THE EVALUATION OF SCIAMACHY CO AND CH_4 SCIENTIFIC DATA PRODUCTS, USING GROUND-BASED FTIR MEASUREMENTS

B. Dils[(1)], M. De Mazière[(1)], J. F. Müller[(1)], M. Buchwitz[(2)], R. de Beek[(2)], C. Frankenberg[(3)], A. Gloudemans[(4)], H. Schrijver[(4)], M. Van den Broek[(4)] and contributing NDSC FTIR teams

(1) Belgian Institute for Space Aeronomy (BIRA-IASB), Ringlaan 3, 1180, Brussels, Belgium, E-mail:Bart.Dils@oma.be
(2) Institute of Environmental Physics (IUP) / Institute of Remote Sensing (IFE), University of Bremen FB1, Otto Hahn Allee 1, 28334 Bremen, Germany
(3) Institute of Environmental Physics, University of Heidelberg, Heidelberg, Germany
(4) SRON, Sorbonnelaan 2, 3584 CA Utrecht, Netherlands

ABSTRACT

In the framework of the European EVERGREEN project, three scientific algorithms, namely WFM-DOAS, IMAP-DOAS and IMLM, have been developed to retrieve the total column amounts of key atmospheric trace gases including CO and CH_4 from SCIAMACHY nadir observations in its near-infrared channels. These channels offer the capability to detect trace gases in the planetary boundary layer, potentially making the associated retrieval products suited for regional source-sink studies.
The retrieval products of these three algorithms, in their present status of development, have been compared to independent data from a ground-based quasi-global network of Fourier-transform infrared (FTIR) spectrometers, for the year 2003. Comparisons have been made for individual data, as well as for monthly averages. To maximize the number of coincidences that satisfy the temporal and spatial collocation criteria, the individual SCIAMACHY data points have been compared with a 3rd order polynomial interpolation of the ground-based data with time. Particular attention has been paid to the question whether the products reproduce correctly the seasonal and latitudinal variabilities of the target species. We present an overall assessment of the data quality of the currently available latest versions of the CO and CH_4 total column products from the three scientific retrieval algorithms.

1 INTRODUCTION

The purpose of the current validation is to identify quantitatively to what extent the scientific SCIAMACHY [1-3] NIR products, WFM-DOAS [4-8], IMAP-DOAS [9-12] and IMLM [13-16], generated by various institutes in Europe can be exploited for global geophysical studies. This is done by comparing the available SCIAMACHY data with correlative, i.e., close in space and time, independent data – *in casu* from a remote-sensing network of ground-based FTIR spectrometers. The ground-based (g-b) correlative data are collected from 11 FTIR spectrometers that are operated at various stations of the Network for the Detection of Stratospheric Change (NDSC, http://www.ndsc.ws). For comparison purposes, all data have been converted to average volume mixing ratios (vmrs) using ECMWF pressure data.

Table 1. Spatial coordinates of the ground-based FTIR stations.

Station	Lat N	Lon E	Alt.(m)
NY.ALESUND	78.91	11.88	20
KIRUNA	67.84	20.41	419
HARESTUA	60.22	10.75	580
ZUGSPITZE	47.42	10.98	2964
JUNGFRAUJOCH	46.55	7.98	3580
EGBERT	44.23	-79.78	251
TORONTO	43.66	-79.40	174
IZAÑA	28.30	-16.48	2367
WOLLONGONG	-34.45	150.88	30
LAUDER	-45.05	169.68	370
ARRIVAL.HEIGHTS	-77.85	166.78	190

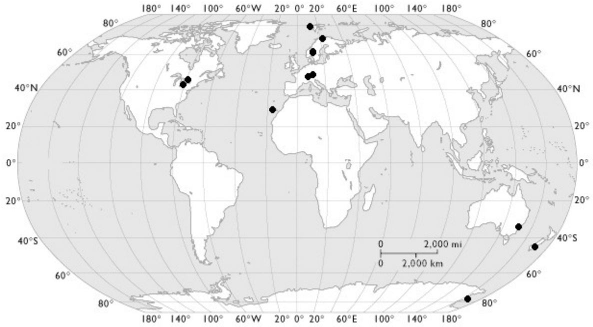

Fig.1. Distribution of stations

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2 METHOD

Due to the inherent different properties of FTIR and SCIAMACHY measurements, the validation is not straightforward and several issues needed to be resolved in order to perform a proper inter-comparison.

