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Comparisons between SCIAMACHY and ground-based FTIR data for total columns of CO, CH_4, CO_2 and N_2O

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Abstract. Total column amounts of CO, CH_4, CO_2 and N_2O retrieved from SCIAMACHY nadir observations in its near-infrared channels have been compared to data from a ground-based quasi-global network of Fourier-transform infrared (FTIR) spectrometers. The SCIAMACHY data considered here have been produced by three different retrieval algorithms, WFM-DOAS (version 0.5 for CO and CH_4 and version 0.4 for CO_2 and N_2O), IMAP-DOAS (version 1.1 and 0.9 (for CO)) and IMLM (version 6.3) and cover the January to December 2003 time period. Comparisons have been made for individual data, as well as for monthly averages. To maximize the number of reliable coincidences that satisfy the temporal and spatial collocation criteria, the SCIAMACHY data have been compared with a temporal 3rd order polynomial interpolation of the ground-based data. Particular attention has been given to the question whether SCIAMACHY observes correctly the seasonal and latitudinal variability of the target species. The present results indicate that the individual SCIAMACHY data obtained with the actual versions of the algorithms have been significantly improved, but that the quality requirements, for estimating emissions on regional scales, are not yet met. Nevertheless, possible directions for further algorithm upgrades have been identified which should result in more reliable data products in a near future.

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1 Introduction

The SCIAMACHY instrument (Burrows et al., 1995; Bovensmann et al., 1999, 2004) onboard ENVISAT makes nadir observations in the near-infrared (NIR; 0.8–2.38 μm) of the most important greenhouse gases such as water vapour (H_2O), carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O), and of the ozone precursor gas carbon monoxide (CO), which also acts as an important indirect greenhouse gas as it significantly impacts the OH budget. SCIAMACHY is among the first satellite instruments that can measure greenhouse gases in the troposphere on a global scale. Its predecessor instrument GOME (Global Ozone

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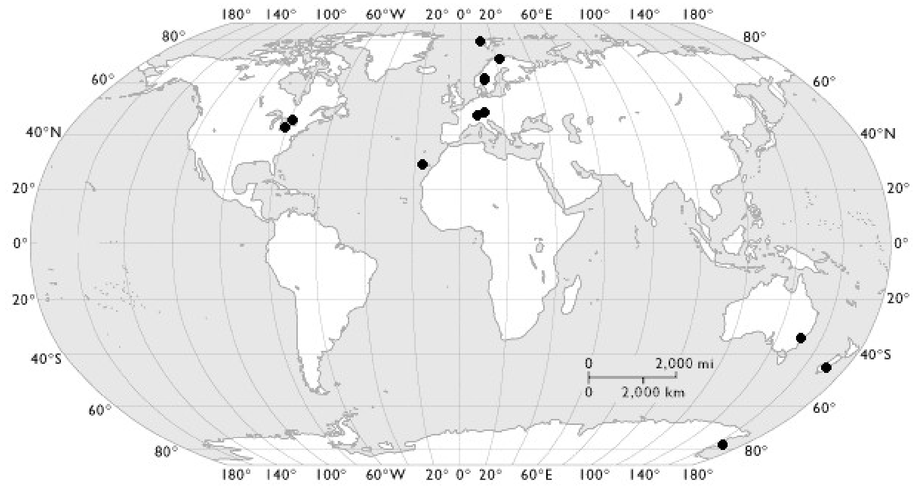

Fig. 1. Distribution of stations contributing to the delivery of correlative g-b FTIR data for comparisons with SCIAMACHY products – see also Table 1.

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

Station	Lat N	Lon E	Altitude(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

Monitoring Experiment) does not include the channels in the NIR (Burrows, et al., 1999). IMG (Interferometric Monitor of Greenhouse Gases) flew onboard ADEOS in 1997 to make nadir measurements in the thermal infrared (TIR), but failed after a few months of operation (Kobayashi et al., 1999). At present, MOPITT (Measurements Of Pollution In The Troposphere, Drummond and Mand, 1996) is delivering only CO profile data retrieved from the TIR channels; the expected CH_4 products are still unavailable due to instrument calibration problems (MOPITT Web site http://eosweb.larc.nasa.gov/PRODOCS/mopitt/table_mopitt.html). SCIAMACHY measurements in the NIR have the important advantage over TIR measurements that they are sensitive down to the earth's surface, where most emission sources are located, whereas thermal infrared measurements have a reduced sensitivity in the boundary layer. It is very important therefore to thoroughly investigate the potential capabilities of SCIAMACHY in its NIR channels.

The purpose of the current validation is to identify quantitatively to what extent the SCIAMACHY NIR products generated by various scientific institutes in Europe can be exploited for global geophysical studies. It therefore addresses the consistency of the data to represent the variations of the CO, CO_2, CH_4 and N_2O fields with season, latitude, etc. 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. Other complementary validation efforts have been made, such as comparisons with data from other satellites, e.g., with CO data from MOPITT, or with analyses from global chemistry models such as TM3 (Heimann and Körner, 2003) or TM5 (Krol et al., 2004), and have been reported by Buchwitz et al. (2005a) and de Beek et al. (2006); Gloudemans et al. (2005); Straume et al. (2005).

The SCIAMACHY data for CO, CH_4, CO_2 and N_2O total columns investigated in this paper have been produced by the algorithms WFM-DOAS v0.5 and v0.4 (Weighting Function Modified DOAS, Institute for Environmental Physics, University of Bremen (Buchwitz et al., 2000, 2004, 2005a, b; de Beek et al., 2006)), IMLM v6.3 (Iterative Maximum Likelihood Method, SRON (Schrijver, 1999; Gloudemans et al., 2005, 2004; de Laat et al., 2006)) and IMAP-DOAS v1.1 and v0.9 (Iterative Maximum A Posteriori-DOAS, University of Heidelberg (Frankenberg et al., 2005a, c)). So far, CO_2 and N_2O data products have been provided by WFM-DOAS v0.4 only. Only those retrieval products which are open to public use have been validated. The data provided for this validation exercise cover the January to December 2003 time period, and thus offer a much better basis for validation than the limited data set that was available for previous exercises (De

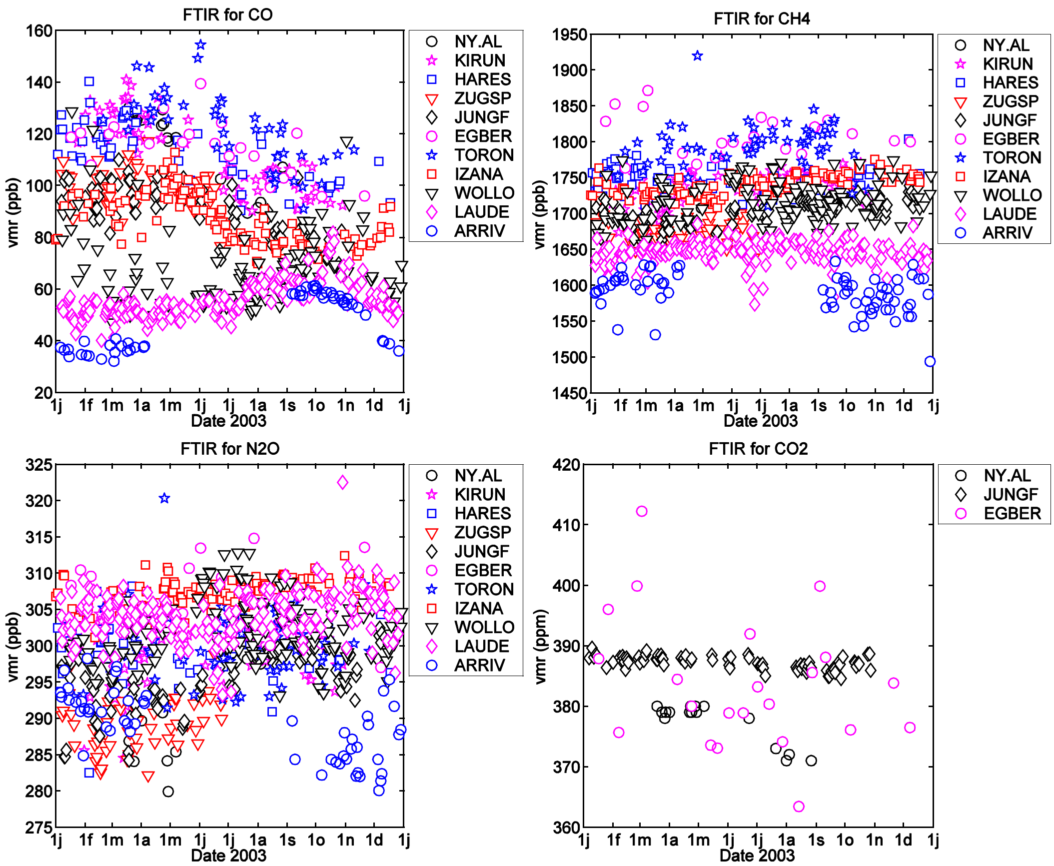

Fig. 2. Ground-based NDSC FTIR data of column averaged volume mixing ratios of **(a)** CO, **(b)** CH_4, **(c)** N_2O and **(d)** CO_2 for the year 2003 compiled at BIRA-IASB for the present validation exercise. In the plots the total column amounts have been converted to volume mixing ratios using ECMWF pressure data (see text).

Mazière et al., 2004). Since then, some algorithm updates have also been implemented. For more in depth information about the SCIAMACHY retrieval algorithms and data products, the reader is referred to the above cited references.

The characteristics of the correlative ground-based FTIR data are described in the next section. Section 3 presents the conditions that have been verified for carrying out the comparisons. The comparison methodology and the results of the comparisons are discussed in Sect. 4, successively for CO, CH_4 and N_2O and CO_2. Conclusions are drawn in Sect. 5.

2 The ground-based correlative data

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). They have been submitted to the Envisat Cal/Val database at NILU or directly to BIRA-IASB and have been compiled by us as part of the commitment in the Envisat AO ID 126 “Validation of ENVISAT-1 level-2 products related to lower atmosphere O_3 and NO_y”. Figure 1 and Table 1 identify the locations of the contributing stations. While the stations cover almost the entire global latitude band, several regions of specific interest (the tropics, Central Africa, China) are not covered.

The g-b FTIR data are obtained from daytime solar absorption measurements under clear-sky conditions. G-b FTIR data can also be obtained from lunar absorption measurements at near full noon, e.g., in polar night conditions at high northern and southern latitude stations: such lunar absorption data are not included in the present data set however.

Figure 2 shows the database of the CO, CH_4, N_2O and CO_2 g-b data products, respectively, available at BIRA-IASB for the present validation exercise, and the stations for which the respective data was available. For comparison purposes, all data have been converted to average volume mixing ratios (vmrs) using ECMWF pressure data, as explained hereinafter (Eq. 1).

Regarding CO (Fig. 2a) seasonal variations are quite pronounced (amplitude of about 50%), with a maximum by the end of local spring, determined by the availability of OH, which is the major sink for CO. Large excursions in the CO

Table 2. Average TM4 profile correction factors for CO and CH_4 over the year 2003.

station	CO mean correction	CH_4 mean correction
Ny Alesund	1.0013	1.0004
Kiruna	1.0052	1.0015
Harestua	1.0006	1.0001
Zugspitze	0.8486	0.9811
Jungfraujoch	0.7882	0.9703
Egbert	1.0078	1.0007
Toronto	1.0384	1.0028
Izaña	0.9107	0.9854
Wollongong	1.0052	1.0005
Lauder	1.0074	1.0022
Arrival heights	0.9989	0.9993

column amounts are observed at Wollongong: they can probably be attributed to biomass burning events. Also, the g-b FTIR data (Fig. 2b) clearly illustrate the interhemispheric gradient of CH_4 that amounts to ~15% going from the South Pole (Arrival Heights) to the maximum values at northern latitudes (Izaña). One also observes a small seasonal variation of CH_4 (of the order of 5%) that is more distinct in the Northern Hemisphere than in the southern one. The CH_4 minimum in the Northern Hemisphere occurs at the beginning of the year, i.e., around mid-winter. N_2O has a very small seasonal variation; also the variability over the entire data set is less than 15%. The CO_2 data set is limited to 3 ground stations, with only very few data at Ny Alesund as seen in Fig. 2d.

Due to the inherent different properties of FTIR and SCIAMACHY measurements, the validation is not straightforward and several issues need to be resolved in order to perform a proper intercomparison. These issues are, (1), how to deal with different ground station altitudes, (2), the data availability, (3) the precision and accuracy of the data, and (4) the difference in observed air masses.

