Satellite validation of column-averaged methane on global scale: Harmonized data from 13 FTIR ground stations versus last generation ENVISAT/SCIAMACHY retrievals

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ABSTRACT: Global measurements of column-averaged methane have recently shown a step forward in data quality via year 2003 and 2004 retrievals from two different processors, namely IMAP-DOAS ver. 49 and WFM-DOAS ver. 1.0. Accuracy and precision have approached the order of 1 %, and can be considered for inverse modelling of sources and sinks. This means at the same time that the quality requirements for ground-based validation data have become higher. In order to guarantee a station-to-station consistency of <1 % we performed a harmonization effort for 13 selected globally distributed mid-infrared FTIR stations. Station-to-station biases are eliminated by using identical micro-windows, spectroscopic line lists, retrieval parameters, sources of ancillary data like pressure-temperature profiles, and water vapor data for deriving dry air columns. Furthermore, a geophysically consistent set of prior information for the retrievals at all stations was established. Our network validation study utilizes the validation strategy developed during the first validation of ENVISAT/SCIAMACHY column-averaged methane by FTIR (Sussmann et al., 2005). The outcome of the new study is the accurate determination of the satellite-ground station biases as a function of latitude on global scale, as well as an assessment of the ability of ENVISAT/SCIAMACHY to measure true day-to-day variability.

1 PREVIOUS WORK – VALIDATION OF SCIAMACHY CHANNEL 6 RETRIEVALS

In 2005 methane total-vertical column retrievals from ground-based solar FTIR measurements at the Permanent Ground-Truthing Station Zugspitze (47.42 °N, 10.98 °E, 2964m a.s.l.), Germany had been used to validate column averaged methane retrieved from ENVISAT/SCIAMACHY spectra by WFM-DOAS (WFMD) version 0.4 and 0.41 for 153 days in 2003 (Sussmann et al., 2005). From the FTIR time series of XCH_4 an atmospheric day-to-day variability of 1% was found, and a sinusoidal annual cycle with a »1.6% amplitude. The bias was WFMD v0.4/FTIR=1.008±0.019 and WFMD v0.41/FTIR=1.058±0.008. WFMD v0.41 was significantly improved by a time-dependent bias correction. It could still not capture the natural day-to-day variability, i.e., the standard deviation calculated from the daily-mean values is 2.4% using averages within a 2000-km radius, and 2.7% for a 1000-km radius. These numbers were dominated by a residual time dependent bias in the order of 3%/month.

2 NEW GENERATION SCIAMACHY RETRIEVALS (CHANNEL 8)

Briefly after our 2005 validation study the SCIAMACHY icing problem was overcome by switching the retrieval algorithms from channel 8 to channel 6, which is not impacted by the icing issue. Channel 6 retrievals were pioneered via IMAP-DOAS and subsequently implemented in WFM-DOAS. This step forward in data quality leads us to the following 3 questions/requirements as to revisiting SCIAMACHY validation for the new algorithms IMAP-DOAS v49 (Frankenberg et al., 2008) and WFM-DOAS v1.0 (Schneising et al., 2009):

- Can the newest SCIAMACHY channel 6 retrievals now capture true day-to-day variability?
- Can the newest SCIAMACHY channel 6 retrievals now reflect the annual cycles as seen by FTIR?

- Since the dominant source of error in 2005, namely the time-dependent biases due to icing (3%/month with channel 8) have been overcome with the channel 6 retrievals, it makes now sense to perform a global validation of biases. The question is: is there a latitudinal dependency of biases for IMAP-DOAS v49 and WFM-DOAS v1.0?

3 HARMONIZED FTIR RETRIEVAL STRATEGY FOR CH4 COLUMNS AND PROFILES AT 13 FTIR STATIONS

3.1 *Harmonized retrieval settings*

Validation of the new high-accuracy and precision SCIAMACHY retrievals require that correlative CH_4 columns are retrieved consistently at the globally distributed ground-based FTIR stations operated within the Network of the Detection of Atmospheric Composition Change (NDACC).
An assessment of consistency between different FTIR stations of the network in May 2008 has shown major drawbacks as to consistency. Therefore, a harmonized retrieval strategy has been developed which comprises:

