validated. Independent scientific algorithms from three different institutes are available for the retrieval of CH_4 and CO total columns. The total columns from each of these scientific algorithms are similar, but significant differences still remain. A short description of each of these algorithms is given in the following sections (see also EVERGREEN document: TN-EVG-TASK1-RET-001).

2.1 The IMLM Retrieval Algorithm

The IMLM retrieval method is based on an **I**terative **M**aximum **L**ikelyhood **M**ethod and is developed at SRON. The retrieval uses a fixed set of climatological atmospheric profiles based on the US standard atmosphere (1976) to compute a model spectrum in terms of optical depths. For each SCIAMACHY ground pixel these profiles are corrected for the mean surface elevation of the pixel, by cutting off the part of the profile below the surface.

Once the optical depths are calculated, the earth radiance can be computed in a forward model ([6]), which is then transformed by an instrument model to represent the radiation detected by the instrument detectors. This modelled spectrum is then fitted to the measured spectrum in an iterative way. The instrument model includes a dedicated dead and/or bad pixel mask, as well as dark signals for every orbit, available in the SRON database set up by Quintus Kleipool (Q. Kleipool, private communication). A first correction for the broadening of the slit function is also included, as well as a correction for the variation of the dark signal within an orbit. Improvements on these corrections are still under investigation. At present, only a fixed temperature profile has been used, but the inclusion of a temperature profile shift in the IMLM retrieval algorithm is almost completed. Scattering in the atmosphere is not included in the forward model, but is expected to introduce only small corrections ([7]). A simple cloud mask based on the SCIAMACHY PMDs B, C, and D has been included in the IMLM algorithm. Cloudy pixels have been removed and are not taken into account in the analyses presented in this paper.

For the retrieval of CH_4 and CO total columns a subwindow of channel 8 ranging from 2354 to 2370 nm has been used.

2.2 The WFM-DOAS Retrieval Algorithm

The Weighting Function Modified Differential Optical Absorption Spectroscopy (WFM-DOAS) retrieval algorithm has been mainly developed for the retrieval of total columns of CO, CH_4, CO_2, H_2O, and N_2O, from the SCIAMACHY near-infrared nadir spectra. A detailed description of the algorithm can be found in [8], [7], and [9].

WFM-DOAS is based on fitting the logarithm of 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 (observed sun-normalized radiance). The fit parameters are the trace gas vertical columns plus other parameters such as a temperature profile shift. In order to avoid time consuming on-line radiative transfer calculations WFM-DOAS has been implemented as a look-up table scheme.

2.3 The IMAP-DOAS Retrieval Algorithm

The IMAP algorithm used at Heidelberg is a modified DOAS algorithm that uses an iterative scheme for maximizing the *a posteriori* probability density function of the trace gases to be retrieved ([10]). The linearization point of the algorithm is a profile based on the US-standard atmosphere from which the optical depth of the atmosphere is derived. Derivatives of these optical depths with respect to perturbations of the absorbing trace gases in different height layers are computed and fitted to optical depths measured by SCIAMACHY. Derivatives for a temperature change in the profile are also included.

Especially for channel 8, a flexible dead/bad pixel mask and daily dark measurement readouts are used for the calibration of the raw spectra. It is also planned to use a time-dependent slit function for channel 8. The following wavelength regions are chosen for the retrieval of CH_4 and CO: for CH_4 channel 6: 1630.6–1669.9nm; CH_4 channel 8: 2261.9–2276.1nm; CO channel 8: 2324.2–2334.9nm.

Channel 6 turned out to be a good alternative for the methane retrieval although the spectral resolution is worse than in channel 8. It is planned to use both channels for the methane retrieval in the future. With the new calibration of the dark signal reasonable CO columns can now be retrieved.

Due to the availability of only a limited amount of data in Heidelberg, only a few orbits could be analyzed prior to the workshop. Therefore, no detailed comparisons of the IMAP total columns to model calculations or satellite measurements could be performed. At the time of

