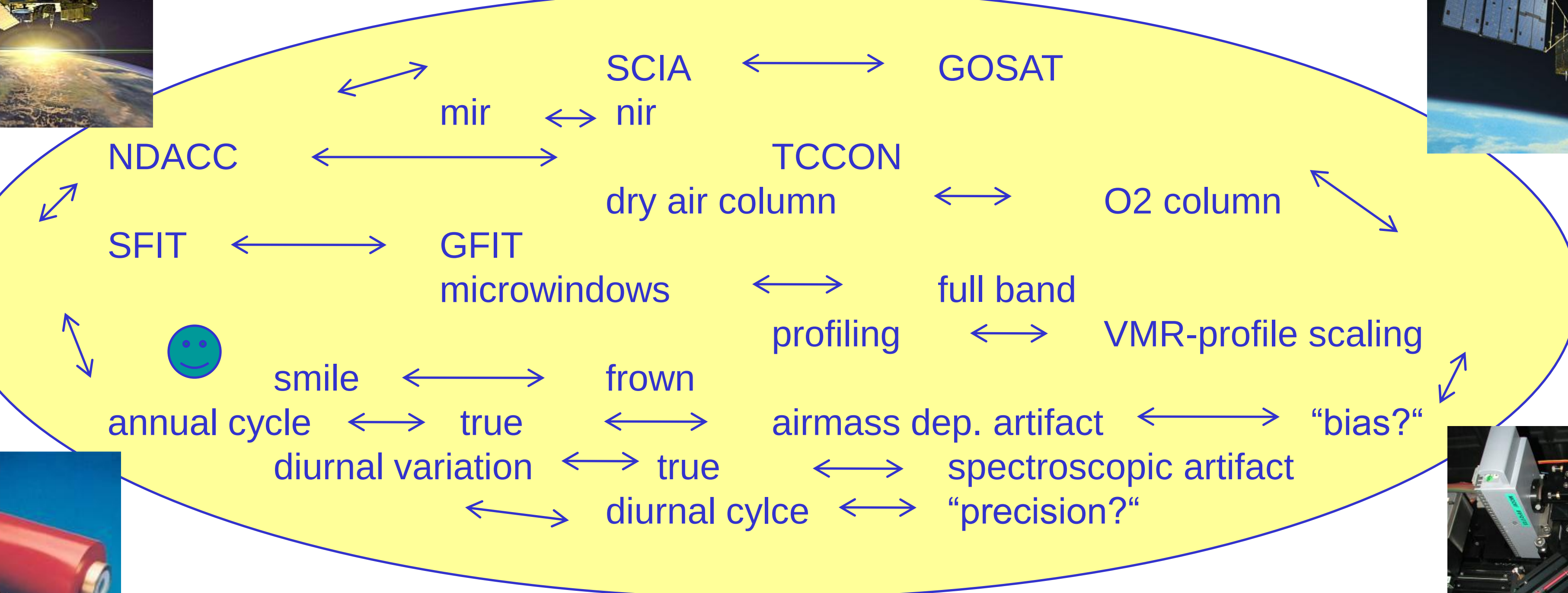
Global intercomparison of SCIAMACHY XCH4 with NDACC FTS – what can we learn for GOSAT validation by TCCON FTS?

R. Sussmann, M. Rettinger, F. Forster, T. Borsdorff

… took some notes from observations “beside the road“:



Research Center Karlsruhe, IMK-IFU Garmisch-Partenkirchen

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Outline:

- global intercomp. of SCIA XCH4 versus 12 NDACC MIR-FTIR stations
- first GFIT results from nearly 2 years TCCON operations at Garmisch
- annual cycles: SCIA versus g.-b. MIR versus g.-b. NIR
- diurnal variations: g.-b. MIR versus g.-b. NIR
- summary

Conclusions from ACP (2005)*: SCIA WFMD v0.41 versus Zugspitze MIR-FTIR

Zugspitze FTIR:

- **precision of daily means is ≈0.4 %**

⇒ can retrieve true annual-cycle amplitude: ≈1 %

⇒ can retrieve true day-to-day variability: ≈1 %

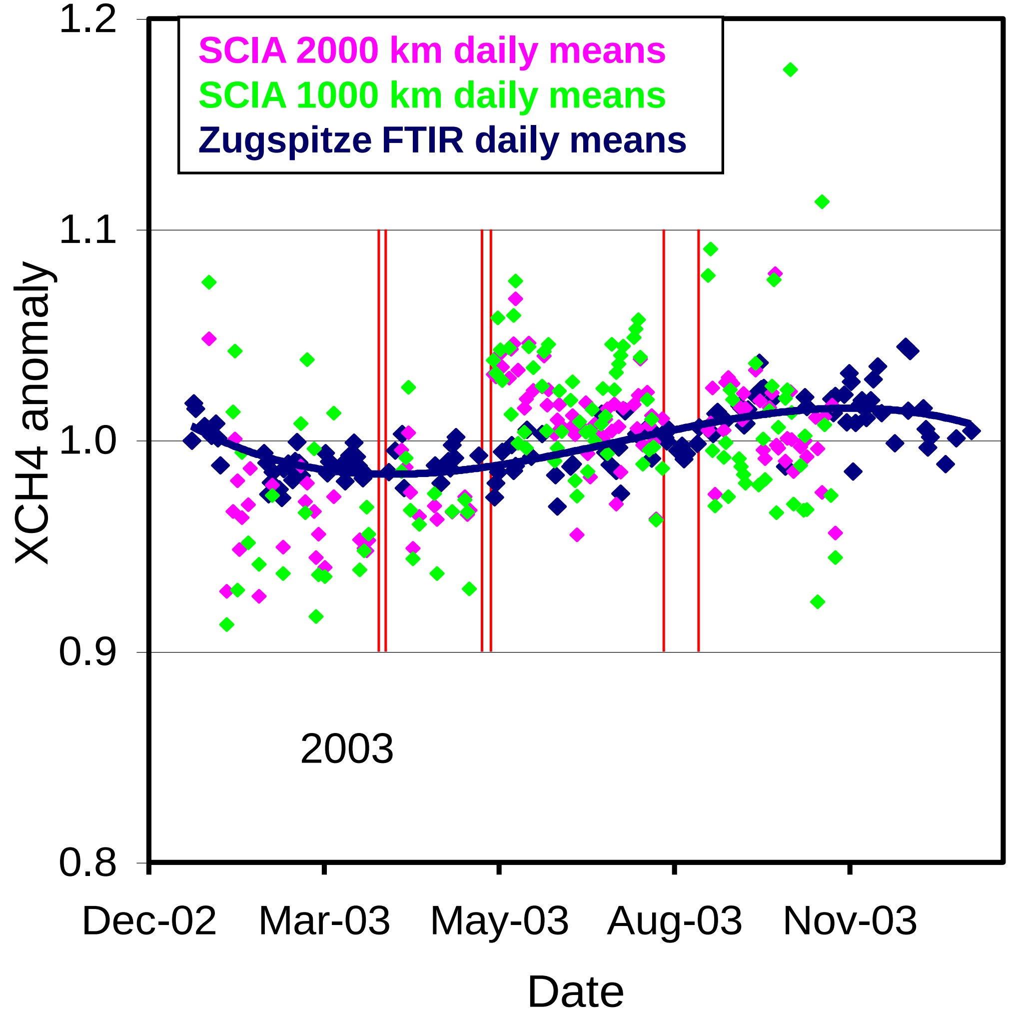
SCIAMACHY WFMD v0.41:

- **time-dependent biases ≈3 %/month due to icing problems in channel 8**

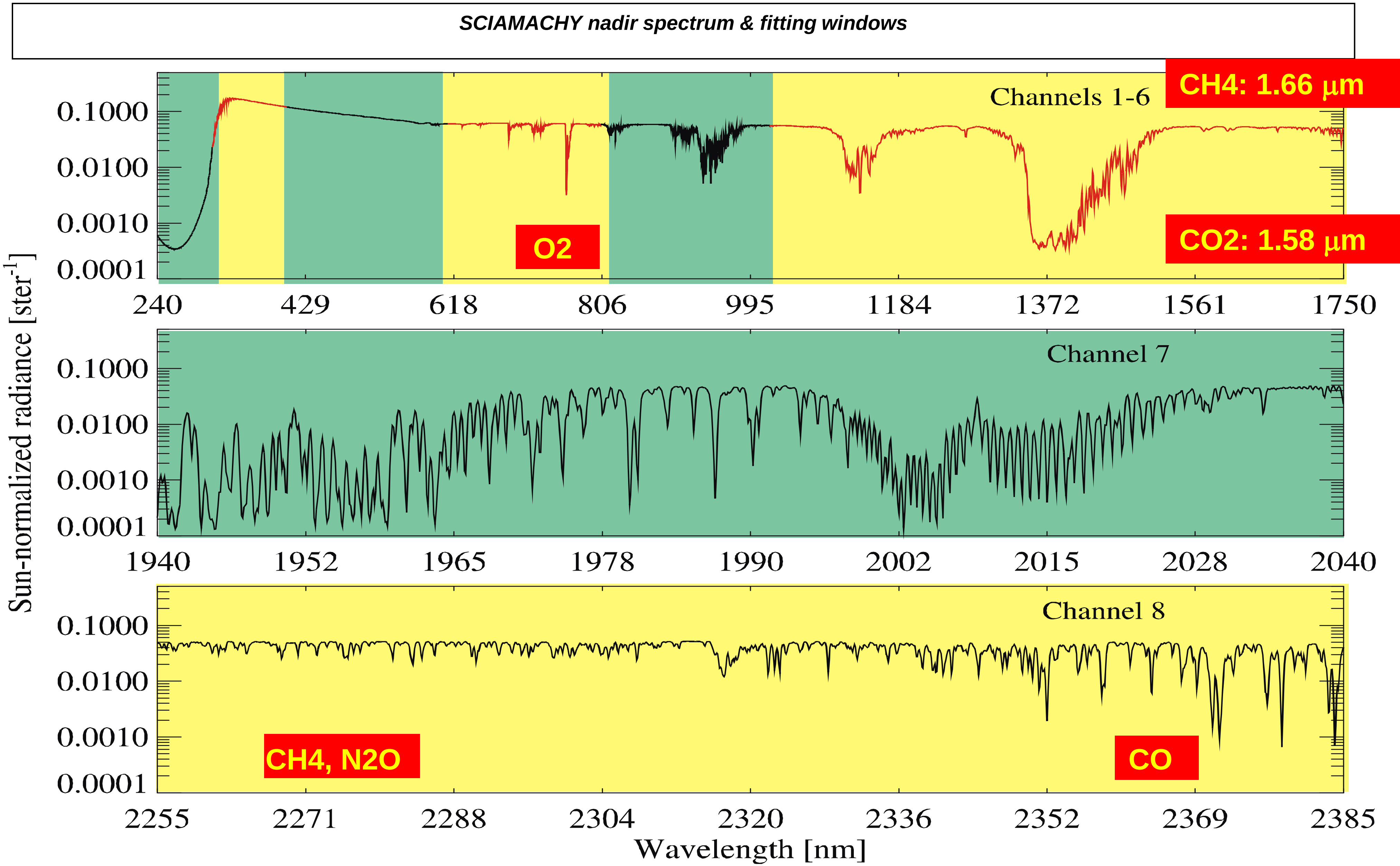
⇒ could not retrieve true day-to-day variability

- ***"precision of the daily means ≈ 0.6 % (calculated from the individual pixels, 1000-km selection radius) would be sufficient to capture true day-to-day variability and the annual cycle***

- if the icing issue could be eliminated".



* Sussmann, Stremme, Buchwitz, de Beek, Atmos. Chem. Phys, 5., 2419–2429, 2005



SCIAMACHY nadir spectrum & fitting windows
Channels 1-6
CH4: 1.66 μm
CO2: 1.58 μm
O2
Channel 7
Channel 8
CH4, N2O
CO
Sun-normalized radiance [ster⁻¹]
Wavelength [nm]
0.1000
0.0100
0.0010
0.0001
240
429
618
806
995
1184
1372
1561
1750
1940
1952
1965
1978
1990
2002
2015
2028
2040
2255
2271
2288
2304
2320
2336
2352
2369
2385

New questions for validating SCIA IMAP-DOAS v49 & WFM-DOAS v1.0

After validation in 2005, the SCIAMACHY icing issue was overcome by re-implementing SCIA retrievals from channel 8 to channel 6.

Two years of SCIA data are now available: 2003 & 2004.

⇒ Possible to revisit the questions

1: Can the new SCIA channel 6 retrievals capture true day-to-day variability?

2: Can the new SCIA retrievals reflect annual cycles as seen by FTIR?