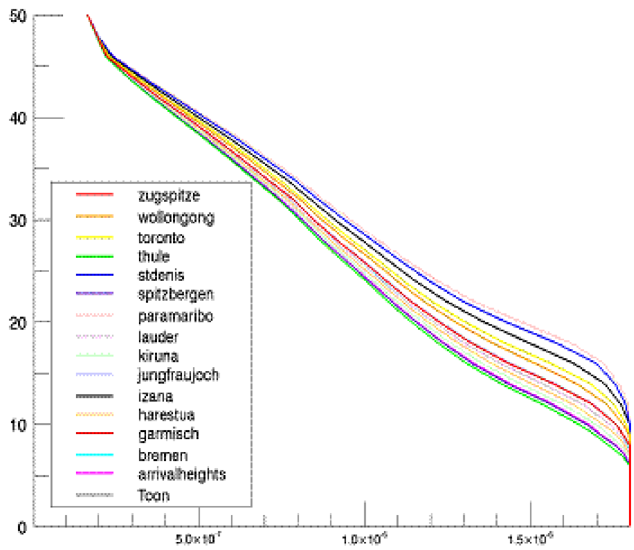

Fig. 1. Harmonized set of CH_4 a priori profiles for different FTIR stations: Toon CH_4 balloon profile adapted for mean (NCEP) tropopause altitude of the different stations via the linear transformation described by Meier (1997).

- one common micro-window set for CH_4 (5 windows, i.e., 2613.7-2615.4 cm^{-1}, 2650.6-2651.3 cm^{-1}, 2835.5-2835.8 cm^{-1}, 2921.0-2921.6 cm^{-1})
- one identical spectroscopic line list (HITRAN 2004 with “Hase update”)
- one common source of pT-input profiles (NCEP)
- one common a priori profile adapted to the mean NCEP tropopause altitude of the different sites (Fig. 1)
- one consistent set of regularization matrices (Tikhonov $\mathbf{L_1}$ applied to per cent changes of retrieved VMR profiles) and altitude grids (1.5 km equidistant):

$$\mathbf{R} = \mathbf{S}_a^{-1} = \alpha\, \mathbf{L}_1^T \mathbf{L}_1 = \alpha \times \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ -1 & 2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2 & -1 \\ 0 & \cdots & 0 & -1 & 1 \end{pmatrix} \in \Re^{n\times n}$$

Tests have shown, that it is a good choice to apply the Tikhonov $\mathbf{L_1}$ regularization to percentage changes (scaling factors) of the individual layers of the VMR profiles to be retrieved (another choice would be the application of $\mathbf{R}$ to profiles given in units of absolute VMR). An important argument for the implementation of $\mathbf{L_1}$ in units of percentage profile changes is, that this leads to the limiting case of a VMR-profile scaling, in case the regularization strength a is tuned towards infinity (dofs°1): VMR-profile scaling (e.g., used in SFIT 1) is one of the best-tested retrieval approaches and well known to yield very robust retrieval results for total columns.
The harmonized retrieval strategy was implemented for 13 FTIR stations (Table 1) and subsequently applied to CH_4 retrievals for the years 2003 and 2004.

Table 1. The 13 FTIR stations of the globally harmonized SCIAMACHY validation effort.

station	latitude	longitude	station altitude	number of columns in 2003/2004	tropopause height
Spitzbergen	78.92 °N	11.92 °E	20 m	113	8.95 km
Thule	76.53 °N	68.74 °W	225 m	177	8.51 km
Kiruna	67.84 °N	20.41 °E	419 m	338	9.62 km
Harestua	60.22 °N	10.75 °E	596 m	1234	10.20 km
Bremen	53.11 °N	8.85 °E	29 m	179	10.74 km
Zugspitze	47.42 °N	10.98 °E	2964 m	999	11.25 km
Garmisch	47.48 °N	11.06 °E	745 m	498	11.25 km
Jungfrauj.	46.55 °N	7.99 °E	3580 m	702	11.38 km
Toronto	43.66 °N	79.40 °W	174 m	185	13.25 km
Izaña	28.30 °N	16.48 °W	2367 m	207	14.44 km
Paramaribo	5.81 °N	55.21 °W	7 m	64	16.36 km
St-Denis	20.90 °S	55.48 °E	50 m	141	15.66 km
Wollongong	34.41 °S	150.88 °E	40 m	633	12.53 km

3.2 *Calculation of the dry air column*

We use NCEP pressure temperature profiles and NCEP water vapor profiles to calculate the dry air column. The CH_4 columns from the MIR retrievals are then divided by the daily dry air column.