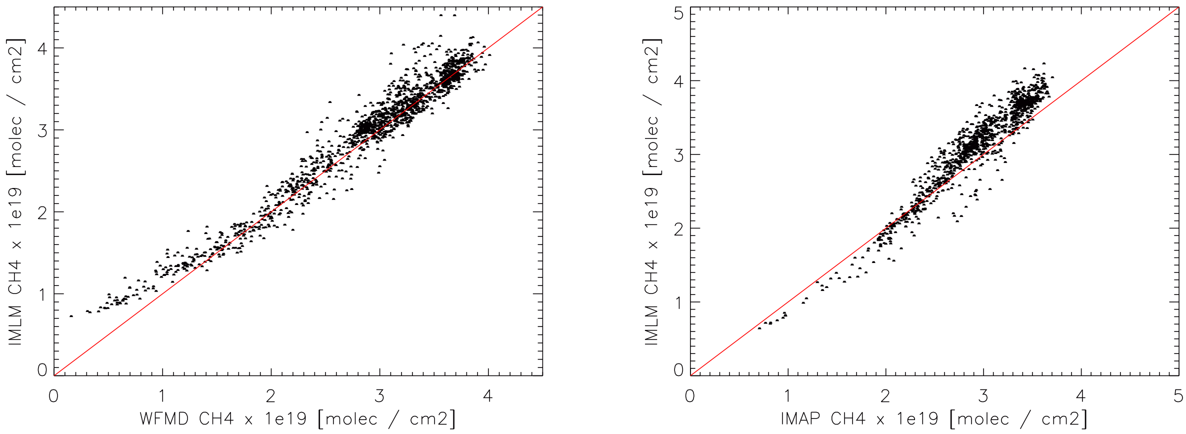

Figure 1. Left: IMLM versus WFM-DOAS CH_4 total columns for orbit 4714 on January 24, 2003. Only ground pixels with errors $\leq 2\times10^{18}$ molec/cm^2 are shown and no cloud mask has been applied. The red line shows the expected 1:1 correlation. The correlation coefficient is 0.98 and the number of comparisons is 1566. Right: CH_4 total columns for orbit 4700 on January 23, 2003. Only ground pixels with errors $\leq 2\times10^{18}$ molec/cm^2 are shown and no cloud mask has been applied. The red line shows the expected 1:1 correlation. The correlation coefficient is 0.96 and the number of comparisons is 1144. (From: EVERGREEN document TN-EVG-TASK1-RET-001).

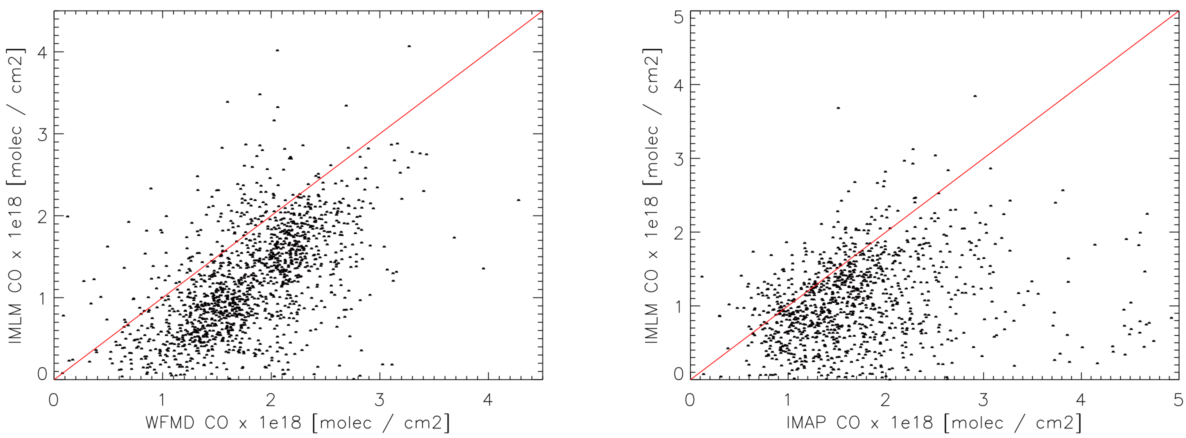

Figure 2. Left: IMLM versus WFM-DOAS CO total columns for orbit 4714 on January 24, 2003. Only ground pixels with errors $\leq 1.5\times10^{18}$ molec/cm^2 are shown and no cloud mask has been applied. The red line shows the expected 1:1 correlation. The correlation coefficient is 0.57 and the number of comparisons is 1423. Right: IMLM versus IMAP CO total columns for orbit 4700 on January 23, 2003. Only ground pixels with errors $\leq 1.5\times10^{18}$ molec/cm^2 are shown and no cloud mask has been applied. The red line shows the expected 1:1 correlation. The correlation coefficient is 0.25 and the number of comparisons is 1089. (From: EVERGREEN document TN-EVG-TASK1-RET-001).

writing, more data has become available, allowing such comparisons to be made in the near future.

3. INTERCOMPARISON OF RETRIEVAL ALGORITHMS

So far, only a limited number of comparisons between the three independent scientific retrieval algorithms have been performed. This is mainly due to the fact that each institute has processed different data sets with only few overlapping orbits. However, the comparisons that could be made clearly show a good agreement between the scientific algorithms for both CH_4 and CO (EVERGREEN document: TN-EVG-TASK1-RET-001). More extensive comparisons will be done in the near future.