(1) The first issue concerns the difference in altitude between the SCIAMACHY ground pixel height and the FTIR measurement location. 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 (P) into mean volume mixing ratios:

$$C_{vmr} = C_{\mathrm{totcol}}/(P * 2.12118e11) \quad (1)$$

Herein C_{vmr} is the mean volume mixing ratio (in ppbv), C_{totcol} the measured total column value (in molec cm^{-2}), and, for the FTIR g-b data, P the pressure at station altitude (in Pa). The factor converts pressure (Pa) into total column (molec cm^{-2}) values. The same normalisation has been applied to the overpass SCIAMACHY data, using the pressure corresponding to the mean altitude of the observed ground pixel, for these data sets which do not have so-called dry air normalised data products (see Sect. 3). The use of this normalisation procedure to improve the comparisons relies on the assumption that the volume mixing ratio of the considered species is constant as a function of altitude, which is the best assumption at hand in the absence of auxiliary information, but still relatively crude. The approximation is best for CO_2, having a nearly constant volume mixing ratio throughout the whole atmosphere, relatively good for CH_4 and N_2O with an almost constant tropospheric vmr, but worse for CO that has a more variable vmr in the troposphere. An error assessment study using TM4 CO and CH_4 profile data has taught us that for the three high altitude stations (Jungfraujoch, Zugspitze and Izaña) the errors associated with this approximation can be as large as 20% for CO and 3% for CH_4. To compensate for these relatively large errors, all CO and CH_4 SCIAMACHY vmrs are multiplied by a profile correction factor prior to any further comparison. This factor was derived by taking the ratio of the calculated TM4 (Meirink et al., 2006) vmr above the mountain station altitude and above ground level (as determined by the model's orography) at the stations geo-location. Note that the spatial resolution of the model ($2\times3°$) does not correspond with that of a SCIAMACHY pixel and thus the correction can never be perfect. We thus opted to keep the correction as simple and clear as possible. Therefore it is not calculated at the SCIAMACHY pixel geo-location for each measurement individually. We did however calculate this correction ratio for each 2003 day since for several stations a small but clear seasonal dependence of this factor was noticeable (see Fig. 3). The impact of such a correction is only significant for the three high altitude stations as one can see from their mean values listed in Table 2 and on their bias values only. It did not have any significant impact on the scatter or seasonality. No model profile N_2O and CO_2 data was available, but the impact is deemed to be far less important, nor is any deviational behaviour for the high altitude stations observed.

(2) The second issue (data availability) concerns the amount of available g-b data. One must remember that the g-b FTIR observations require clear-sky conditions. Consequently the g-b FTIR database does not represent a daily coverage, even if most stations are operated on a quasi-continuous basis. This limits of course the number of possible coincidences with SCIAMACHY overpasses. Moreover for some ground-based stations the available data sets do not cover the entire January till December 2003 time period. To maximize data overlap between SCIAMACHY observations and FTIR g-b measurements, and to ensure a statistically significant correlative data set, the SCIAMACHY data that meet the spatial collocation criteria (see Sect. 3) are not compared on the basis of temporal overlap with the g-b data. Instead, we developed an alternative method in which the

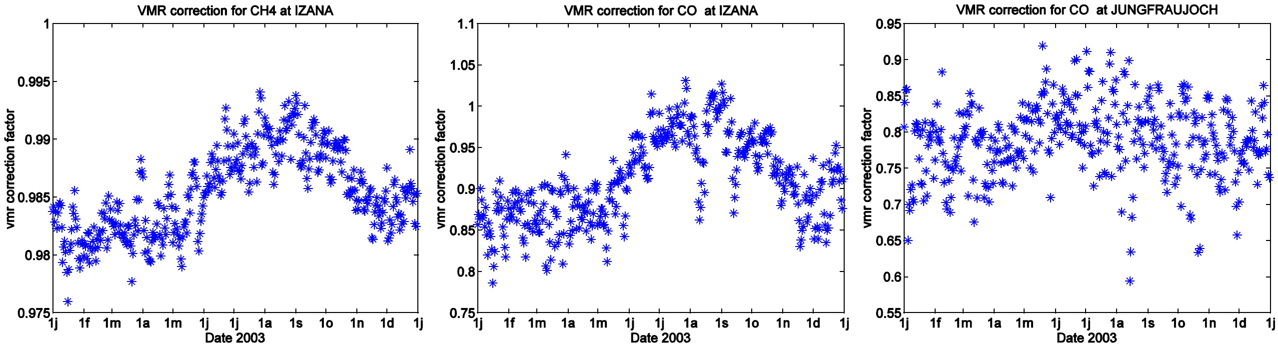

Fig. 3. Typical examples of TM4 profile correction factors as a function of time. **(a, b)** TM4 profile correction factor for CH_4 and CO Izaña, exhibiting exceptionally strong seasonality. **(c)** TM4 profile correction factor for CH_4 and CO Jungfraujoch, exhibiting a moderate seasonality (an example of Jungfraujoch CH_4 is given in Fig. 4b).

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. To ensure consistency between all stations, all FTIR data points, if not already daily averages, have been converted to daily averages prior to any further manipulations such as the normalisation using ECMWF daily pressure data and the subsequent 3rd order polynomial fitting procedure. This third order polynomial fit gives a good representation of the seasonal variability (see example in Fig. 4a), but loss of information as to daily variability and as to possible short term events cannot be avoided. Furthermore, locations with strong daily variability may exhibit differences/biases between SCIAMACHY and FTIR if the time of a significant number of FTIR measurements differs a lot from 10:00 h local time, i.e. the SCIAMACHY overpass time. The data comparisons have been limited to the time periods during which g-b data are available to avoid gross extrapolation errors. This explains why there are no g-b data available for inter-comparisons during the polar night at high-latitude stations. This method, which significantly increases the number of coincident data, allows us to study the latitudinal dependence over a wider range of stations whereas the usual validation method, considering only daily coincidences, failed to provide sufficient, if at all, overlapping data, especially for stations near the poles where the amount of SCIAMACHY data points is limited. The latter is due to the difficulties of cloud filter algorithms to distinguish between ice and clouds and to the high solar zenith angles over these regions leading to low signal to noise ratios, and thus larger errors in the retrieved total columns.

The standard deviations of the ground-based data with respect to their 3rd order fit, or

$$std\left(\frac{y_i^{GB}-y_i^{PF}}{y_i^{PF}}\right) \quad (2)$$

(with y_i^{GB} the individual ground-based daily averaged volume mixing ratios on day i, and y_i^{PF} the corresponding values from the 3rd order polynomial fit) are, on average, 9.5% for CO (the average standard deviation drops to 7.0% when excluding the Wollongong measurements), 1.15% for CH_4, and 1.16% for N_2O and 1.12% CO_2. The individual values per station are provided in Tables 6–9 hereinafter.

Table 3. Percentage scatter on the daily mean FTIR and SCIAMACHY data, collocated on the large spatial grid. Also indicated are the target precisions set for the SCIAMACHY data. Data marked by * are dry air normalised products, typically denoted by an X such as XCH_4.

	FTIR	WFM-DOAS	IMLM	IMAP	Desired precision
CO	9.49	25.1	22.4	23.5*	5–10
CH_4	1.15	1.93*	3.14	1.09*	1
N_2O	1.16	9.31*			10
CO_2	1.12	3.78*			1

(3) The third issue, that of data precision and accuracy, has been discussed partially above. Individual g-b FTIR data for N_2O, CO, CO_2 and CH_4 have a precision in the order of a few percent (<5%). Because of the adopted approach to use interpolated (fit) values instead of original measurement data, the effective precision of the g-b correlative data is set by the values listed in Table 3. It is important to realise that the thus obtained scatter includes the natural day-to-day variability.

Conservative estimates for the accuracies considering the entire FTIR network are 3% for N_2O and CO_2, and 7% for CO and CH_4. Network accuracies are continuously improved over time by adopting some agreements among the contributing stations regarding the choice of spectral data analysis parameters. For example, this has been done recently in the UFTIR project for CO, N_2O and CH_4 (http://www.nilu.no/uftir).

Table 4. Selection of spectral channels and microwindows for the retrieval of CO, CH_4, N_2O and CO_2 in the different retrieval methods considered.

	WFMDv0.5 (v0.4 for N_2O and CO_2)	IMLMv6.3	IMAPv1.1 (v0.9 for CO)
CO	Channel 8: 2324.2–2334.9 nm	Channel 8: 2324.5–2337.9 nm	Channel 8: 2324.2–2334.9 nm
CH_4	Channel 6: 1629.0–1671.0 nm	Channel 8: 2324.5–2337.9 nm	Channel 6: 1630.0–1670.0 nm
N_2O	Channel 8: 2265.0–2280.0 nm		
CO_2	Channel 6: 1558.0–1594.0 nm		

(4) An additional difference between FTIR and SCIAMACHY, 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. For Channel 8 products (see further in Sect. 3), the pixel size is $30\times120\,km^2$, for Channel 6 products $30\times60\,km^2$ (see Table 4 for the used SCIAMACHY channels for each algorithm). Consequently, for example for a mountainous g-b station, the SCIAMACHY column also samples to some extent the valleys around the station that often harbour significantly higher concentrations of pollutants compared to the mountain site. This might create an apparent bias between the FTIR and SCIAMACHY measurements. Additionally, to obtain a statistically significant data set, the spatial collocation criteria include all SCIAMACHY pixels centred within $\pm2.5°$ latitude and $\pm5°$ or $\pm10°$ longitude of the FTIR ground-station coordinates (for the small grid and large grid collocation, respectively – see Sect. 4), thus covering an even wider area, which in turn may influence the data scatter as compared to that of the FTIR g-b measurements. 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.

3 The SCIAMACHY data and selection criteria for comparison

The retrieval methods discussed in this paper (WFM-DOAS (henceforth called WFMD), IMLM and IMAP-DOAS (henceforth called IMAP)) not only use different mathematical retrieval algorithms, but also obtain their data for CO, CH_4, N_2O and CO_2 from different spectral channels and wavelength regions: an overview hereof is given in Table 4. Each of the channels/windows has its own distinct features and associated problems. For instance the SCIAMACHY NIR Channels 7 and 8 are affected by ice layer build-up on the detectors, which is countered by regular decontamination of the instrument (Bovensmann et al., 2004). Also, not all the SCIAMACHY data sets considered for the present comparisons cover the complete year 2003: the IMLM data set contains no data for July and August, and WFMD only contains data from January till October. While the CH_4 IMAP data set covers the entire 2003 time period their CO data set lacks measurements for August. Due to the fact that the January to December 2003 time frame includes periods of lower transmission and ice decontamination of the SCIAMACHY instrument, differences in the considered time periods may lead to apparent differences in the final comparison results when evaluating the algorithms. Some differences may also occur because of the seasonal variation of the inter-hemispheric latitudinal gradient of some species, notably CO.

It must also be noted that for WFMD and IMAP, the final data products, henceforth denoted as XCH_4, XCO_2, XN_2O and XCO, are the total column values of said species divided by the total column values of either CO_2 (for XCH_4), O_2 (XCO_2 and XN_2O) or CH_4 (XCO), all scaled to be a proxy for dry air. Thus the dry air normalized product is equal to its measured total column value multiplied by the ratio of the expected vmr of the dry air proxy (a constant) over its measured total column value. For instance XCH_4 (ppb)=CH_4 (molec cm^{-2})*368e3 (ppb)/CO_2 (molec cm^{-2}). The only exception is WFMD CO, which uses CH_4 measurements (from the same fitting window) to correct the total column values but does not provide dry air normalized XCO vmrs (de Beek et al., 2006). This normalisation should improve the data quality, given the fact that systematic retrieval errors, such as residual cloud contamination, are eliminated to a large extent from the ratio product. In order to maximize the possibility for such cancellation of retrieval errors, the spectral windows for the retrieval of the species and its dry air proxy must be as close as possible. In the case of XCO and XCH_4, the dry air proxies CH_4 and CO_2 respectively are derived from the same spectral channel. For XCO_2 and XN_2O, O_2 is retrieved from another channel (Channel 4). An additional (small) error is introduced into the normalized product by treating the expected dry air proxy vmr as a constant, neglecting its seasonal and latitudinal variability. Therefore this constant scaling factor is sometimes, but not for this validation, replaced by a variable expected vmr based on a global model (Frankenberg et al., 2006). For the purpose of this validation, in those cases where dry air normalised products are available, these products are used instead of the total column measurements scaled by the ECMWF pressure.

Table 5. Selection criteria associated with accepted error levels for the SCIAMACHY data included in the comparisons with ground-based data.