Because the target molecules have most of their total concentration in the lower troposphere, the total column amount is strongly dependent on the observatory's or pixel's mean altitude. To eliminate any apparent differences or variations in the data set that are due to this altitude dependence, we have normalised all total column data using ECMWF operational pressure data into mean volume mixing ratios. The same normalisation has been applied to the overpass SCIAMACHY data, for those datasets which do not have so-called dry air normalised data products (see further). Additionally all SCIAMACHY vmrs are multiplied by a profile correction factor, derived from TM4 model data (see [17]).

To maximize data overlap between SCIAMACHY observations and FTIR g-b measurements, and to ensure a statistically significant correlative data set, the SCIAMACHY measurements are compared with the corresponding (in time) interpolated value of a third order polynomial fit through the FTIR g-b data, rather than with the FTIR data themselves. This third order polynomial fit gives a good representation of the seasonal variability, but loss of information as to daily variability and as to possible short term events cannot be avoided. To asses the representation of the seasonality, weighted monthly averages are calculated.

An additional difference between FTIR and SCIAMACHY data, for which no obvious solution is available, is the fact that the column measured by SCIAMACHY is an average column above the area covered by a SCIAMACHY pixel which extends beyond the location of the g-b station. This might create an apparent bias between the FTIR and SCIAMACHY measurements. Additionally, to obtain a statistically significant dataset, the spatial collocation criteria include all SCIAMACHY pixels centred within ±2.5° latitude and ±5° or ±10° longitude of the FTIR ground-station coordinates (for the small grid and large grid collocation, respectively), thus covering an even wider area. Unfortunately there is no way around this inherent difference and thus when interpreting all validation results, one must always keep this point in mind. To have an indication of the impact of spatial collocation, all parameters have been calculated for both the small and large spatial collocation grid. In this paper only results for the large grid are shown. A more detailed description concerning the methodology and all results are shown in [17].

3 THE SCIAMACHY DATA

The data products from different algorithms differ greatly among themselves. For IMAP, the final data products, henceforth denoted as XCH_4 and XCO, are the total column values of said species divided by the total column values of either CO_2 (for XCH_4) or CH_4 (XCO), all scaled to be a proxy for dry air. WFMD also provides XCH4 vmr values. However while their CO product uses CH_4 measurements (from the same fitting window) to correct the total column values, it does not provide XCO vmrs. Both IMLM CO and CH_4 products are total column values only. For the purpose of this validation, dry air normalised products are used in stead of the total column measurements scaled by the ECMWF pressure, whenever they are available. Furthermore, not all scientific data products are derived from the same spectroscopic channel, nor do they use the same error thresholds or other quality selection criteria. Most notably IMLM CH_4 is derived from Channel 8 affected by build-up of ice, while both IMAP and WFMD XCH_4 are taken from Channel 6. Therefore this validation only deals with the scientific end products and not the algorithms behind these products. Moreover during the course of this validation it became apparent that the WFM-DOAS XCH4 data required a solar zenith angle correction. All results shown here apply to the corrected data.

4 RESULTS

Table 2 gives a summary of the statistical comparison results for the year 2003. Bias is the calculated weighted (the weight = $1/(err)^2$, in which err is the error on the individual measurement as given by the data providers) bias (in %) of the individual SCIAMACHY data relative to the 3^{rd} order polynomial fit through the ground-based FTIR data. The indicated errors represent the corresponding weighted standard errors (3*std/sqrt(N)). N is the number of correlative individual SCIAMACHY data. σ_{scat} is the percentage 1σ weighted standard deviation of the daily averaged SCIAMACHY measurements with respect to the polynomial interpolation of the daily FTIR data, corrected for the bias. R is the correlation coefficient between the weighted monthly mean SCIAMACHY and FTIR data. Also given are the scatter of the daily averaged FTIR data points relative to their corresponding polynomial fit values (σ_{FTIR}) and the target precisions (TP) needed for inverse modelling on a regional scale.

4.1 CO

For CO, the results look promising. The correlation coefficients between g-b FTIR and SCIAMACHY data are relatively high and in general the time series capture the overall seasonal variation. However the relatively high scatter, combined with periods or regions with relatively scarce data (near the poles, southern hemisphere, January and August) can cause serious aberrations in the data output of which the data user should be aware.

Table 2. Summary of all results (from Dils et al. (2006)).