3.3 *Harmonized quality selection*

Quality selection of FTIR spectra is performed using the rms of the spectral fitting residuals as a criterion. Harmonized rms thresholds are obtained via elbow plots, see Fig. 3.

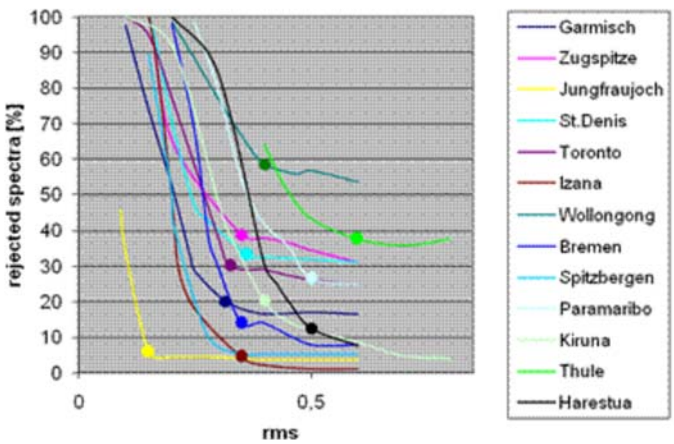

Fig. 2. Thresholds for quality selection of FTIR retrieval results.

4 VALIDATION STRATEGY

4.1 *Coincidence criteria*

Temporal coincidence. SCIAMACHY data and FTIR measured within the same day have been used. The reasons are i) that SCIAMACHY overpasses at one site are limited to one certain hour of a day, and ii) that there is a significant day-to-day variability of XCH4 in the order of 1 %, while there is no comparable true diurnal variation of XCH4 (Sussmann et al., 2005).

Spatial coincidence. The question of the appropriate size of spatial co-location criteria cannot be uniquely solved, as many discussions on satellite validation workshops have proven. Therefore in Sussmann et al. (2005) we have demonstrated a strategy of using different collocation criteria in parallel and, thereby, analyse their impact on the validation results. In this study we use three different pixel selection radii, i.e., of 200 km, 500 km, and 1000 km for all sites in parallel.

4.2 *Altitude correction*

The altitude of a FTIR located at a mountain or a valley site may differ significantly from the mean altitude of its surroundings measured by SCIAMACHY. This altitude effect leads to a difference between the CH_4 column measured by the FTIR and the mean column derived from SCIAMACHY data within a certain pixel selection radius around this site.

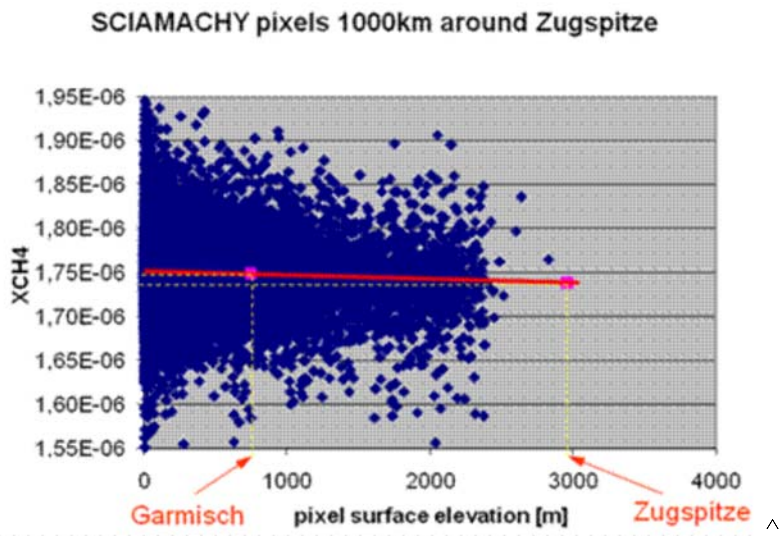

Fig. 3. Altitude correction of XCH4 for high-altitude FTIR sites.

The altitude effect is reduced by considering column-averaged mixing ratios instead of column densities. However, the effect is perfectly eliminated only in the special case of an altitude constant VMR profile (e.g., approximately eliminated for XCO2). In case of XCH4, there is still a residual altitude effect in the order of up to a few percent, due to the gradient of the CH_4 profile above the tropopause.