Algorithm	Selection criteria (in addition to spatial and temporal collocation criteria)
WFMD	For XN_2O and XCO_2: Cloud-free, Over land (altitude >0), Solar Zenith Angle <85 deg, Error (fitting) <10% for CO_2, <60% for N_2O, only forward scan pixels. For XCH_4 and CO: Only data that are marked as good by the v0.5 data file quality flag
IMLM	Cloud-free, Albedo ≥0.01, Instrument-noise related Error <2E18 molec cm^{-2} for CH_4 (∼5%) and <1.5E18 molec cm^{-2} for CO, Solar Zenith Angle <80 deg
IMAP	For CH_4 data: [Vertical Column Density of CO_2/exp(-surface elevation(m)/8500)]>7E21 molec cm^{-2} and variance of fit residual <0.5% For CO data: variance of the fit residual (without weighting) <0.017, weighted variance of the fit residual between 10 and 0.1, error <7E17 molec cm^{-2} and <30%

The data products for SCIAMACHY give reliable values only for cloud-free pixels because clouds are not transparent in the NIR (Buchwitz et al., 2000, 2004; Gloudemans et al., 2005; Straume et al, 2005) and thus effectively take over the role of the earth's surface. Since the highest concentrations of the target species are found close to the earth's surface, where the air pressure is the highest and where the sources and sinks are located, interpreting cloud-contaminated columns as total columns can lead to large errors in the analysis. The different algorithms investigated here use different cloud detection schemes (Buchwitz et al., 2004, 2005a; de Beek et al., 2006; Gloudemans et al., 2005) resulting in different cloud masks and methods dealing with clouds. In some cases they do not mask all cloudy pixels and in other cases they may be too restrictive, because they cannot distinguish between ice- or snow-covered surfaces and clouds, resulting in loss of data. This implies that some comparisons with g-b FTIR data may still suffer from the presence of clouds in the SCIAMACHY observation. The current IMAP method does not contain a cloud detection algorithm for CO. For XCH_4, IMAP and WFMD filter their measurements based on a lower threshold for the height-corrected CO_2 column: the column must be at least 89% of the expected total column assuming constant CO_2. This method effectively filters high-altitude clouds, while the dry air normalisation should reduce the impact of remaining low altitude cloud contamination. WFMD CO uses a similar scheme using CH_4 total column data (see de Beek et al., 2006).

In addition to the above, for low albedo values, the precision of the cloud-free SCIAMACHY data is strongly influenced by the albedo of the observed ground-pixel, because it determines to a large extent the signal-to-noise ratio of the corresponding observed spectra. This explains why data over ocean (water) are less reliable than data over land. Also measurements with a high solar zenith angle (typically at the Earth's poles), lead to low signal to noise ratios, and thus larger errors in the retrieved total columns. A restriction on the accepted solar zenith angles therefore further limits the size of the comparison data set at northern and southern high-latitude stations.

The criteria adopted for temporal and spatial 'collocation' stem from choosing the best compromise between achieving better or worse statistics and keeping more or less natural variability in the data. Spatial collocation has been defined as data being within ±2.5° latitude and ±10° longitude of the FTIR ground station (hereinafter indicated as the large collocation grid). Data that have been taken closer to each other (within ±2.5° latitude and ±5° longitude, hereinafter indicated as the small collocation grid) have been looked at in particular. The spatial collocation criteria adopted here are loose; however making those more stringent would have made the number of coincidences too small, especially at the high-latitude stations.

Additional selection criteria have been applied to the SCIAMACHY data, based on confidence limits as described in the Product Specification Document (available at http://www.sciamachy.org/validation/) or given by the data providers. These confidence limits are different for the different algorithms, because they estimate the errors differently. For example, WFMD includes spectral fit errors in the final error estimate, whereas the error reported by IMLM only accounts for instrument-noise related errors, and therefore appears to be smaller. The additional selection criteria that have been applied to the SCIAMACHY data from each algorithm are listed in Table 5.

In summary, the comparisons are made for dry air normalised products, hereinafter simply called the data, and are limited to (1) cloud-free SCIAMACHY data, according to the individual cloud detection schemes from individual algorithms, (2) having the centre of the SCIAMACHY pixel within the spatial collocation area around the location of the g-b site, as outlined above, and (3) satisfying the additional selection criteria listed in Table 5. Temporal coincidence has been defined as data being taken at the same time, in which the real g-b FTIR data set has been approximated by a continuous set of interpolated values, as explained in Sect. 2.

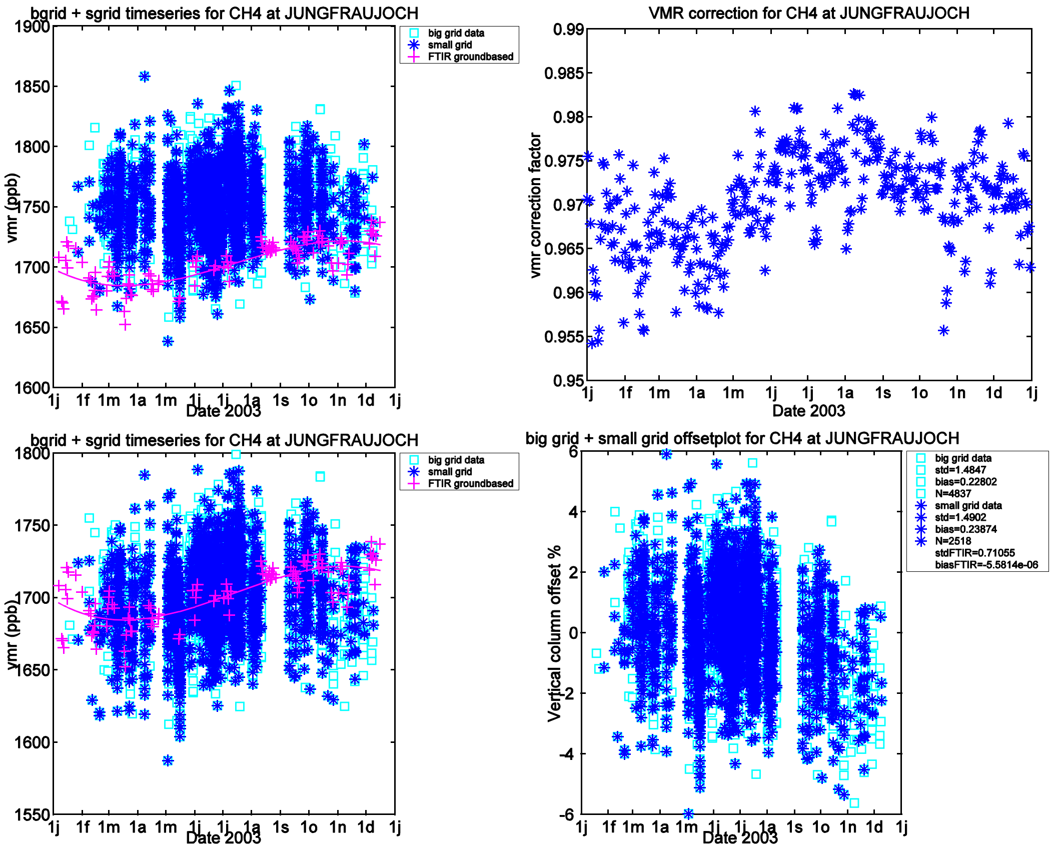

Fig. 4. Time series of CH_4 measurements at Jungfraujoch from g-b FTIR (+) and SCIAMACHY IMAP-DOAS (open squares for large collocation grid; * for small collocation grid). **(a)** original XCH_4 data points (symbols) and 3rd order polynomial fit through the FTIR ground-based data (solid line). **(b)** TM4 profile correction factor as a function of time. **(c)** XCH_4 data points (symbols) after the application of the correction factor and 3rd order polynomial fit through the FTIR ground-based data (solid line). **(d)** Corresponding time series of relative biases, (SCIAMACHY-FTIR)/FTIR, of IMAP-DOAS versus g-b interpolated data. Listed in the legend are the average bias, the standard deviation and the number of data points for the IMAP-DOAS data sets as well as the average bias and standard deviation of the FTIR data relative to their polynomial fit.

Before making the comparisons, we have verified that the total column averaging kernels of both data products (g-b FTIR and SCIAMACHY) are very similar, showing a rather uniform sensitivity close to 1 from the ground to the stratosphere (Buchwitz et al., 2004; Sussmann and Buchwitz, 2005; Sussmann et al., 2005). The associated smoothing errors for both data sets are negligible compared to the observed differences between them. Therefore we have compared the data products as such, without taking the averaging kernels explicitly into account.

4 The comparisons between timeseries of g-b FTIR network and SCIAMACHY data of CO, CH_4, CO_2 and N_2O total column amounts

4.1 Comparison methodology

Time series of the relative differences between the selected SCIAMACHY individual mean vmrs (x_j^{SCIA}) and the corresponding values from the 3rd order polynomial interpolation through the normalised g-b FTIR daily network data (x_j^{PF}), i.e., $[(x_j^{\mathrm{SCIA}} - x_j^{\mathrm{PF}})/x_j^{\mathrm{PF}}]$ have been made for all the different SCIAMACHY algorithms and target products. An example for CH_4 from the IMAP algorithm at the Jungfraujoch station is shown in Fig. 4. An overall weighted bias over the considered time period, b, was calculated for each target product, algorithm and station, following

$$b = \mathrm{mean}_{\mathrm{w}} \left(\frac{\mathrm{x}_{\mathrm{j}}^{\mathrm{SCIA}} - \mathrm{x}_{\mathrm{j}}^{\mathrm{PF}}}{\mathrm{x}_{\mathrm{j}}^{\mathrm{PF}}} \right) \tag{3}$$

in which the weighted mean, mean_w, of a data set which consists of N elements x_j is given by the general expression

$$\text{mean}_w(x)=\bar{x}_w=\frac{\sum_{j=1}^{N} w_j x_j}{\sum_{j=1}^{N} w_j} \tag{4}$$

with w_j the weight of the individual data. In our case $w_j=1/(err_j)^2$ in which err_j is the error on the individual measurement as given by the data providers. Note that the definition of the error changes with each algorithm and may or may not include instrument and/or fitting errors. The thus calculated biases are listed in Tables 6 to 9. A globally averaged weighted bias (i.e., a mean over all stations) was calculated as well and is also listed in the same corresponding Tables. The weighted standard errors on the biases reported in Tables 6 to 9 are given by

$$\frac{3}{\sqrt{N}} \times sd_w\left(\frac{x_j^{\text{SCIA}}-x_j^{\text{PF}}}{x_j^{\text{PF}}}\right) \tag{5}$$

in which the weighted standard deviation, sd_w, of a data set which consists of N elements x_j is given by the general expression:

$$sd_w(x)=\sqrt{\frac{N' \sum_{j=1}^{N} w_j\left(x_j-\bar{x}_w\right)^2}{\left(N'^{-1}\right)\sum_{j=1}^{N} w_j}} \tag{6}$$

with N', the number of non-zero weights.

It should be mentioned that the number of correlative data points can vary greatly from station to station (from 0 to several thousands). Due to different selection criteria and cloud filtering procedures for the three algorithms the number of collocations also varies between algorithms and thus precisions may vary accordingly. These numbers of correlative data points are indicated also in Tables 6 to 9. It must be kept in mind that the obtained absolute value of the overall bias can often be explained by slightly wrong slit functions and/or spectral parameters (Gloudemans et al, 2005); in some cases (WFMD v0.4 XN_2O and XCO_2) the SCIAMACHY data have been scaled according to a chosen reference value (Buchwitz et al., 2005a) (0.66 for N_2O and 1.27 for CO_2). Similarly the associated error is strongly influenced by the exact choice of error criteria.

We have also evaluated the scatter of the selected SCIAMACHY measurements, σ_{scat}, for each station, algorithm and target species, for comparison with the corresponding ones of the FTIR data. To this end, the individual normalised SCIAMACHY measurements and their respective weights have been weighted averaged per day in order to be comparable with the scatter of the daily averaged FTIR data. Note that while the daily averages for the FTIR data are pure averages in time, the SCIAMACHY averages (y_i^{SCIA}) are also spatial averages over the collocation grid around the FTIR station. Thus the scatter is influenced by the natural variability within the collocation grid as well as the actual retrieval errors. The latter are strongly related to the solar zenith angle and surface albedo, thus considerable station to station differences of the scatter are not unlikely.

A bias of the daily-averaged measurements, y_i, called b_{day} hereinafter, has then been calculated using the daily averaged SCIAMACHY values, as

$$b_{\text{day}}=\text{mean}_w\left(\frac{y_i^{\text{SCIA}}-y_i^{\text{PF}}}{y_i^{\text{PF}}}\right) \tag{7}$$

Analogous to Eq. (3) σ_{scat} is then obtained as the statistical 1σ weighted standard deviation, of the daily averaged SCIAMACHY data (y_i^{SCIA}) with respect to the polynomial interpolation of the daily FTIR data, corrected for the daily bias (b_{day}), according to:

$$\sigma_{\text{scat}}=sd_w\left(\frac{y_i^{\text{SCIA}}-\left(1+b_{\text{day}}\right)y_i^{\text{PF}}}{\left(1+b_{\text{day}}\right)y_i^{\text{PF}}}\right) \tag{8}$$

The resulting values of σ_{scat} for the large collocation grid are summarized in Table 3, together with the scatter on the g-b FTIR data and the desired target precision for each species. These targets have been set in order to accurately detect the global sources and sinks of these species, and their evolutions (Barrie et al., 2004; Bréon et al., 2003). The complete set of σ_{scat} values, including those from small grid collocated measurements, are listed in Tables 6 to 9.

To have a clearer view on the ability of SCIAMACHY to reproduce temporal variations, an important data quality requirement, we have calculated the weighted monthly averages, z_k, of both the original ground-based data (without a polynomial fitting procedure) and the SCIAMACHY data, on the large collocation grid and satisfying all selection criteria. Time series of these SCIAMACHY monthly averages have been plotted in Figs. 7, 10, 11, 12 and 13, again for all target products, algorithms and stations. The errors depicted on these figures represent the weighted statistical errors on these monthly averages and do not represent the measurement and retrieval errors on the individual data

$$\frac{3}{\sqrt{N_k}} \times sd_w\left(x_{j,k}^{\text{SCIA}}\right) \tag{9}$$

in which N_k is the number of individual SCIAMACHY measurements, $x_{j,k}^{\text{SCIA}}$, for month k.