3: Is there a latitudinal dependency of biases for IMAP-DOAS v49 and WFM-DOAS v1.0?

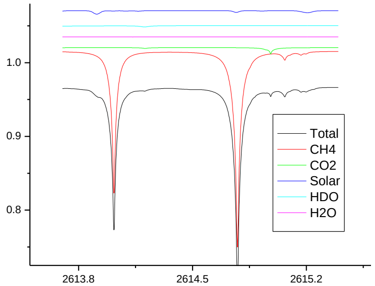
⇒ Make sure that g.-b. CH_4 columns are retrieved in a perfectly consistent manner at all globally distributed ground-based MIR-FTIR stations.

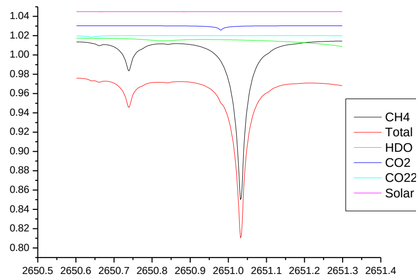
The 12 NDACC-MIR-FTIR stations of our SCIA – MIR-FTIR intercomp. study

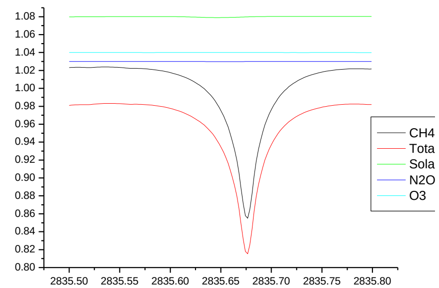
station	latitude	longitude	station altitude	Number of columns in 2003/2004	tropopause height
Spitzbergen	78.92 N	11.92 E	20 m	113	8.95 km
Thule	76.53 N	68.74 W	225 m	177	8.51 km
Kiruna	67.84 N	20.41 E	419 m	338	9.62 km
Harestua	60.22 N	10.75 E	596 m	1234	10.20 km
Bremen	53.11 N	8.85 E	29 m	179	10.74 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
Jungfraujoch	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
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

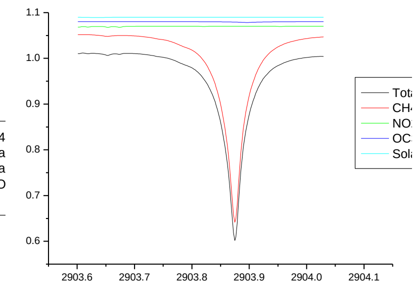
MIR-FTIR CH4 retrieval homogenization:

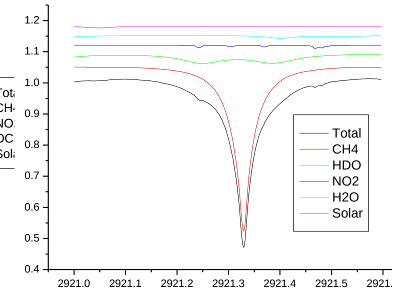
- one common micro-window set: <u>5 windows 2613 - 2921 cm^{-1}</u>











- harmonized treatment of interfering species: <u>same binput-file</u>
- identical spectroscopy for all: <u>same cfgls (HIT04 & Hase update)</u>
- common source of pT-input profiles: <u>NCEP</u>
- one consistent set of a priori profiles: <u>Toon with Meier correction</u>
- one consistent set of regularization matrices and altitude grids: <u>Tikhonov-L_1 on the %-VMR scale</u>

Harmonizing the g.-b. MIR XCH4 data set: how to calculate the air column

- in situ p measurements not continuously available at all sites for 2003/2004

- radio sondes not available for all sites

- NEP p-profiles and ECMWF in situ p available

- NCEP favored because:

  - The forward model of the g.-b. FTIR retrievals uses NCEP pressure profiles to calculate the airmass-profile (“fas.mas” file) which is internally used to transfer VMR profiles to partial column (CH4) profiles

  - I.e., the air columns calculated from NCEP are i) readily available, and ii) perfectly consistent to the CH4 total columns retrieved.

Harmonizing the g.-b. MIR XCH4 validation data set: dry versus wet XCH4

- previous SCIA validation studies derived XCH4 from FTIR via rationing by <u>wet</u> air columns (derived from pressure data).