Fig 1 (left panel) shows a scatter plot of the IMLM and WFM-DOAS CH_4 total columns for orbit 4714 (January 24, 2003). It can be seen that overall the correlation is very good (correlation coefficient of 0.98), except for low columns, which correspond to measurements above high clouds, where the bulk of the CH_4 column is missing. It is still under investigation where this difference comes from. Comparisons between IMLM and WFM-DOAS for January 23, 2003, give similar results.

A comparison between the CH_4 columns from the IMLM and IMAP algorithms for orbit 4700 on January 23, 2003 is shown in Fig. 1 (right panel). The correlation is good, even for low columns, with a correlation coefficient of 0.96. However, the slope of the IMLM to IMAP total columns is somewhat steeper than the expected 1:1 relationship. This is under investigation.

Similar scatter plots have been made for CO. Fig. 2 (left panel) shows the comparison between IMLM and WFM-DOAS for orbit 4714, on January 24, 2003. It can be seen that the IMLM and WFM-DOAS CO columns are less correlated than the CH_4 columns. The IMLM and IMAP CO columns for orbit 4700 on January 23, 2003 (Fig. 2, right panel) are also less correlated than the CH_4 columns and the comparison is somewhat worse than the IMLM versus WFM-DOAS plot: the IMAP CO columns show a larger spread. Recently, improvements have been made to the IMAP algorithm, which have not yet been investigated, but are expected to lead to a better correlation.

4. VALIDATION OF SCIAMACHY CO AND CH_4 COLUMNS

In order to obtain accurate global distributions of CH_4 and CO from SCIAMACHY observations, the retrieved columns need to be validated. One of the most important validation techniques used for satellite measurements are comparisons with ground-based stations. However, total columns of CH_4 and CO are only measured by a limited number of stations, of which a significant fraction is situated at elevated locations ([4]). Since most of the CH_4 and CO resides in the lower parts of the troposphere, measurements from elevated ground stations mostly sample less CH_4 and CO compared to the columns retrieved from the large SCIAMACHY ground pixels. Furthermore, the CH_4 and CO sources and sinks are located in the atmospheric boundary layer. SCIAMACHY total columns, sampling deeper into the atmosphere, will therefore often show larger variations than the columns measured at the elevated ground-based stations. This complicates the validation with ground-based measurements. Therefore, comparisons with chemistry transport models and independent satellite observations are required to obtain a complete validation of the SCIAMACHY CH_4 and CO total column products.

In the case of CH_4, SCIAMACHY is currently the only satellite-based instrument that successfully measures the total column of this species. Therefore, satellite intercomparisons can only be presented for CO. At present, the only other instrument that can measure CO total columns from space is the MOPITT instrument. Whereas SCIAMACHY measures CO in the near-infrared, MOPITT observes CO in the thermal infrared. In addition, MOPITT uses gas-correlation spectroscopy, based on pressurized cells ([1]), whereas SCIAMACHY uses a grating spectrometer. Thus, measurements from these satellites provide two independent sets of CO column products, making them very suitable for validation. The disadvantage of MOPITT is however that measurements in the thermal infrared have a low sensitivity to the boundary layer. Comparisons with chemical transport models have the disadvantage that these models do not contain up-to-date emissions. Especially for CO, which has strong temporal and spatial variations, this makes satellite intercomparisons a very valuable validation technique. Therefore, for CO only comparisons with MOPITT are reported here, although comparisons with chemistry transport models have also been performed.

5. COMPARISONS WITH SATELLITE OBSERVATIONS - CO

A thorough validation of SCIAMACHY data products can only be obainted if large data sets are investigated in order to get good statistics. In this paper, two different approaches are discussed. The first describes the analysis of a large number of daily data, the second analyzes monthly averaged data.

5.1 Daily Data Sets

An example of a comparison of daily SCIAMACHY CO data with the corresponding MOPITT measurements is shown in Fig. 3. This figure presents the CO total columns retrieved with the WFM-DOAS algorithm for January 30, 2003. It can be seen that there is an overall good agreement, e.g. over North Africa. The agreement is however somewhat less over South America and South Africa.