In the case of CO, we have also calculated monthly mean MOPITT CO data taken over a 2.5 by 10° collocation grid. The MOPITT profile data is used to calculate the total column values above station altitude after which ECMWF pressure data at these station altitudes is used to convert the MOPITT CO total columns into volume mixing ratios. So it was

Table 6. Summary of statistical results of comparisons between SCIAMACHY and FTIR g-b data for (X)CO. Bias is the calculated weighted bias (in %, see Eq. 3) of the SCIAMACHY data relative to the 3rd order polynomial fit through the ground based FTIR data for CO, using the small grid (SG=±2.5° LAT, ±5° LON) and large grid (LG=±2.5° LAT, ±10° LON) spatial collocation criteria. The indicated errors represent the weighted standard errors of the ensemble of individual weighted biases (see Eq. 5). n is the number of correlative individual SCIAMACHY data. σ_{scat} is the percentage 1σ weighted standard deviation of the daily averaged SCIAMACHY measurements towards the bias corrected polynomial FTIR fit (see Eq. 8). R is the correlation coefficient between the monthly mean SCIAMACHY and FTIR data and P is the probability of no-correlation.

Algorithm → Station ↓		WFMD, SG CO v0.5	WFMD, LG CO v0.5	IMLM, SG CO v6.3	IMLM, LG CO v6.3	IMAP, SG XCO v0.9	IMAP, LG XCO v0.9
Ny Alesund	Bias	−7.99±3.16	−8.30±2.23	−5.62±37.8	−1.07±33.0	−2.34±2.62	−2.67±1.83
	n	1091	2131	22	30	783	1575
($\sigma_{scat\,FTIR}$=2.57)	σ_{scat}	21.6	16.7	7.14	15.8	24.7	21.9
Kiruna	Bias	−7.68±3.78	−8.25±2.55	−8.51±25.0	−7.41±17.8	−2.35±3.05	−2.27±2.00
	n	994	1956	40	76	632	1252
($\sigma_{scat\,FTIR}$=5.97)	σ_{scat}	30.4	21.9	40.7	42.4	29.6	22.8
Harestua	Bias	−2.57±3.54	−4.75±2.62	6.92±20.7	6.07±18.4	−2.03±3.17	−2.99±2.00
	n	1035	1847	111	141	700	1466
($\sigma_{scat\,FTIR}$=6.38)	σ_{scat}	29.2	26.1	64.4	60.1	27.6	23.7
Zugspitze	Bias	−5.29±4.88	−3.96±3.16	11.7±7.30	6.10±4.44	−18.8±2.76	−18.3±1.86
	n	668	1459	523	1283	610	1329
($\sigma_{scat\,FTIR}$=5.96)	σ_{scat}	25.5	18.3	36.0	26.2	26.0	24.7
Jungfraujoch	Bias	−2.49±3.23	−2.00±2.24	−4.50±4.91	−7.71±3.32	−9.77±3.17	−10.7±2.13
	n	1580	3339	950	2137	725	1675
($\sigma_{scat\,FTIR}$=7.71)	σ_{scat}	25.2	22.4	40.8	30.7	28.9	27.5
Egbert	Bias	−1.15±2.98	−1.34±2.20	8.67±5.97	7.02±3.98	−8.13±2.22	−9.47±1.72
	n	1440	2830	774	1705	976	1873
($\sigma_{scat\,FTIR}$=6.51)	σ_{scat}	25.5	23.7	33.4	28.3	27.5	25.0
Toronto	Bias	−4.99±3.00	−4.92±2.22	6.98±5.70	4.58±3.81	−8.58±2.12	−9.91±1.74
	n	1337	2699	806	1723	770	1519
($\sigma_{scat\,FTIR}$=6.94)	σ_{scat}	27.2	26.1	32.7	26.7	27.3	25.3
Izaña	Bias	8.39±3.56	5.65±1.90	−13.5±3.12	−14.8±1.33	−2.01±1.95	−4.58±1.13
	n	1493	3757	410	2290	1097	2910
($\sigma_{scat\,FTIR}$=6.83)	σ_{scat}	32.9	24.8	14.2	13.7	18.9	17.9
Wollongong	Bias	25.7±13.2	18.8±6.02	−19.4±3.95	−21.4±2.15	34.8±11.5	19.2±5.86
	n	219	814	894	2396	116	432
($\sigma_{scat\,FTIR}$=18.1)	σ_{scat}	39.2	28.1	32.0	28.4	26.0	28.0
Lauder	Bias	18.9±8.25	22.6±5.83	28.1±31.9	28.7±31.7	40.0±9.00	48.9±6.96
	n	610	1257	66	67	136	364
($\sigma_{scat\,FTIR}$=8.43)	σ_{scat}	29.3	26.7	64.0	63.7	22.3	22.8
Arrival Heights	Bias	12.7±23.1	18.7±13.9	52.1±38.2	58.6±27.2	56.7±49.5	54.7±31.5
	n	100	273	123	234	12	23
($\sigma_{scat\,FTIR}$=4.34)	σ_{scat}	35.4	41.6	67.1	54.7	34.4	30.8
Global	**Bias**	**−0.61±1.28**	**−0.004±0.87**	**−11.1±1.76**	**−14.7±0.90**	**−4.47±0.99**	**−4.99±0.68**
	$\boldsymbol{n}$	**10 567**	**22 362**	**4719**	**12 082**	**6557**	**14 418**
($\boldsymbol{\sigma_{scat\,FTIR}}$=**9.49**)	$\boldsymbol{\sigma_{scat}}$	**28.2**	**25.1**	**26.5**	**22.4**	**25.8**	**23.5**
	$\boldsymbol{R}$	**0.79**	**0.86**	**0.79**	**0.83**	**0.53**	**0.53**
	$\boldsymbol{P}$	**3.85E-19**	**4.12E-27**	**1.81E-13**	**2.30E-16**	**5.33E-6**	**1.64E-6**

not necessary to make an altitude correction using TM4 profile data. The MOPITT values are included in Fig. 7.

It is also very important to verify whether SCIAMACHY is able to reproduce the seasonal and latitudinal variations of the target species. A separate look at the latitudinal variation in the SCIAMACHY data can be easily derived from Tables 6 to 9 (in combination with Table 1) and is illustrated in Figs. 5 and 8, showing the bias as a function of latitude, per algorithm, for CO and CH_4 respectively.

Table 7. Summary of statistical results of comparisons between SCIAMACHY and FTIR g-b data for sza corrected and uncorrected WFMD XCH_4. Bias is the calculated weighted bias (in %) of the SCIAMACHY data relative to the 3rd order polynomial fit through the ground based FTIR data for WFMD XCH_4 before (v0.5) and after the solar zenith angle correction (cor), using the small grid (SG =±2.5° LAT, ±5° LON) and large grid (LG =±2.5° LAT, ±10° LON) spatial collocation criteria (see Eq. 3). The indicated errors represent the weighted standard errors of the ensemble of individual weighted biases (see Eq. 5). n is the number of correlative individual SCIAMACHY data. σ_{scat} is the weighted percentage 1σ standard deviation of the daily averaged SCIAMACHY measurements towards the bias corrected polynomial FTIR fit (see Eq. 8). R is the correlation coefficient between the monthly mean SCIAMACHY and FTIR data and P is the probability of no-correlation.

Algorithm → Station ↓		WFMD, SG XCH_4 v0.5	WFMD, LG XCH_4 v0.5	WFMD, SG XCH_4 cor	WFMD, LG XCH_4 cor
Ny Alesund	Bias	−3.94±1.90	−5.28±1.33	0.13±1.69	−1.26±1.16
	n	39	90	39	90
($\sigma_{scat\,FTIR}$=0.62)	σ_{scat}	2.44	3.17	1.81	2.61
Kiruna	Bias	−6.18±0.31	−5.76±0.24	−2.48±0.23	−2.07±0.17
	n	2600	4486	2600	4486
($\sigma_{scat\,FTIR}$=1.27)	σ_{scat}	4.47	4.19	2.37	2.20
Harestua	Bias	−4.98±0.37	−4.82±0.33	−2.50±0.27	−2.33±0.25
	n	1848	2186	1848	2186
($\sigma_{scat\,FTIR}$=1.12)	σ_{scat}	4.50	4.40	2.44	2.35
Zugspitze	Bias	−2.20±0.31	−1.95±0.20	−2.02±0.21	−1.50±0.13
	n	1529	3741	1529	3741
($\sigma_{scat\,FTIR}$=0.76)	σ_{scat}	3.52	3.39	1.67	1.19
Jungfraujoch	Bias	−3.78±0.18	−3.11±0.12	−3.74±0.12	−3.21±0.08
	n	4247	8525	4247	8525
($\sigma_{scat\,FTIR}$=0.71)	σ_{scat}	2.91	3.02	1.28	1.31
Egbert	Bias	−3.93±0.19	−4.22±0.14	−4.56±0.13	−4.75±0.09
	n	3774	7516	3774	7516
($\sigma_{scat\,FTIR}$=1.41)	σ_{scat}	3.21	3.16	1.86	1.63
Toronto	Bias	−2.64±0.17	−2.80±0.12	−3.19±0.14	−3.32±0.10
	n	3781	7426	3781	7426
($\sigma_{scat\,FTIR}$=1.69)	σ_{scat}	2.58	2.51	2.06	1.90
Izaña	Bias	−2.18±0.16	−2.95±0.09	−3.45±0.12	−5.19±0.08
	n	852	4397	852	4397
($\sigma_{scat\,FTIR}$=0.55)	σ_{scat}	1.57	1.57	1.17	1.33
Wollongong	Bias	−4.90±0.32	−4.96±0.19	−3.99±0.26	−4.12±0.12
	n	484	1809	484	1809
($\sigma_{scat\,FTIR}$=1.56)	σ_{scat}	1.78	2.29	1.14	0.83
Lauder	Bias	−5.28±0.66	−5.28±0.66	−0.77±0.49	−0.77±0.49
	n	426	426	426	426
($\sigma_{scat\,FTIR}$=0.99)	σ_{scat}	4.01	4.01	1.86	1.86
Arrival Heights	Bias	−8.40±2.09	−9.99±0.38	−1.19±1.99	−2.89±0.38
	n	41	1470	41	1470
($\sigma_{scat\,FTIR}$=1.52)	σ_{scat}	4.24	3.17	3.96	2.83
Global	**Bias**	**−4.05±0.09**	**−4.09±0.06**	**−3.24±0.07**	**−3.28±0.05**
	$\boldsymbol{n}$	**19 621**	**42 072**	**19 621**	**42 072**
($\sigma_{scat\,FTIR}$=1.15)	$\boldsymbol{\sigma_{scat}}$	**3.58**	**3.36**	**2.09**	**1.93**
	$\boldsymbol{R}$	**0.68**	**0.72**	**0.80**	**0.80**
	$\boldsymbol{P}$	**1.92E-12**	**4.93E-16**	**1.79E-19**	**2.02E-21**

Another useful marker for the ability to reproduce seasonal and latitudinal variations is the correlation coefficient (R) between the SCIAMACHY and FTIR monthly averages. Only monthly mean SCIAMACHY values which have been derived from at least 10 individual measurements have been taken into account. It turns out to be impossible to produce meaningful R values for the individual stations, given the limited temporal variation of the g-b data and the limited number of data points. However, the overall correlation coefficient per retrieval method over all stations and time does

Table 8. Summary of statistical results of comparisons between SCIAMACHY and FTIR g-b data for (X)CH_4. Bias is the calculated weighted bias (in %) of the SCIAMACHY data relative to the 3rd order polynomial fit through the ground based FTIR data for (X)CH_4, using the small grid (SG=±2.5° LAT, ±5° LON) and large grid (LG=±2.5° LAT, ±10° LON) spatial collocation criteria (see Eq. 3). The indicated errors represent the weighted standard errors of the ensemble of individual weighted biases (see Eq. 5). n is the number of correlative individual SCIAMACHY data. σ_{scat} is the weighted percentage 1σ standard deviation of the daily averaged SCIAMACHY measurements towards the bias corrected polynomial FTIR fit(see Eq. 8). R is the correlation coefficient between the monthly mean SCIAMACHY and FTIR data and P is the probability of no-correlation.