In order to reduce this effect Dils et al. (2006) have applied an altitude correction factor to the SCIAMACHY XCH4 data using the ratio of TM4 model data at the station´s altitude and the TM4 VMR at the ground level (as determined by the model´s orography). However, the spatial resolution of the model (2´3 °) does not correspond with that of a SCIAMACHY pixel and, thus, the correction can never be perfect (Dils et al., 2006).

In order to avoid any additional uncertainty introduced by using model data we developed a statistical altitude correction using a big ensemble of individual SCIAMACHY XCH4 measurements. A linear fit is performed to individual-pixel SCIAMACHY XCH4 values plotted as a function of ground-pixel altitude (Fig. 2). The difference in XCH4 derived from this Figure for 745 m a.s.l. and 2964 m a.s.l. is 0.52 %, and agrees very well to the bias of 0.30 % derived from coincident ground-based soundings of the Garmisch FTIR (745 m a.s.l.) and the Zugspitze FTIR (2964 m a.sl.). I.e., the altitude dependency of SCIAMACHY is consistent with the ground-based FTIR and thus can be used for the altitude correction of FTIR mountain stations (Jungfraujoch, Zugspitze, Izana, see Table 1).

4.3 *Treatment of intercomparison error*

In order to reduce intercomparison errors, the retrieved FTIR CH_4 vertical profiles (dofs ≈2-3) were folded by the total column averaging kernels from the SCIAMACHY retrievals (dofs = 1).

5 VALIDATION RESULTS

Correlative validation data sets (daily means - satellite versus ground) have been set up separately for
- IMAP-DOAS v49 and WFM-DOAS v1.0
- 3 different pixel selection radii (200 km, 500 km, 1000 km around each FTIR station)
- 2003 and 2004 data
- 13 FTIR stations

So there are 2´3´2´13 = 156 validation data sets. We grouped the 156 validation data sets into 52 validation plots each containing the 3 SCIA data sets for the three selection radii (200 km, 500 km, 1000 km). See Fig. 4 below for some examples. From each of the 156 data sets the statistics of the diurnal variation, the pixel to-pixel variation, day-to-day variability, and biases has been derived.