A more quantitative analysis is presented in Fig. 4. It shows that, although there is a significant spread in both data sets, the data sets seem to have a good correlation. A

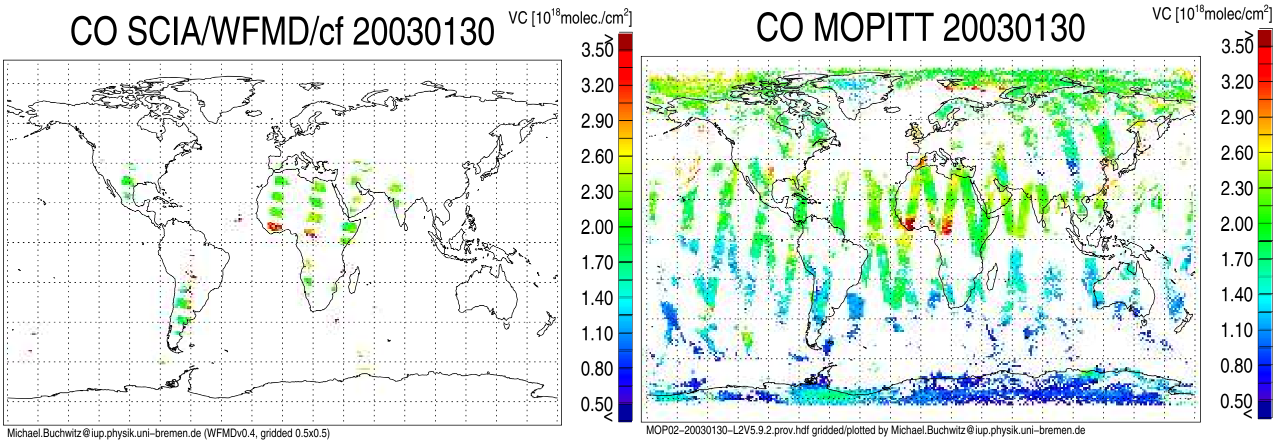

Figure 3. Left: CO total columns from the WFM-DOAS retrieval algorithm for January 30, 2003. Only cloud-free pixels are shown. Right: The corresponding CO total columns as measured with the MOPITT instrument (from: http://www.eos.ucar.edu/mopitt/data/plots/mapsv3.html). Note that both figures use the same vertical scale (from: [9]).

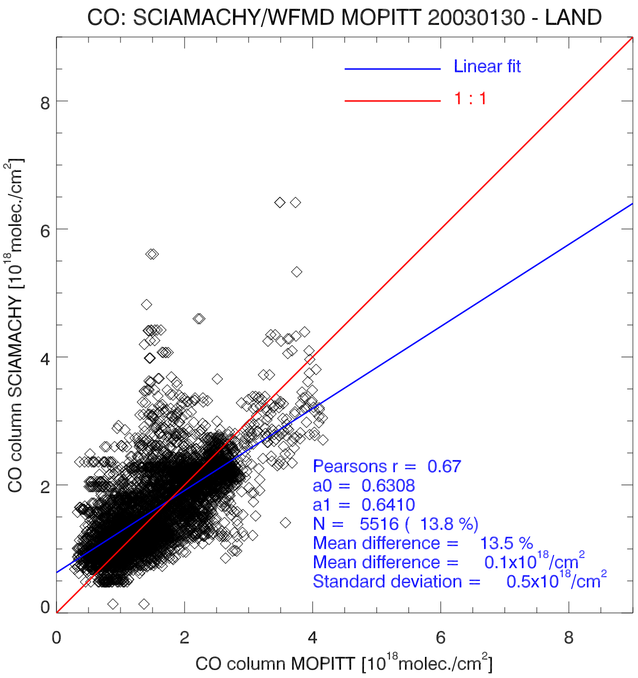

Figure 4. Comparison of the column-averaged CO concentrations from the WFM-DOAS algorithm and those measured by the MOPITT measurements for January 30, 2003. Note that the WFM-DOAS data have been multiplied by a factor 0.5 as explained in [9]. Only pixels over land are shown.

more detailed analysis of the WFM-DOAS CO results is given in [9].

5.2 Monthly Averaged Data Sets

Fig. 5 shows the monthly distribution of CO for February 2004. The upper panel shows the monthly averaged SCIAMACHY data as retrieved with the IMLM scientific algorithm. Only cloud-free pixels with instrument noise related errors $< 1.5\times10^{18}$ molec/cm^2 have been included. The latter results in the removal of most data over the oceans, since the low surface albedo leads to large retrieval errors. The lower panel shows the corresponding distribution as observed with the MOPITT instrument. A first qualitative comparison of both data sets shows that there is an overall good agreement. Both show a clear North-South gradient and enhanced CO columns in West and Central Africa (bio-mass burning), Asia and North-America (pollution from industrial areas). But also large differences are observed, e.g. over India and South America. Part of this difference may come from the fact that the MOPITT measurements are not sensitive to the boundary layer resulting in lower CO total columns. A more detailed comparison of these two sets of satellite measurements will be performed in close collaboration with the National Center for Atmospheric Research (NCAR).