Algorithm → Station ↓		WFMD, SG XCH_4 cor	WFMD, LG XCH_4 cor	IMLM, SG CH_4 v6.3	IMLM, LG CH_4 v6.3	IMAP, SG XCH_4 v1.1	IMAP, LG XCH_4 v1.1
Ny Alesund	Bias	0.13±1.69	−1.26±1.16	/	/	0.09±0.16	0.04±0.11
	n	39	90	0	0	511	1105
($\sigma_{scat\,FTIR}$=0.62)	σ_{scat}	1.81	2.61	/	/	0.80	0.78
Kiruna	Bias	−2.48±0.23	−2.07±0.17	−2.94±5.97	−2.63±4.42	−0.29±0.23	−0.004±0.16
	n	2600	4486	16	27	458	819
($\sigma_{scat\,FTIR}$=1.27)	σ_{scat}	2.37	2.20	5.39	4.55	1.22	1.03
Harestua	Bias	−2.50±0.27	−2.33±0.25	−4.94±6.22	−4.33±5.84	0.66±0.25	0.96±0.18
	n	1848	2186	19	21	393	682
($\sigma_{scat\,FTIR}$=1.12)	σ_{scat}	2.44	2.35	9.71	9.59	1.12	1.10
Zugspitze	Bias	−2.02±0.21	−1.50±0.13	−2.42±0.97	−1.86±0.58	2.39±0.15	2.56±0.10
	n	1529	3741	351	945	1063	2387
($\sigma_{scat\,FTIR}$=0.76)	σ_{scat}	1.67	1.19	6.65	6.49	1.01	1.18
Jungfraujoch	Bias	−3.74±0.12	−3.21±0.08	−4.75±0.61	−4.62±0.41	0.24±0.09	0.23±0.06
	n	4247	8525	748	1585	2518	4837
($\sigma_{scat\,FTIR}$=0.71)	σ_{scat}	1.28	1.31	5.13	4.65	1.09	1.23
Egbert	Bias	−4.56±0.13	−4.75±0.09	−5.58±0.78	−6.10±0.54	−2.21±0.14	−2.36±0.10
	n	3774	7516	426	923	1142	2379
($\sigma_{scat\,FTIR}$=1.41)	σ_{scat}	1.86	1.63	4.72	4.37	1.27	1.18
Toronto	Bias	−3.19±0.14	−3.32±0.10	−4.24±0.82	−4.74±0.55	−1.55±0.16	−1.67±0.11
	n	3781	7426	428	960	1108	2315
($\sigma_{scat\,FTIR}$=1.69)	σ_{scat}	2.06	1.90	5.13	4.43	1.42	1.33
Izaña	Bias	−3.45±0.12	−5.19±0.08	−1.58±0.41	−2.29± 0.15	−1.52±0.07	−1.51±0.04
	n	852	4397	400	2275	1880	5929
($\sigma_{scat\,FTIR}$=0.55)	σ_{scat}	1.17	1.33	2.17	2.12	0.69	0.69
Wollongong	Bias	−3.99±0.26	−4.12±0.12	−3.40±0.35	−3.24±0.19	−0.63±0.17	−0.52±0.10
	n	484	1809	927	2474	798	2093
($\sigma_{scat\,FTIR}$=1.56)	σ_{scat}	1.14	0.83	3.07	2.54	1.44	1.43
Lauder	Bias	−0.77±0.49	−0.77±0.49	0.24±2.58	0.24±2.58	3.08±0.27	3.18±0.22
	n	426	426	41	41	257	393
($\sigma_{scat\,FTIR}$=0.99)	σ_{scat}	1.86	1.86	5.71	5.71	1.36	1.35
Arrival Heights	Bias	−1.19±1.99	−2.89±0.38	−4.61±4.71	−4.69±5.23	4.35±2.33	4.83±1.83
	n	41	1470	16	72	2	15
($\sigma_{scat\,FTIR}$=1.52)	σ_{scat}	3.96	2.83	4.30	12.1	1.05	1.49
Global	**Bias**	**−3.24±0.07**	**−3.28±0.05**	**−2.86±0.21**	**−2.83±0.10**	**−0.48±0.06**	**−0.62±0.04**
	n	**19 621**	**42 072**	**3372**	**9323**	**10 130**	**22 954**
($\sigma_{scat\,FTIR}$=1.15)	**σ_{scat}**	**2.09**	**1.93**	**3.20**	**3.14**	**1.07**	**1.09**
	R	**0.80**	**0.80**	**0.52**	**0.71**	**0.76**	**0.70**
	P	**1.79E-19**	**2.02E-21**	**2.45E-4**	**3.62E-9**	**1.15E-14**	**1.91E-12**

provide useful information. The value of this correlation coefficient depends not only on the effective correlation but also on the number of overlapping monthly mean data points. Next to the correlation coefficient R, we also tested for the hypothesis of no correlation. The latter is expressed by the P-value, also given in Tables 6 to 9, which is the probability of getting a correlation R as large as the observed value by random chance, supposing the true correlation is zero. If P is small, say less than 0.05, then the correlation R is significant. The P-value is computed by transforming the correlation to a t-statistic having n-2 degrees of freedom, with n the number of data points. The calculated R and P values give us a clear indication of how successful SCIAMACHY is in reproducing the overall variations in the g-b FTIR data. These

Table 9. Summary of statistical results of comparisons between SCIAMACHY and FTIR g-b data for WFMD XN_2O and XCO_2. Bias is the calculated weighted bias (in %) of the SCIAMACHY data relative to the 3rd order polynomial fit through the ground based FTIR data for WFMD XCO_2 and XN_2O, using the small grid (SG =±2.5° LAT, ±5° LON) and large grid (LG=±2.5° LAT, ±10° LON) spatial collocation criteria (see Eq. 3). The indicated errors represent the weighted standard errors of the ensemble of individual weighted biases (see Eq. 5). n is the number of correlative individual SCIAMACHY data. σ_{scat} is the weighted percentage 1σ standard deviation of the daily averaged SCIAMACHY measurements towards the bias corrected polynomial FTIR fit (see Eq. 8). R is the correlation coefficient between the monthly mean SCIAMACHY and FTIR data and P is the probability of no-correlation.

Species → Station ↓		WFMD, SG XN_2O v0.4	WFMD, LG XN_2O v0.4	WFMD, SG XCO_2 v0.4	WFMD, LG XCO_2 v0.4
Ny Alesund*	Bias	−7.84±0	−10.2±7.58	−5.83±1.49	−6.09±1.25
($\sigma_{scat\,FTIRCO_2}$=0.23)	n	1	2	130	194
($\sigma_{scat\,FTIRN_2O}$=1.40)	σ_{scat}	0	3.98	4.07	5.36
Kiruna	Bias	−3.30±2.84	−2.29±2.18		
	n	219	406		
($\sigma_{scat\,FTIRN_2O}$=1.40)	σ_{scat}	8.88	13.8		
Harestua	Bias	−3.36±3.05	−3.11±2.60		
	n	257	351		
($\sigma_{scat\,FTIRN_2O}$=1.42)	σ_{scat}	12.6	11.0		
Zugspitze	Bias	−1.11±2.54	0.43±1.70		
	n	255	540		
($\sigma_{scat\,FTIRN_2O}$=0.99)	σ_{scat}	8.06	7.35		
Jungfraujoch*	Bias	−2.68±1.36	−1.71±0.93	−7.62±0.28	−7.70±0.18
($\sigma_{scat\,FTIRCO_2}$=0.21)	n	848	1755	1896	4289
($\sigma_{scat\,FTIRN_2O}$=1.01)	σ_{scat}	8.99	8.70	3.40	3.29
Egbert*	Bias	2.47±2.12	1.84±1.39	−6.09±0.27	−5.92±0.19
($\sigma_{scat\,FTIRCO_2}$=2.63)	n	570	1183	1580	3221
($\sigma_{scat\,FTIRN_2O}$=1.55)	σ_{scat}	8.37	7.63	3.58	3.41
Toronto	Bias	4.06±2.26	3.42±1.41		
	n	543	1167		
($\sigma_{scat\,FTIRN_2O}$=1.59)	σ_{scat}	10.24	9.11		
Izaña	Bias	4.59±1.62	1.72±0.67		
	n	516	1656		
($\sigma_{scat\,FTIRN_2O}$=0.55)	σ_{scat}	4.84	4.81		
Wollongong	Bias	−3.62±1.99	−3.52±1.09		
	n	136	480		
($\sigma_{scat\,FTIRN_2O}$=1.24)	σ_{scat}	4.90	8.37		
Lauder	Bias	0.95±7.35	0.95±7.35		
	n	73	73		
($\sigma_{scat\,FTIRN_2O}$=1.08)	σ_{scat}	15.2	15.2		
Arrival Heights	Bias	/	/		
	n	0	0		
($\sigma_{scat\,FTIRN_2O}$=1.14)	σ_{scat}	/	/		
Global	**Bias**	**0.13±0.77**	**0.20±0.46**	**−6.91±0.20**	**−6.95±0.14**
($\sigma_{scat\,FTIR\,CO_2}$= 1.12)	***n***	**3418**	**7613**	**3606**	**7704**
($\sigma_{scat\,FTIR\,N_2O}$=1.16)	**σ_{scat}**	**9.51**	**9.31**	**3.57**	**3.78**
	R	**0.61**	**0.51**	**0.38**	**0.42**
	P	**4.89E-6**	**4.04E-5**	**0.088**	**0.057**

*CO_2 g-b measurements available for these stations only

variations include the temporal variations as well as the latitudinal variations (with the latter dominating).

Hereinafter the results summarized in the tables and figures are discussed in detail, per molecule.

4.2 Results for CO

All results for CO are listed in Table 6 and shown in Figs. 5 to 7. First of all it must be noted that, while both WFMD and IMLM CO products have been normalised for this validation

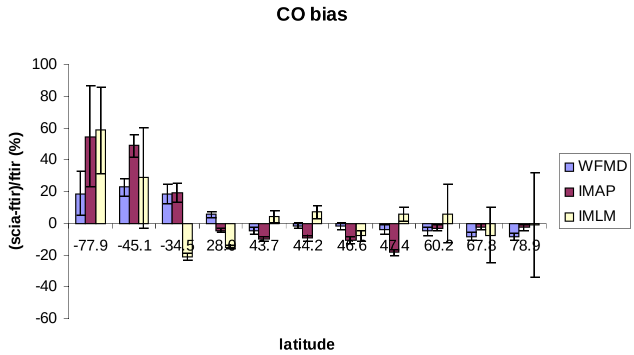

Fig. 5. The calculated percentage bias for CO as a function of latitude for a large grid collocation, for all three algorithms. Notice that the horizontal scale is not linear with latitude.

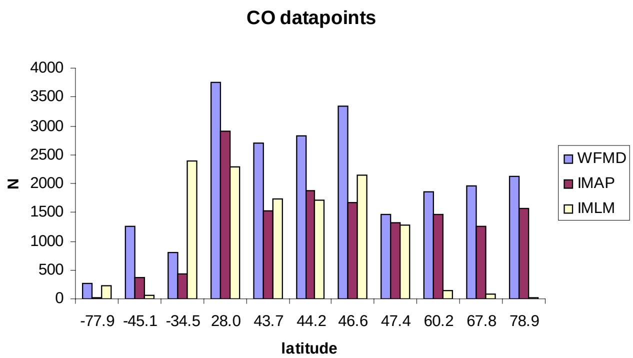

Fig. 6. The number of overlapping data points for CO as a function of latitude for a large grid collocation, for all three algorithms. Notice that the horizontal scale is not linear with latitude.

with ECMWF pressure data, IMAP XCO is a dry air normalised product using CH_4 as a proxy for dry air.

The TM4 profile CO data, yielded average correction factors for the normalisation with altitude of 0.85 for Zugspitze, 0.79 for Jungfraujoch and 0.91 for Izaña. All other stations had factors well below 1%, with the notable exception of Toronto (3.8%), which, given its altitude of a mere 174 meters, indicates strong boundary layer concentrations of CO in the model. All mean correction values are listed in Table 2 and typical examples are shown in Fig. 3.

When looking at Fig. 5, the obtained bias is far from constant as a function of latitude. Both IMLM and IMAP seem to exhibit an increasingly larger bias when moving down through the Southern Hemisphere. This effect is less gradual for WFMD, but a clear difference between the Southern Hemisphere and Northern Hemisphere data is noticeable for all algorithms. However, one has to keep in mind the very limited amount of data points for these Southern Hemisphere stations (see Fig. 6), which make an honest quality assessment, let alone the assessment of a trend, very difficult. These bias increases could be related to the difficulties of accurately acquiring the low Southern Hemisphere CO concentrations. Also immediately noticeable is the large difference between the small and large grid IMLM overall biases. As already mentioned, the geographical collocation area can have a significant impact upon the bias. Also the other algorithms exhibit differences in the bias between small and large grids when looking at the data per station. In some cases (Wollongong, which could be related to local biomass burning events) these differences can be substantial, but most differences remain within the order of a few percent.

The overall data scatter around the bias-shifted FTIR polynomial fit, $\sigma_{SCAT,}$ for all algorithms ranges around 23.5% (23.5 for IMAP, 25.1 for WFMD and 22.4 for IMLM), for the large collocation grid, which is ~2.3 times the desired 10% target precision on CO as well as the scatter of the ground-based FTIR data (9.5%). When taking the smaller spatial collocation grid, the scatter increases to around 27%, due to the decrease in data points, which apparently offsets the potential scatter decrease associated with less atmospheric variability in a smaller geographical area. Note that also the scatter, especially for IMLM which has a very limited amount of data points near the poles, can vary strongly from station to station (between 15.8 and 63.7%). Although WFMD measurements exhibit the highest scatter, they also clearly have the highest R (0.86) and lowest P values among the three retrieval methods. Also IMLM exhibits high R values, while those of IMAP are considerably lower. Note that IMAP XCO is derived with an older version of the algorithm (v0.9) than the one used for the XCH_4 product (v1.1).