	CO			CH_4		
	WFMD CO v0.5	**IMLM CO v6.3**	**IMAP XCO v0.9**	**WFMD XCH_4 v0.5 cor**	**IMLM CH_4 v6.3**	**IMAP XCH_4 v1.1**
Bias (%)	0.00 ± 0.87	-14.7 ± 0.90	-4.99 ± 0.68	-3.28 ± 0.05	-2.83 ± 0.10	-0.62 ± 0.04
N	22362	12082	14418	42072	9323	22954
σ_{scat} (%)	25.1	22.4	23.5	1.93	3.14	1.09
R	0.86	0.83	0.53	0.80	0.71	0.70
σ_{FTIR} (%)	9.49			1.15		
TP (%)	5(10)			1		

The scatter on the CO data is still at least a factor 2 worse than that of the g-b FTIR measurements and target precision of 10%. Part of the large scatter may be due to natural variability (also present in the FTIR scatter) and part due to low precision of individual SCIAMACHY measurements. The calculated biases for the southern hemisphere stations are significantly larger than for the northern hemisphere data. This could be related to a large drop in data availability (as is also indicated by the sharp increase of the standard errors) [17]. For those stations where one expects significant boundary layer concentrations (Toronto and Egbert) the MOPITT CO data agree surprisingly well with the FTIR g-b data. It would be of great benefit to the scientific community if a comparison between MOPITT, SCIAMACHY and independent data could be performed at additional sites where considerable boundary layer CO concentrations are expected.

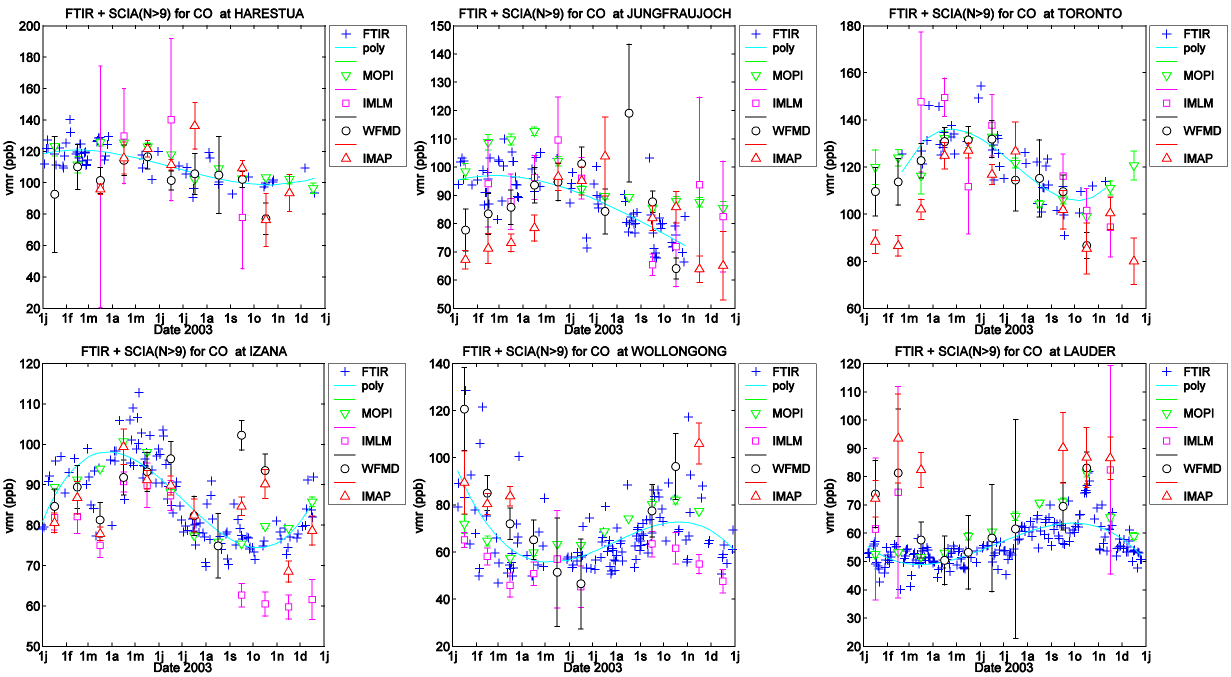

Fig 2. Examples of weighted monthly mean vmrs for (X)CO as a function of time for the year 2003 (for other stations see [17]), for the 3 algorithms together with the daily averaged FTIR measurements and corresponding 3rd order polynomial fit. The error bars on the monthly mean values represent the standard error. Monthly mean data are not shown for months with fewer than 10 SCIAMACHY measurements.(from Dils et al. (2006))