A more quantitative, although preliminary, analysis is presented in Fig. 6. This figure uses the monthly data as shown in Fig. 5 and divides the globe in five degree latitude bins. Then, all monthly SCIAMACHY data within each latitude bin have been averaged and compared to the average of the corresponding MOPITT CO total columns within the same latitude bin. Only data between longitudes 30° W and 60° E have been taken into account. This region is chosen because the Sahara and South-Africa are mostly cloud-free and have a high surface albedo, allowing accurate retrievals. It can be seen that there is a good agreement over South-Africa (between

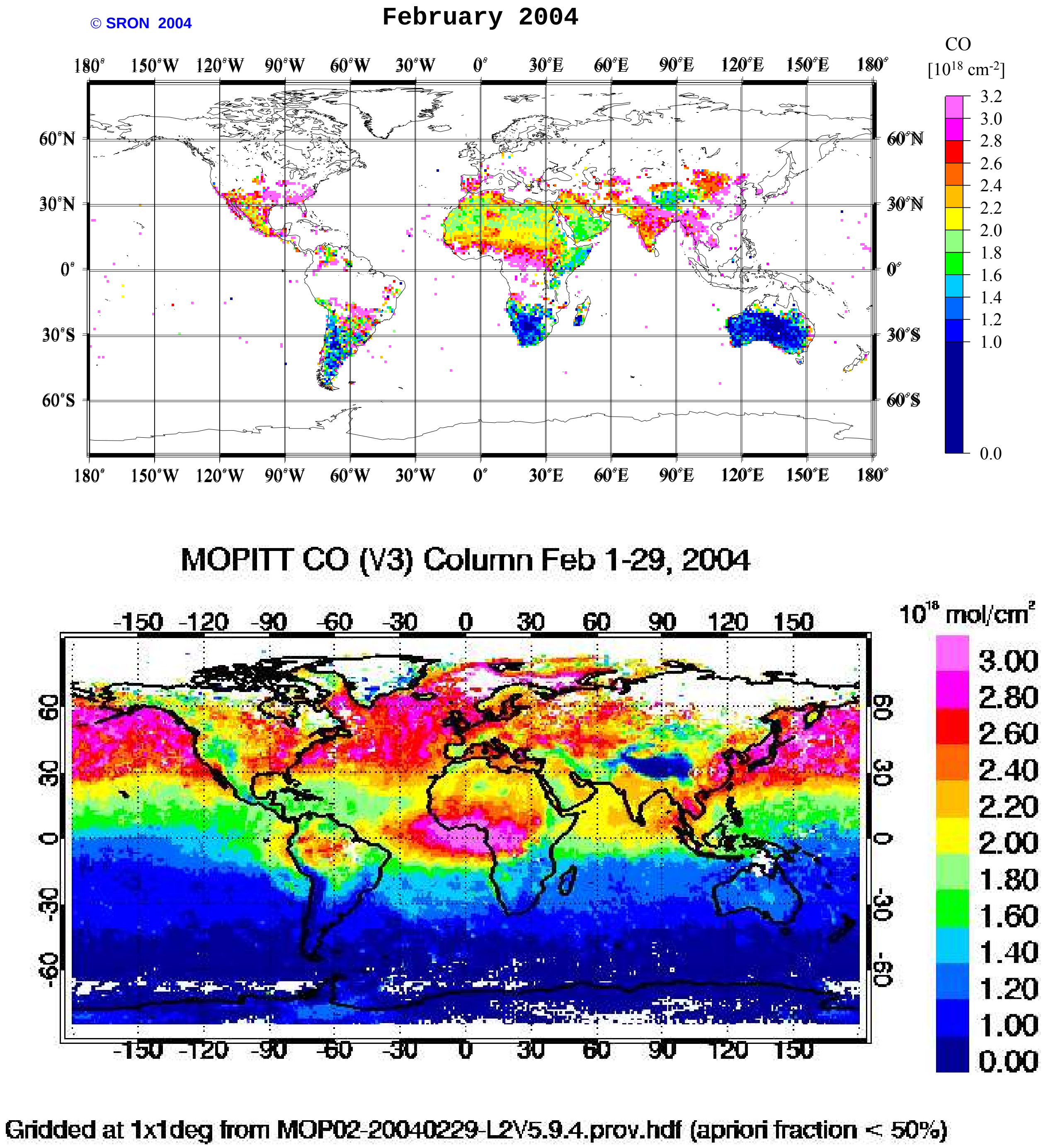

Figure 5. Top: Monthly averaged CO total columns from the IMLM retrieval algorithm for February 2004. Only cloud-free pixels with instrument noise related errors $< 1.5\times10^{18}$ molec/cm^2 have been included. The daily SCIAMACHY data have been regridded on a 1° by 1° grid before averaging all available data for this month. Bottom: The corresponding monthly averaged CO total columns as measured by the MOPITT instrument also on a 1° by 1° grid (taken from: http://www.eos.ucar.edu/mopitt/data/plots/mapsv3_mon.html). Note that both figures use the same vertical scale.