Having such a relatively high scatter complicates the evaluation of the time series of all algorithms (Fig. 7), certainly for those months for which only a limited amount of data is available. Therefore Figs. 7, 10, 11, 12 and 13 do not show months for which there were less than 10 data points available (nor are they included in the calculation of R and P). Also included in Fig. 7, are monthly mean MOPITT CO values.

All algorithms appear to have potential given a further decrease in the amount of data scatter. However there are certainly a number of points which need to be looked at more closely. For WFMD for instance, the January (and February) data seems consistently too low for the Northern Hemisphere and too high for the Southern Hemisphere, with respect to the other WFMD data points. The same can be said for IMAP XCO where the underestimation seems to linger into March. In most cases, IMLM has too few data in this period to make a statement. Aberrant behaviour is sometimes also observed for August (Jungfraujoch). In many cases, the September-October data for WFMD and IMAP look suspiciously high. Both January and August feature ice layer decontamination periods and the amount of data for these months are scarce which could (to some extent) be an explanation for the above mentioned deviations. It is hard to detect any systematic offsets for IMLM but significant deviations (although more at random) do occur. From Fig. 6 one can also clearly see that IMLM only retains significant data (due to their strict cloud

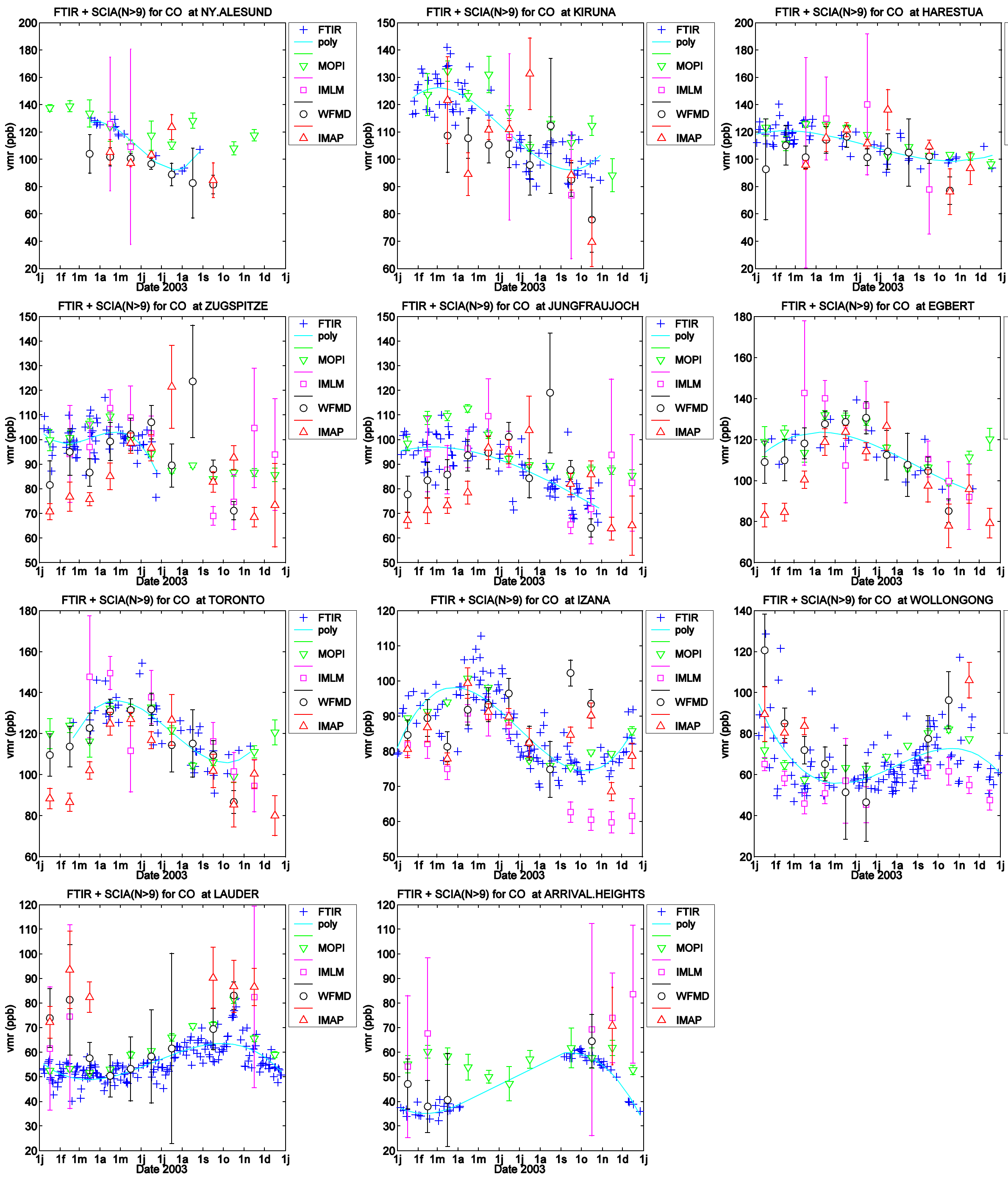

Fig. 7. Weighted monthly mean vmrs for (X)CO at all stations as a function of time for the year 2003, for the 3 algorithms together with the daily averaged FTIR measurements and corresponding 3rd order polynomial fit. The large grid was chosen for the spatial collocation criteria. The error bars on the monthly mean values represent the standard error, see Eq. (9). No monthly mean data is shown for months which contained fewer than 10 SCIAMACHY measurements.

filtering algorithm) for mid latitude stations. MOPITT CO on the other hand follows the FTIR seasonality almost perfectly. The correlation coefficient R between the monthly mean MOPITT and FTIR values over the entire network is 0.96, while P=8.15e-55, which is still better than for any of the SCIAMACHY algorithms. Only for the high latitude Ny Alesund and Arrival Heights stations do we notice a considerable deviation. MOPITT CO however measures in

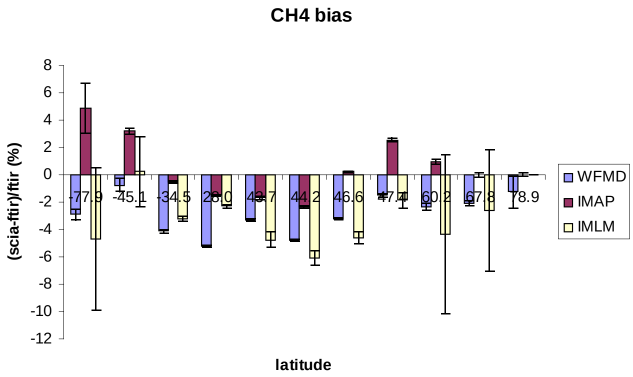

Fig. 8. The calculated percentage bias for CH_4 as a function of latitude for a large grid collocation, for all three algorithms. Notice that the horizontal scale is not linear with latitude.

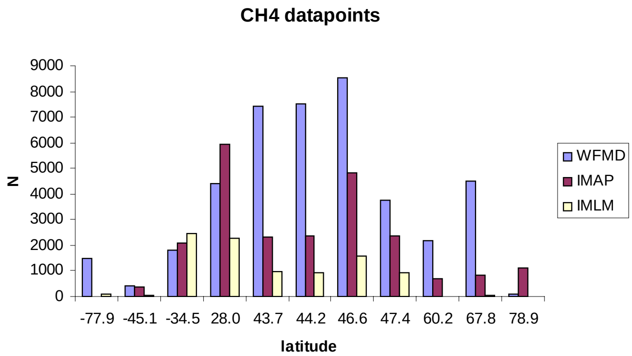

Fig. 9. The number of overlapping data points for CH_4 as a function of latitude for a large grid collocation, for all three algorithms. Notice that the horizontal scale is not linear with latitude.

the thermal infrared and unlike SCIAMACHY near-infrared capability is unable to look into the boundary layer where the strong local emission sources are located. Most of the current FTIR stations are located at remote areas, where local emission sources are low. However, when we look at the two stations which are not located at such remote locations, Egbert (∼70 km from the city of Toronto) and Toronto itself, we see that MOPITT still captures the seasonality extremely well.

In order to truly asses the different capabilities of MOPITT vs. SCIAMACHY CO, it is clear that more independent measurements, especially taken in regions where substantial boundary layer CO concentrations can be expected, are required.

4.3 Results for CH_4

First of all it must be noted that the differences between the algorithm parameters are considerable in the case of CH_4. Both IMAP and WFMD derive CH_4 from Channel 6, while IMLM derives CH_4 from Channel 8 which is affected by an ice layer. Furthermore, the final IMAP and WFMD CH_4 products are dry air normalised XCH_4 (using CO_2 as a proxy for dry air) products, which also allows both algorithms to eliminate the necessity for a rigid cloud detection algorithm and thus retain much more data points. IMLM only keeps measurements that are 100% cloud free, according to their cloud detection algorithm. This striking difference in data quantity is shown in Fig. 9. Therefore the differences between IMLM and WFMD and IMAP are not necessarily related to the retrieval algorithm itself. Another important point is that the WFMD XCH_4 data products have been corrected to compensate for a clear solar zenith angle (sza) dependence which became apparent during the course of this validation exercise (Buchwitz et al., private communication). The corrected XCH_4 is equal to XCH_4 v0.5(uncorrected) divided by (0.95+0.15cos (sza)). The impact of this correction is shown in Fig. 10 and Table 7. The cause for this dependence is under investigation but might be due to a calibration error of the Channel 6+ (upper ranges of Channel 6) spectra (as it affects CH_4 but not Channel 6 CO_2 total columns). IMAP, which uses the same spectral windows, has not (yet) been corrected for such dependence; in any case the effect of such dependence, if any, seems far less apparent. This having been said both IMAP and WFMD are investigating to what extent their data could be affected and more importantly what the exact cause of this dependence might be.

From Table 8 and Fig. 11, one can also see that all three algorithms exhibit statistically significant, mostly negative, biases. Especially those of WFMD and IMLM are large, making it more difficult to assess the seasonality. One doesn't observe any clear latitudinal dependence of the bias for any of the algorithms. However the variability between stations, with respect to the target precision of 1%, is still considerable. Not all variability should be attributed to the SCIAMACHY retrieval algorithms. FTIR CH_4 retrieval is a challenging task and the end results still depend on the microwindows and other retrieval parameters used. A survey of NDSC Egbert and Toronto CH_4 data by Taylor et al. (2005) has shown that interchanging retrieval parameters and microwindows between these stations, could account for a difference of up to 3.3%.

TM4 profile CH_4 data yielded correction factors for the normalisation with altitude of 0.98 for Zugspitze, 0.97 for Jungfraujoch and 0.985 for Izaña. All other stations had factors well below 0.3%. While these factors for the high altitude stations are far smaller than those for CO, they are still significant because of the extremely strict target precision of 1%.

A striking feature that can be derived from Table 8 is the low scatter for IMAP XCH_4, (1.09%), approaching the 1% target precision and even better than the 1.15% FTIR scatter. Note that the variability per station ranges between 0.69% (Izaña, thus probably capturing high surface albedo measurements over the Sahara desert) and 1.49% (Arrival Heights, Southern Hemisphere polar station with very limited correlative data points). SCIAMACHY measurements with