4.2 CH_4

For CH_4, the scatter has (almost) reached the target precision of 1% in the case of IMAP, while the other algorithms are still a factor 2 to 3 away. It appears that the IMLM data for CH_4 retrieved from channel 8 exhibit more scatter than the data from both other algorithms. They are also less numerous due to the larger footprint of one SCIAMACHY ground scene in channel 8 and the necessity of strict cloud filtering. It is thus very difficult to assess the time series of this product although for those stations for which sufficient data are available it seems to capture the seasonal variability well. Comparisons with ECMWF pressure normalized WFMD and IMAP CH_4, show that the icing problem of Channel 8 is well handled. WFMD XCH_4 still harbours structural problems, prompting a solar zenith angle (SZA) correction factor on the WFMD data. This SZA correction (XCH_4_corrected= XCH_4_v05 / (0.9 + 0.15*cos(SZA)) improved the comparisons tremendously, but it clearly fails in some cases (e.g., at Izaña). IMAP XCH_4 still seems to have problems with southern hemisphere station data.

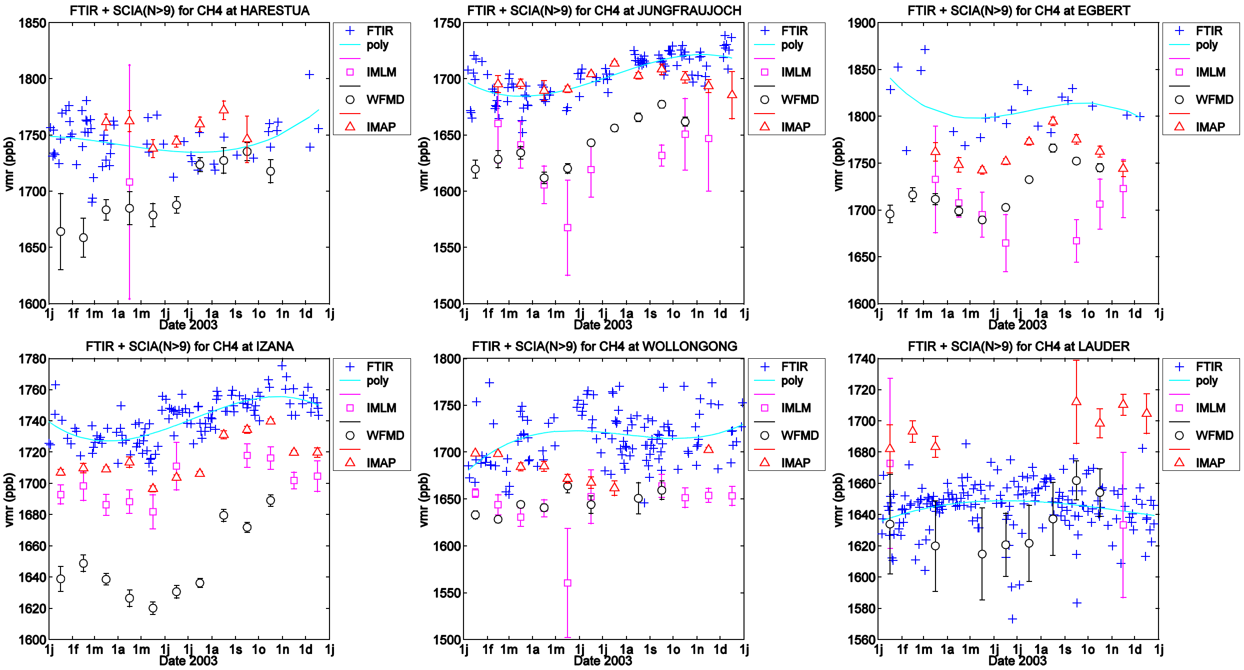

Fig. 3. Examples of weighted monthly mean vmrs for (X)CH_4 as a function of time for the year 2003, for the 3 algorithms (note that for IMLM no XCH4 data was available and ECMWF pressure data is used for the normalisation) together with the daily averaged FTIR measurements and corresponding 3rd order polynomial fit. (for other stations see [17]) The error bars on the monthly mean values represent the standard error. Monthly mean data are not shown for months with fewer than 10 SCIAMACHY measurements. . (from Dils et al. (2006))

5 CONCLUSIONS

Overall, one can state that SCIAMACHY provides an added value to the actually deployed fleet of satellite instruments, especially for tropospheric chemistry research on a global scale. Considerable improvements on the data quality have been achieved but there are still significant remaining issues to be resolved. A more detailed description of this work can be found in [17].

6 ACKNOWLEDGEMENTS

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