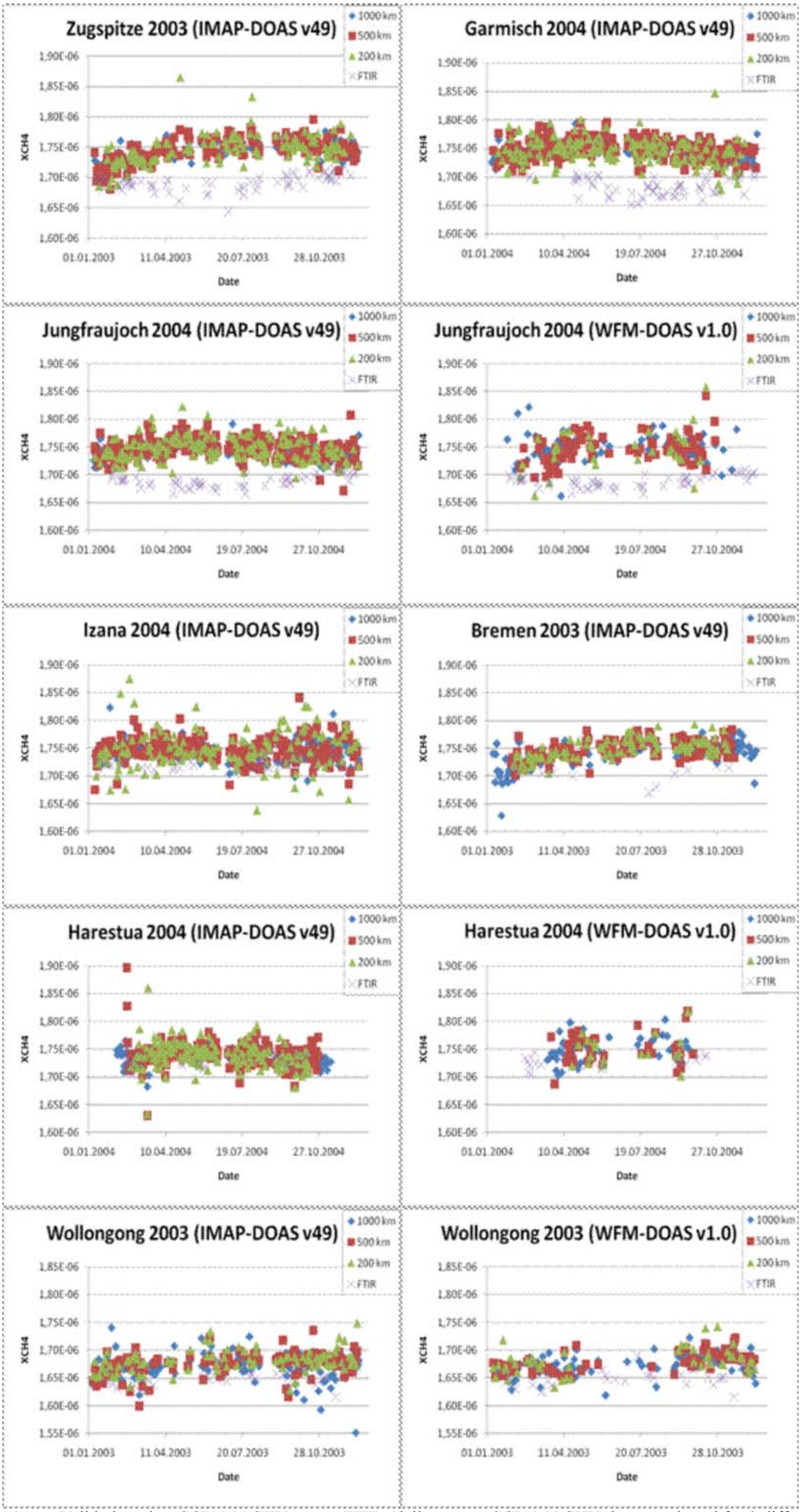

Fig. 4. Validation plots SCIAMACHY versus FTIR (daily means; SCIAMACHY data are plotted for 3 different selection radii around each FTIR ground station).

The latitudinal distribution of the biases is shown in Fig. 5. Further validation results are given in the Summary.

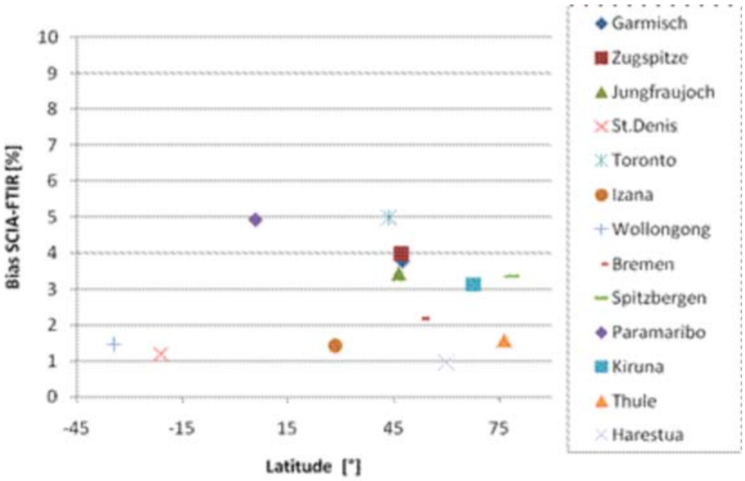

Fig. 5. The bias of each FTIR station relative to SCIAMACHY (IMAP-DOAS v49, 500 km selection radius) plotted against the station's latitude.

SUMMARY AND RESULTS

A station-to-station harmonization of XCH4 retrievals from 13 globally distributed ground-based mid-infrared FTIR spectrometry stations of the NDACC network has been performed. The single pixel column measurement precision of SCIAMACHY XCH4 is »1.5-2.5 % and has improved by a factor 2-4 since 2005 (rel. to WFM-DOAS v0.41). Improved SCIA precision allows to retrieve day-to-day variability (0.7-1.5 %). No significant correlation of the annual cycles between SCIA ("frown"-shaped) and FTIR ("smiley" shape) can be found above clean-air NDACC stations. There is a significant high bias of SCIAMACHY XCH4 of » 2.8±1.4 % (1 sigma uncertainty) relative to the harmonized g.-b. FTIR data set. There is no significant latitudinal dependency of the bias. No significant difference in data quality between IMAP-DOAS v49 and WFM-DOAS v1.0 could be found. WFMD data selection is stricter which leads to a slightly better single-pixel precision at the cost of fewer data.

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