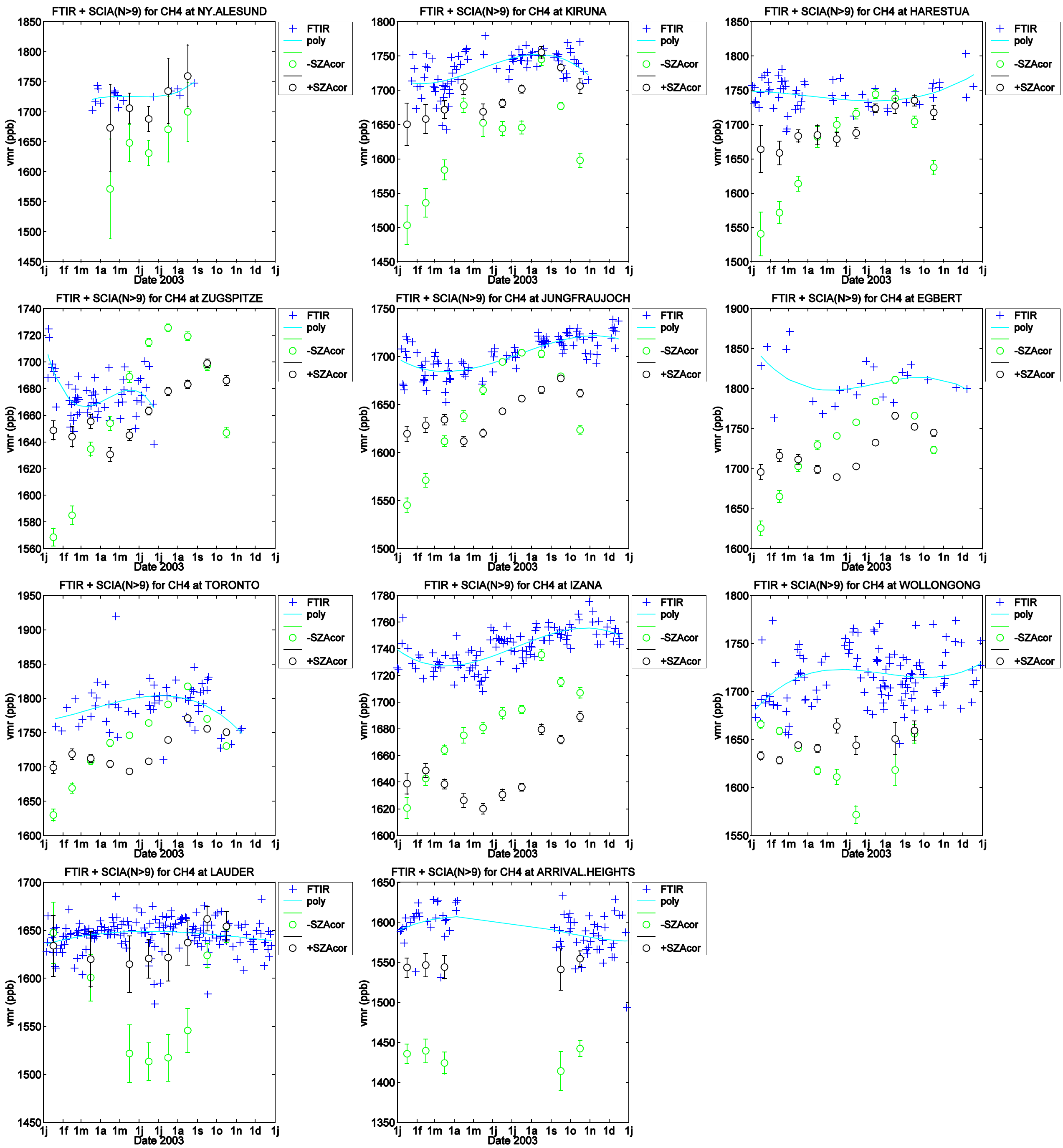

Fig. 10. Weighted monthly mean vmrs for WFMD XCH_4 before (green circles) and after (black circles) the solar zenith angle correction together with the daily averaged FTIR measurements and corresponding 3rd order polynomial fit. The large grid was chosen for the spatial collocation criteria. The error bars on the monthly mean values represent the standard error, see Eq. (9). No monthly mean data is shown for months which contained fewer than 10 SCIAMACHY measurements.

precisions of the order of 1.5 to 2% can already contribute considerably to emission uncertainty reduction (Meirink et al., 2006). Certainly IMAP measurements, but also to a lesser extent WFMD, already reach this more relaxed requirement.

When interpreting these numbers one always has to keep in mind that the scatter is not calculated with respect to the FTIR data themselves but to the polynomial fit through these data. Such an approach is certainly valid in cases where the scatter on the SCIA data is much larger than that on the FTIR

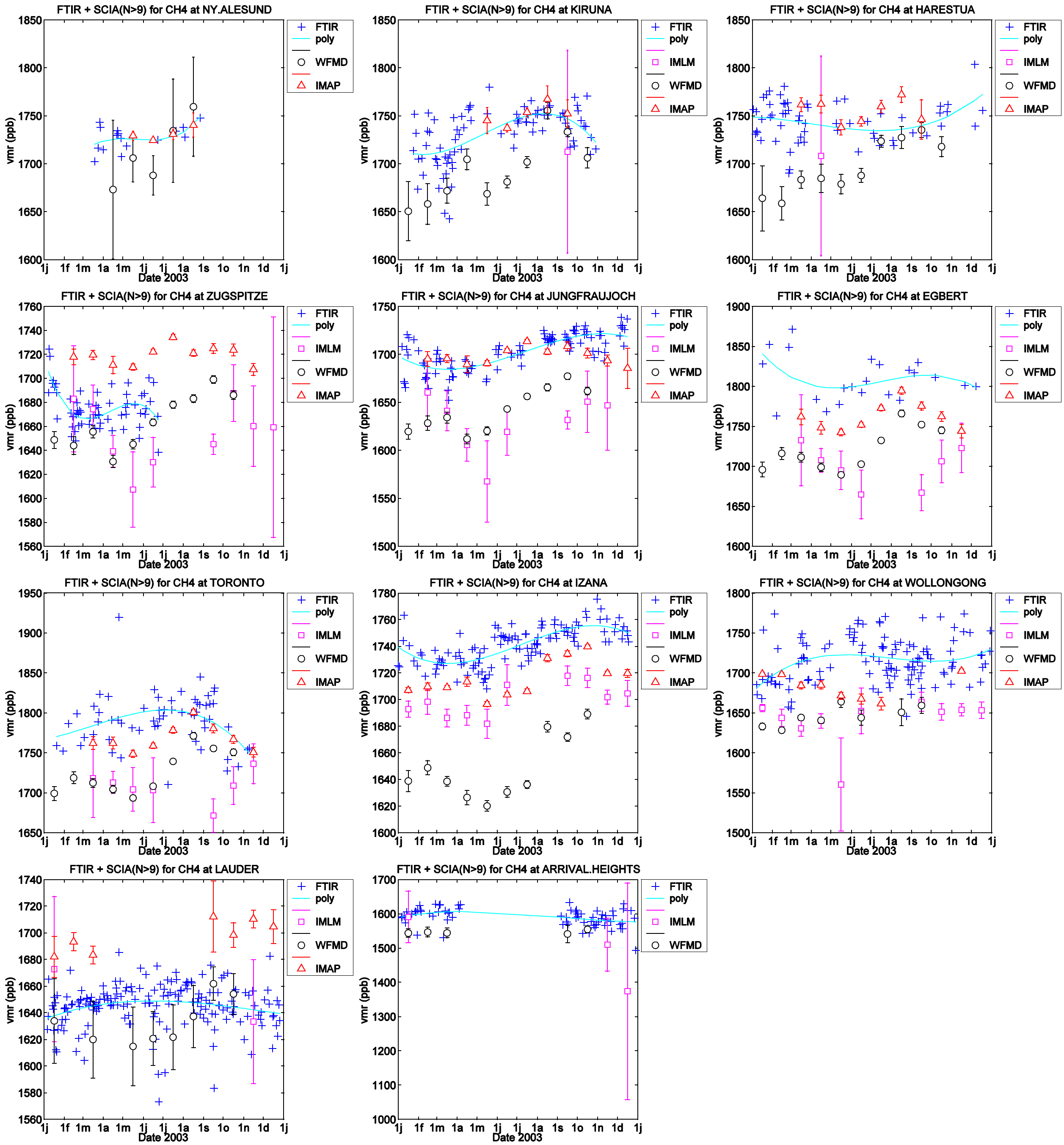

Fig. 11. Weighted monthly vmrs for (X)CH_4 at all stations as a function of time for the year 2003, for the 3 algorithms (note that for IMLM no XCH4 data was available and ECMWF pressure data was used for the normalisation) together with the daily averaged FTIR measurements and corresponding 3rd order polynomial fit. The large grid was chosen for the spatial collocation criteria. The error bars on the monthly mean values represent the standard error, see Eq. (9). No monthly mean data is shown for months which contained fewer than 10 SCIAMACHY measurements.

data itself. When however, the SCIA scatter (1.09%) is becoming similar to that of FTIR (1.15%), as is currently the case, the validity becomes to some extent debatable as one can easily imagine two SCIAMACHY data sets with equal, thus calculated, scatter values, one capturing the FTIR day to day variability perfectly, while the other does the complete opposite. However, as is apparent from Fig. 11, the data quality as it is, while a significant improvement with

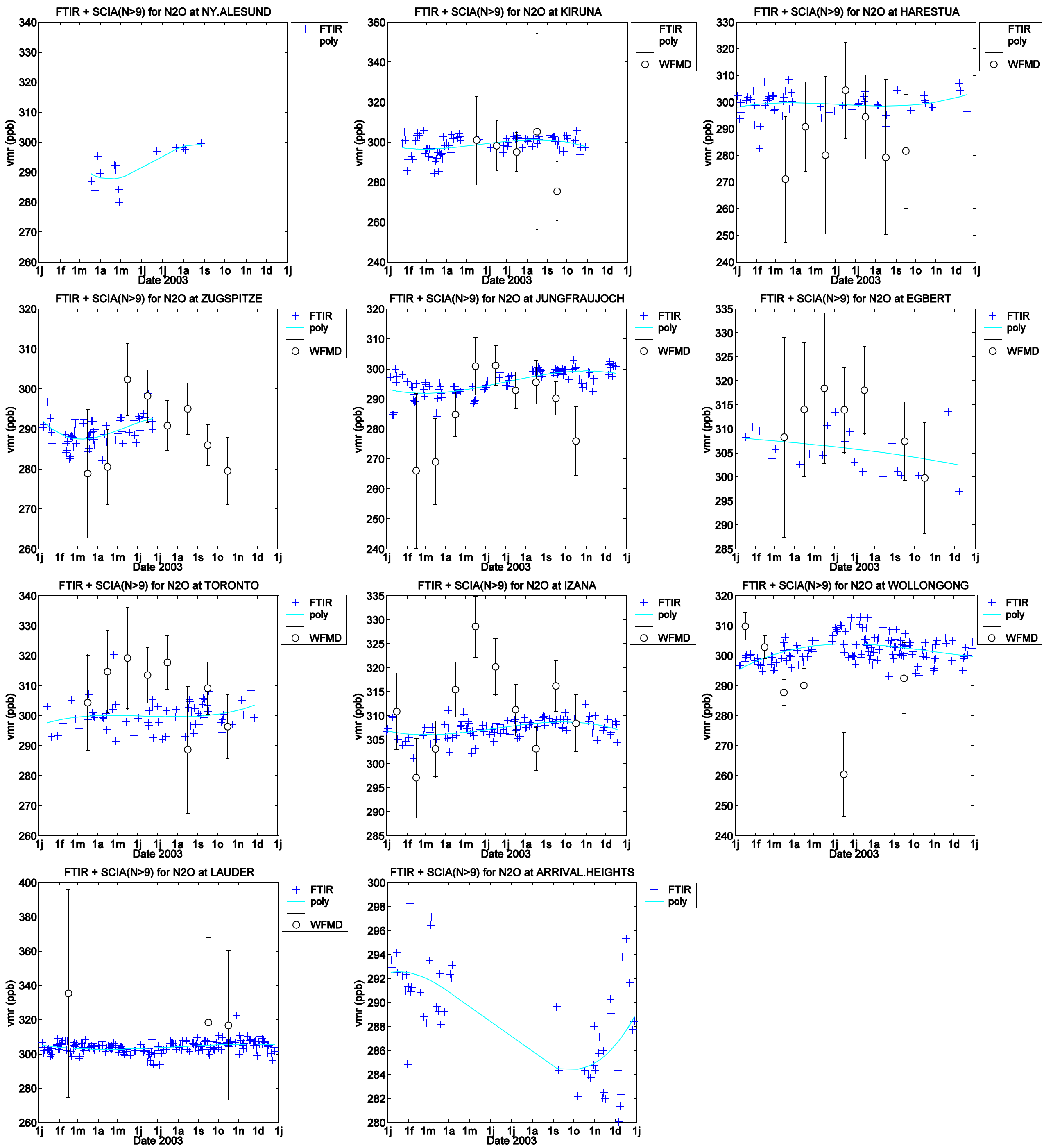

Fig. 12. Weighted monthly mean vmrs for WFMD XN_2O at all stations as a function of time for the year 2003, together with the daily averaged FTIR measurements and corresponding 3rd order polynomial fit. The large grid was chosen for the spatial collocation criteria. The error bars on the monthly mean values represent the standard error, see Eq. (9). No monthly mean data is shown for months which contained fewer than 10 SCIAMACHY measurements.

previous versions, has not yet obtained the level for which day-to-day variability becomes an issue. Regarding IMLM, the scatter on its CH_4 data is the largest, which can to some extent be explained by the fact that the algorithm product is the total CH_4 column and that the normalisation has been made using ECMWF pressure data. When applying this same normalisation procedure to the CH_4 column data from IMAP and WFMD, then all algorithms show comparable results. IMLM data then even becomes slightly better than those from WFMD (For LG: σ_{scat}=3.9% and R=0.33) and IMAP (σ_{scat}=2.1% and R=0.58). It is clear that one should normally apply a strict cloud filtering algorithm, before using ECMWF normalised CH_4 IMAP and WFMD data, and that this would improve the above mentioned IMAP and WFMD statistics. Still, it is clear that the ice issue problems which plague Channel 8 retrievals of IMLM have been well handled but that the benefits of normalisation, using CO_2 as a proxy for dry air, are considerable.