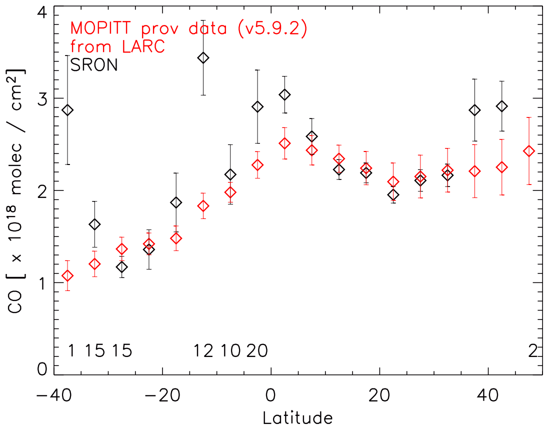

Figure 6. Comparison of the monthly CO total columns for February 2004 as presented in Fig. 5, where all data within a five degree latitude bin have been averaged (see text). The black diamonds denote the IMLM CO total columns, the red diamonds the corresponding MOPITT data. Only cloud-free pixels with instrument noise related errors $< 1.5{\times}10^{18}$ molec/cm^2 have been included. The error bars denote the instrument noise related errors only.

latitudes 30° S and 20° S) and over Northern Africa (between the Equator and 30° N). In both cases the difference between the IMLM columns from the SRON algorithm and the MOPITT measurements is less than 10%. The large difference over Central Africa is probably due to cloudy pixels in the SCIAMACHY data that have not been filtered out. The increase in the SCIAMACHY CO columns over Europe (latitudes $>$ 35° N) is most likely caused by the variation of the dark signal within an orbit, a correction which was not yet implemented in the retrieval at the time this analysis was done (see Sect. 2).

6. COMPARISONS WITH MODEL CALCULATIONS - CH_4

Although chemistry transport models do not contain up-to-date emissions and global distributions are currently only calculated on rather coarse spatial grids (e.g. 2° by 3°), they do provide accurate information on the large scale distribution of the trace gases, such as the North-South gradient. At present, only detailed comparisons with the chemistry transport model TM3, in collaboration with the Royal Netherlands Meteorological Institute (KNMI), have been performed. Both comparisons for daily data and monthly averaged data have been performed. Only results for CH_4 are shown here.

6.1 Daily Data Sets

Fig. 7 shows an example of a comparison of the CH_4 total columns retrieved with the WFM-DOAS algorithm and calculated by the TM3 model for January 24, 2003. There is an overall good agreement, e.g. over the Sahara, South America, and the Himalayas. The agreement is however less over Australia.

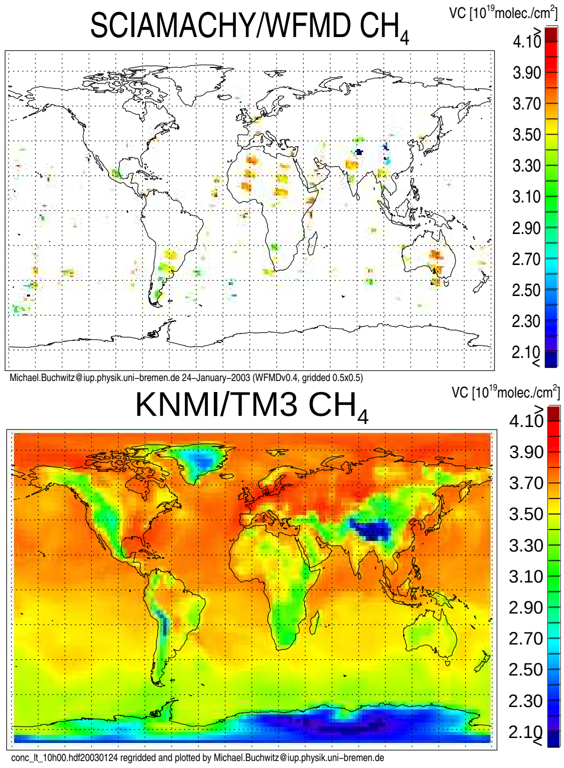

Figure 7. Top: CH_4 total columns from the WFM-DOAS retrieval algorithm for January 24, 2003. Only cloud-free pixels are shown. Bottom: The corresponding CH_4 total columns calculated by the TM3 chemistry transport model on a 2.5° by 2.5° grid. Note that both figures use the same vertical scale.

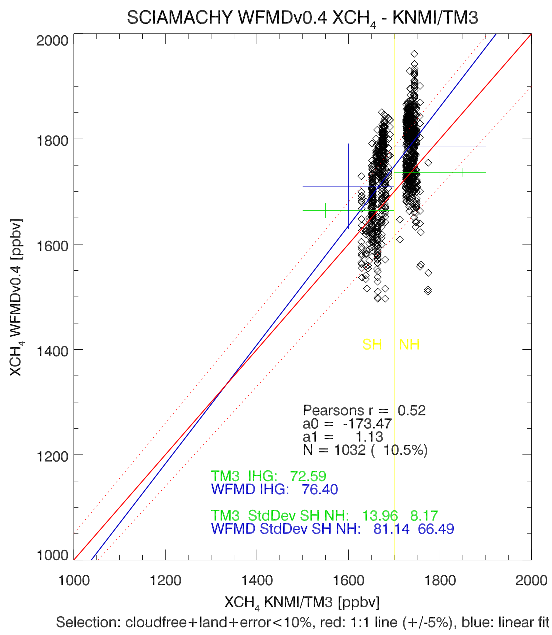

Figure 8. Comparison of the column-averaged CH_4 concentrations from the WFM-DOAS algorithm and those calculated by the TM3 model for January 24, 2003.

A more quantitative analysis is presented in Fig. 8. It shows that, although there is a large spread in the WFM-DOAS results, the North-South gradients (InterHemispheric Gradient; IHG) agree well for both data sets.

6.2 Monthly Averaged Data Sets

Fig. 9 shows the monthly distribution of CH_4 for February 2004. The left panel shows the monthly-averaged SCIAMACHY data as retrieved with the IMLM scientific algorithm. Only cloud-free pixels with instrument noise related errors $< 0.2\times10^{19}$ molec/cm^2 have been included. The daily SCIAMACHY data have been regridded on a 1^o by 1^o grid before averaging all available data for this month. The right-hand panel shows the monthly-averaged CH_4 total columns as calculated by the TM3 model. This Figure shows that such a qualitative comparison shows good agreement between the monthly averaged SCIAMACHY data and the corresponding TM3 calculations. E.g. the North-South gradient is clearly visible in the SCIAMACHY data. In addition, many differences can be seen as well, such as the polluted areas in Eastern USA, and the East coast of Australia, which are hardly visible in the TM3 model. In Central Africa a region with low CH_4 columns is visible which is not in agreement with the TM3 calculations. Since this region is mostly cloudy during this time of the year, this is probably due to cloudy SCIAMACHY pixels that have not been filtered out by the simple cloud mask included in the IMLM retrieval algorithm. Other persistently cloudy areas such as in Brasil can clearly be identified by the lack of SCIAMACHY data, indicating that the cloud mask used does at least a fair job. This can also be seen from comparisons of the IMLM cloud mask with the FRESCO method (not shown here) which generally gives a good agreement.

The lack of data over the oceans is due to the fact that the albedo is too low to perform accurate retrievals. At high latitudes the IMLM retrieval algorithm also produces large errors, due to the high solar zenith angles.

In order to obtain a more quantitative comparison of the monthly-averaged CH_4 total columns from the IMLM algorithm and the TM3 model as shown in Fig. 9, the globe has been divided in five degree latitude bins. Then, all monthly SCIAMACHY data within each latitude bin have been averaged and compared to the average of the TM3 CH_4 total columns within the same latitude bin. The resulting values are shown in Fig. 10 where only data between longitudes 30^o W and 60^o E have been taken into account. This region is chosen because the Sahara and South-Africa are mostly cloud-free and have a high surface albedo, allowing accurate retrievals. It can be seen that there is a good agreement over South-Africa (between latitudes 35^o S and 20^o S) and over Northern Africa (between the Equator and 25^o N). In both cases the difference between the IMLM columns from the SRON algorithm and the TM3 calculations is less than 2%. The large difference over Central Africa is probably due to cloudy pixels in the SCIAMACHY data that have not been filtered out. The deviation from the TM3 model over Europe (latitudes $> 25^o$ N) is most likely caused by the variation of the dark signal within an orbit, a correction which was not yet implemented in the retrieval at the time this analysis was done (see Sect. 2).