The impact of this dry air normalisation is also apparent in the higher R values of both XCH_4 products as compared to IMLM CH_4. Strikingly this difference quickly decreases when considering the IMLM data on a large grid (R=0.70) rather than on the small grid (R=0.52). This large impact of the spatial collocation grid is probably related to the fact that additional monthly mean values for the high latitude stations become valid (derived from more than 9 data points), effectively increasing the range over which the FTIR measurements vary. The sza corrected WFMD data set delivers the best product in this respect, while IMAP XCH_4 exhibits a relatively moderate correlation despite the fact that it clearly has the lowest scatter of all the three algorithms. This could be related to the fact that IMAP has no monthly mean ($n>9$) data for Arrival Heights, again decreasing the variability range and thus R. But more important facts that could have a negative influence on the correlation coefficient R are the clear overestimation of Lauder data, as well as the facts that IMAP XCH_4 often has high values in August, and an apparent opposite seasonal variation in comparison to g-b FTIR at Wollongong.

Due to the limited number of data points for IMLM, one can only do a decent comparison for the mid latitude stations south of Zugspitze to Wollongong and even for those stations the larger scatter complicates matters significantly. This aside, the ability to capture the seasonal variability looks promising, if an increase in data points and reduction in errors could be achieved. Of the three, WFMD, after sza correction, correlates best with the FTIR data, with the very notable exception of Izaña, where the other algorithms clearly outperform WFMD. Also for Toronto, the July–August data look high.

It is clear that there are considerable differences between the three algorithms, all of which show some different weak points. IMLM CH_4 clearly suffers from the limited amount of data points and the higher scatter; this to the extent that drawing definite conclusions from the time series plots would be very premature. IMAP XCH_4 has the lowest scatter, performs well for the Northern Hemisphere stations but exhibits clear problems for the Southern Hemisphere stations. WFMD has been corrected for its sza dependence, resulting in reasonable agreement (ignoring the bias) with the FTIR data for several stations, but less so for others (most notably Izaña). Further developments that can be expected in the near future are the XCH_4 IMLM data retrieved from Channel 6, as well as an in depth investigation into the cause and impact of the solar zenith angle dependence on both IMAP and WFMD algorithms. These developments should further enhance the data quality considerably.

4.4 Results for N_2O and CO_2

For XN_2O and XCO_2, only WFMD v0.4 measurements have been available for the present study. Unlike the version 0.5 WFMD data, the v0.4 measurements are still scaled with a constant factor, which is equal to 1.27 for CO_2 and 0.66 for N_2O. Furthermore, the ground-based data set for CO_2 is limited to three stations only, which makes it impossible to draw any conclusions regarding the latitudinal dependence of the CO_2 measurements. The N_2O ground-based data set covers all stations. Neither for N_2O nor for CO_2 have we applied a correction to the normalisation using the TM4 profile data. For N_2O this profile correction would probably be of the same order as that for CH_4. However given the more relaxed precision criteria (10%) and the fact that we observe no systematically different biases for the high altitude stations in the FTIR – SCIAMACHY comparisons, such a correction would not significantly alter the results of the validation. For CO_2 with its quasi-constant vmr profile with altitude, such a profile correction would have negligible impact.

The biases for XN_2O, which is essentially a by-product of the retrieval of (initial version 0.4) CH_4 in Channel 8, are summarized in Table 9. We observe no obvious systematic latitudinal dependence of the bias and the overall bias isn't statistically significant, although it is statistically significant positive or negative at some individual stations. The spread of the N_2O SCIAMACHY measurements, σ_{scat}, is a considerable 8 times larger than that of the ground-based FTIR measurements, however they do reach the desired 10% target precision. Also the R and P values indicate a moderate correlation.

From the time profile plots in Fig. 12, it is clear that the variability on the monthly mean data is too large to detect any apparent structured deviations from the temporal evolution. However, again, as with CO, it looks as if the initial data points are lower than the remainder, at least for the Northern Hemisphere, or that the late spring data points are relatively high, depending on your point of view. This is especially striking for Zugspitze and Junfraujoch. But again this could be merely statistical scatter. All in all, it is clear that the current data quality of XN_2O needs improvement before it becomes useful for data users, but given the fact that it is a by-product and that efforts to improve its quality are very limited, these initial results are promising for the future development of this product.

For XCO_2, we only obtained ground-based FTIR data from three stations. One of them is near the poles (Ny Alesund), another one is a mountainous station (Jungfraujoch)

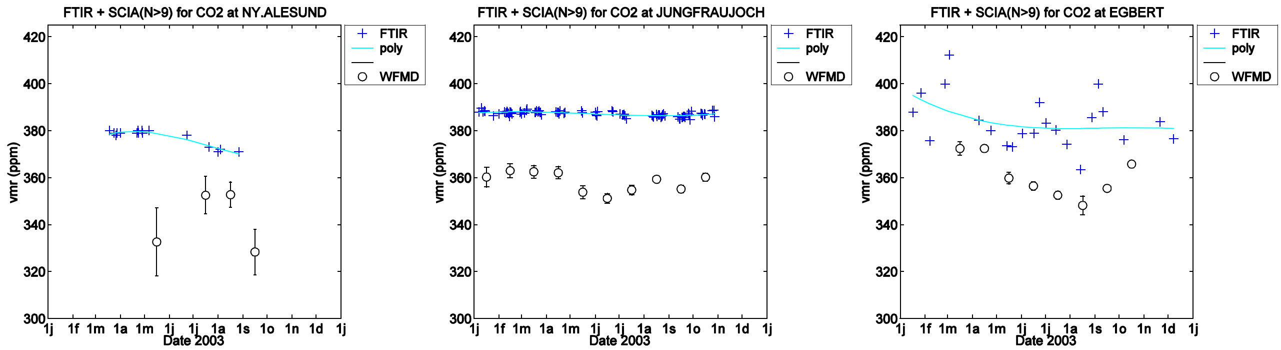

Fig. 13. Weighted monthly mean vmrs for WFMD XCO_2 at all stations as a function of time for the year 2003, together with the daily averaged FTIR measurements and corresponding 3rd order polynomial fit. The large grid was chosen for the spatial collocation criteria. The error bars on the monthly mean values represent the standard error, see Eq. (9). No monthly mean data is shown for months which contained fewer than 10 SCIAMACHY measurements.

and the third one (Egbert) is only 70 km away from a major city (Toronto). Among them, only the Ny Alesund CO_2 data (immediately submitted as vmrs) are retrieved from near infrared spectra while Jungfraujoch and Egbert use observations in the mid infrared . The near-infrared retrieval benefits from the simultaneous retrieval of O_2 data, thus enabling to deliver dry-air normalised products with a precision that is better than 1%. Table 9 also shows that the XCO_2 results for these stations, albeit the limited data set, are fairly consistent among each other, indicating a significant negative bias of the order of 7% of the SCIAMACHY measurements relative to the 3rd order polynomial fit through the ground-based FTIR measurements. The obtained correlation coefficient R indicates that there is only a limited degree of correlation and the probability P is even larger than the 0.05 target value thus stating that the correlation is not statistically significant. This is not surprising given the extremely small number of overlapping monthly mean data points and the corresponding limited variability of the FTIR data. All in all it is extremely difficult to draw conclusions from such a small data set. Figure 13 shows that XCO_2 seems to be correctly capturing the seasonal variations (higher in winter, lower in summer) but also that the SCIAMACHY data exhibit features that are clearly not present in the FTIR data.

The scatter on the XCO_2 data is about 3 times larger than that of the ground-based FTIR measurements and required (target) precision. As with XN_2O, XCO_2 is in the initial phase of its development and still requires significant improvements before becoming a reliable product. Nevertheless this and other validation exercises (de Beek et al., 2006) already show promising results.

5 Conclusions

The present comparisons between SCIAMACHY data for CO, CH_4, CO_2, and N_2O mean volume mixing ratios from three different algorithms (WFM-DOAS v0.5 (v0.4 for XCO_2 and XN_2O), IMLM v6.3, and IMAP v1.1 (v0.9 for XCO)) and correlative FTIR g-b data cover the period January to December 2003. The validation approach uses a polynomial interpolation through the g-b FTIR data to increase the number of collocated data. The comparison results show that scientific teams have significantly improved the retrieval algorithms for deriving the total columns of the above-mentioned target species from the instrument's NIR channels, despite the calibration problems inherent with the spectra (Buchwitz et al., 2000, 2004, 2005a, 2005b; Frankenberg et al., 2005a, 2005c; Gloudemans et al., 2004, 2005).

Overall, for CO and CH_4, all algorithms give relatively good descriptions of the seasonal and latitudinal variability of the gas species involved. Nevertheless, they still exhibit clear flaws which have to be kept in mind by the data user. It is clear that the capturing of the seasonal variability using the spatial overlap criteria and monthly mean averaging as done in this paper is promising but far from perfect. There are several ways of overcoming some of these remaining issues (averaging over larger time periods and/or larger spatial areas, using scaling (fitting) to additional (in-situ) measurements, etc.) depending on the data user's specific needs. Calculating the scatter, see Eq. (8), using the SCIAMACHY and FTIR monthly mean values instead of daily mean SCIAMACHY and FTIR polynomial values, did not improve the result. However, the correlative data set, for 11 stations over one year only, becomes too small to make an honest assessment of whether monthly mean values over our collocation grid do reach the target precision. Quantitative studies for monthly averaged SCIAMACHY CO data on spatial scales of a few degrees are very promising (de Laat et al., 2006). It is however beyond the scope of this article, and often beyond the capabilities of our dataset, to validate any of such approaches.

One must be aware of the fact that, due to the use of a polynomial fitting procedure for the g-b data and the smearing over the collocation grid for the satellite data, the obtained values for the scatter in the SCIAMACHY data include contributions from the natural variability of the considered species. The latter spatial variability includes variations related to topography as well as real variability of the concentrations. This increase of the variability with an enlargement of the collocation grid is often – but not always – offset by an increase in data points.

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. 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.

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, and have the lowest R value of all the algorithms when considering the small grid collocation; they are also less numerous due to 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 ice issue problem of Channel 8 is well handled. WFMD and IMAP XCH_4 still harbour structural problems, prompting a solar zenith angle correction factor on the WFMD data. This sza correction improved the comparisons tremendously, but it clearly fails in some cases (e.g., at Izaña). IMAP XCH_4 seems to have problems with Southern Hemisphere station data. Both groups are currently investigating the possible causes of this dependence and in how far it could impact the IMAP XCH_4 or the future Channel 6 XCH_4 IMLM data.

Both XCO_2 and XN_2O must be looked upon as preliminary data sets as they have received considerably less attention in their development than CO and CH_4. For XCO_2, the data set is simply too small to make any binding conclusions while for XN_2O, even though it has reached the target precision of 10%, the scatter on the data is too large to make any useful comments about possible structural deviations in the time series.

The remaining quantitative uncertainties will probably be reduced in future algorithm improvements, having acquired a better comprehension of the instrument/spectral problems.

Having said that, one must be aware that due to the inherent differences between SCIAMACHY and FTIR observations, the validation is not straightforward. Different measures have been undertaken to limit the impact of these differences but they cannot be completely ignored. Especially the differences in air mass between an FTIR and SCIAMACHY measurement, further accentuated by the necessary use of a relatively large spatial collocation grid, cannot be avoided. With future more accurate SCIAMACHY products, more independent measurements will be needed in order to really make an accurate assessment of SCIAMACHY's ability to capture the day-to-day variability and ability to measure into the boundary layer. The current FTIR network data set is too limited (in time and space) in this respect. 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.

It must also be stressed once more that the actual conclusions are based on a limited number of data coincidences, that the collocation criteria were not very stringent, and that a correction for the surface altitude has been applied that may add additional uncertainties. Some comparisons may still suffer from the presence of clouds because of imperfect cloud algorithms associated with the satellite data retrieval. Additional features that have not been taken into account in the comparisons are possible small sensitivity differences due to slightly different total column averaging kernels, spectroscopic uncertainties, etc. All conclusions drawn from this study therefore relate to the end product (or its monthly mean values), if applicable after normalisation, and profile correction as presented in section 2, and not to the algorithm itself since the differences in algorithm parameters and normalisation method can be significant. It is therefore difficult to make a straightforward evaluation of the performances of the three algorithms among them.

The present results based on comparisons for 11 FTIR stations indicate that it is not yet possible to perform quantitative studies on small spatial and temporal ($<$1 month) scales. In that respect all the data products are to breach a non-negligible gap before reaching the quality requirements for individual SCIAMACHY measurements. However this does not exclude that the actual SCIAMACHY products for CO and CH_4 can be used for performing coarse qualitative studies for which lower precisions than the ones listed in Table 3 are required, provided that the data user takes into consideration the issues raised in this and other SCIAMACHY validation papers (De Mazière et al., 2004; Gloudemans et al., 2004; Sussmann and Buchwitz, 2005; Sussmann et al., 2005). An example hereof is the identification of large source and sink areas for CO and CH_4 on a global scale, the variability of which is of the order of 200 and 10% respectively, as discussed by Frankenberg et al. (2005c, 2005b) and de Beek et al. (2006).

Based on the conclusions drawn here and in other papers in this same volume, 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, that considerable improvements on the data quality have been achieved but that there are still significant remaining issues to be resolved.

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