7. CONCLUSIONS

The SCIAMACHY CH_4 and CO total column products from the scientific algorithms at SRON, IUP/IFE, and the University of Heidelberg have improved significantly since the previous validation workshop in December 2002. Especially, the implementation of a correction for the ice-layer growing on the SCIAMACHY channel 8 detector has improved the total column products. The columns are now in much better agreement with model calculations and independent satellite measurements. The operational products are, however, still off by orders of magnitude, mainly because the ice-layer correction is not yet included (see Sect. 2). All three scientific algorithms presented in this paper give similar CH_4 and CO total columns, although some differences remain. These are currently under investigation. At present, a sufficiently large data set is available for the validation of CH_4 and CO total column products. The first results show that the variability in the daily SCIAMACHY CO total columns agree well with measurements by the MOPITT instrument (see Sect. 5.1). The differences are in some cases up to $\sim$40%, but given the weakness of the CO lines this is expected. Similar results are obtained for the monthly averaged CO data (see Sect. 5.2). The daily SCIAMACHY data for CH_4 are in good agreement with TM3 calculations, with differences of up to $\sim$5%. The expected spacial variability is clearly visible (Sect. 6.1). Similar results, but with slightly smaller differences, are obtained when comparing monthly averaged cloud-free CH_4 data over Africa from February 2004 (Sect. 6.2). Thus, the results from the scientific algorithms are very promising. There is still room for improvement of the instrument calibration and the retrieval algorithms. These improvements will be implemented in the near future.

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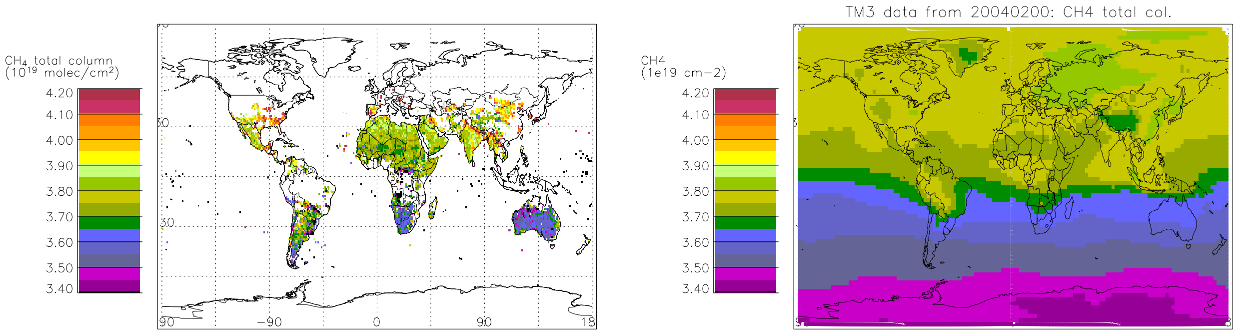

Figure 9. Left: Monthly-averaged CH_4 total columns from the IMLM retrieval algorithm for February 2004. Only cloud-free pixels with instrument noise related errors $< 0.2{\times}10^{19}$ molec/cm^2 have been included. The daily SCIAMACHY data have been regridded on a 1° by 1° grid before averaging all available data for this month. Right: The corresponding monthly-averaged CH_4 total columns calculated by the TM3 chemistry transport model on a 2.5° by 2.5° grid. Both the SCIAMACHY and the TM3 total columns have been normalized to the surface pressure. Note that both figures use the same vertical scale.

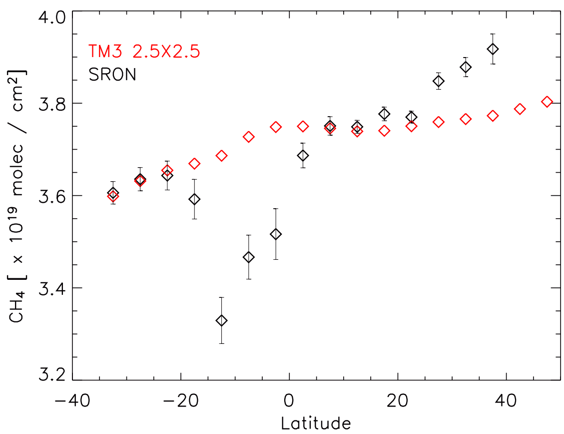

Figure 10. Comparison of the monthly CH_4 total columns for February 2004 as presented in Fig. 9, where all data within a five degree latitude bin have been averaged (see text). The black diamonds denote the IMLM CH_4 total columns, the red diamonds the corresponding TM3 data. Only cloud-free pixels with instrument noise related errors $< 0.2{\times}10^{19}$ molec/cm^2 have been included. The error bars denote the instrument noise related errors only. Both the SCIAMACHY and the TM3 total columns have been normalized to the surface pressure.

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