⇒inconsistency to SCIAMACHY, which retrieves <u>dry</u> XCH4 .

⇒ FTIRs should substract the water vapor column from the air column:

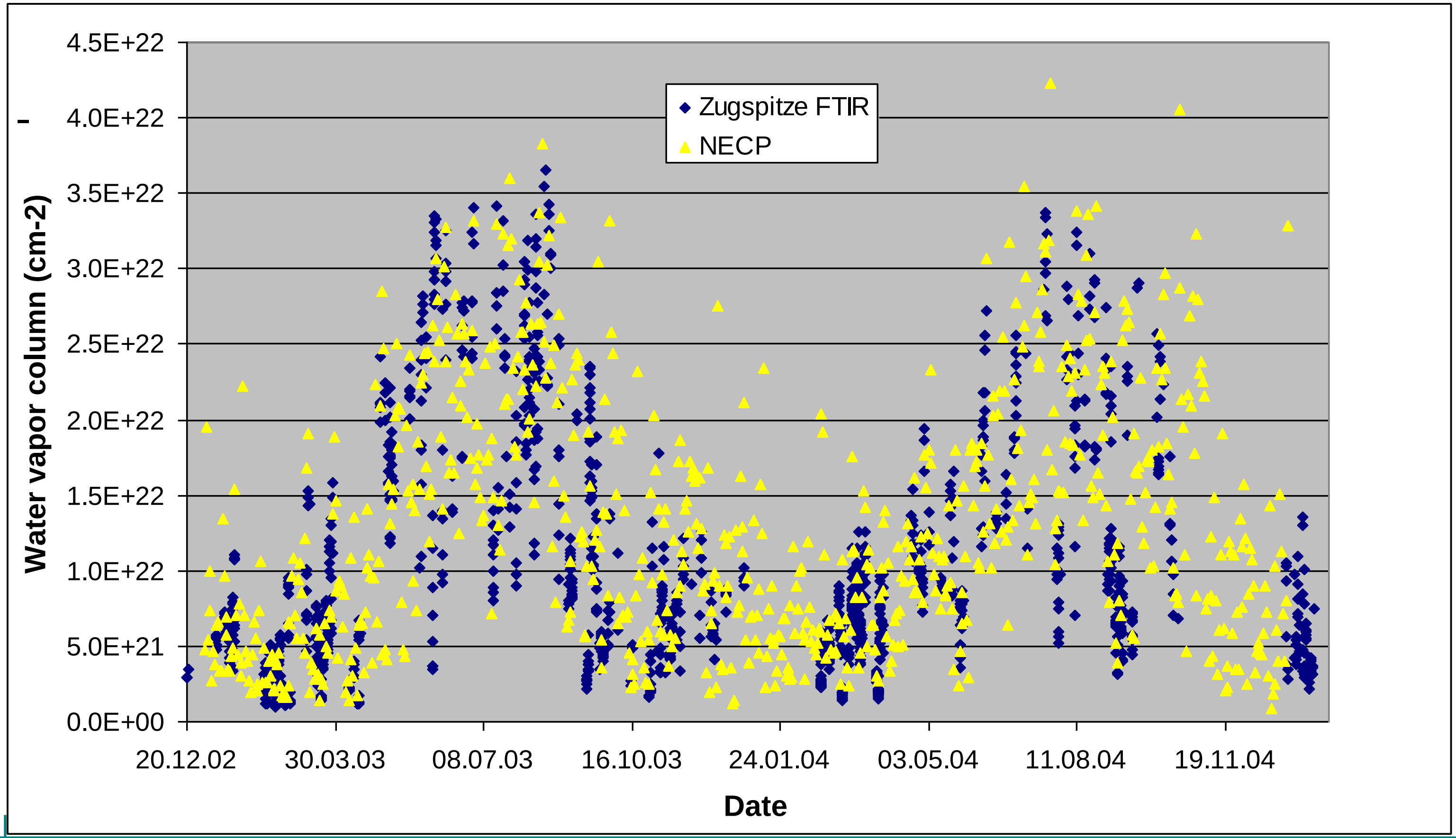
<u>where do we get water columns from?</u>

<u>not all FTIR groups have a maturated FTIR water retrieval;</u>

<u>are NCEP water columns reliable?</u>

Harmonizing the g.-b. MIR XCH4 validation data set: how to calculate dry XCH4

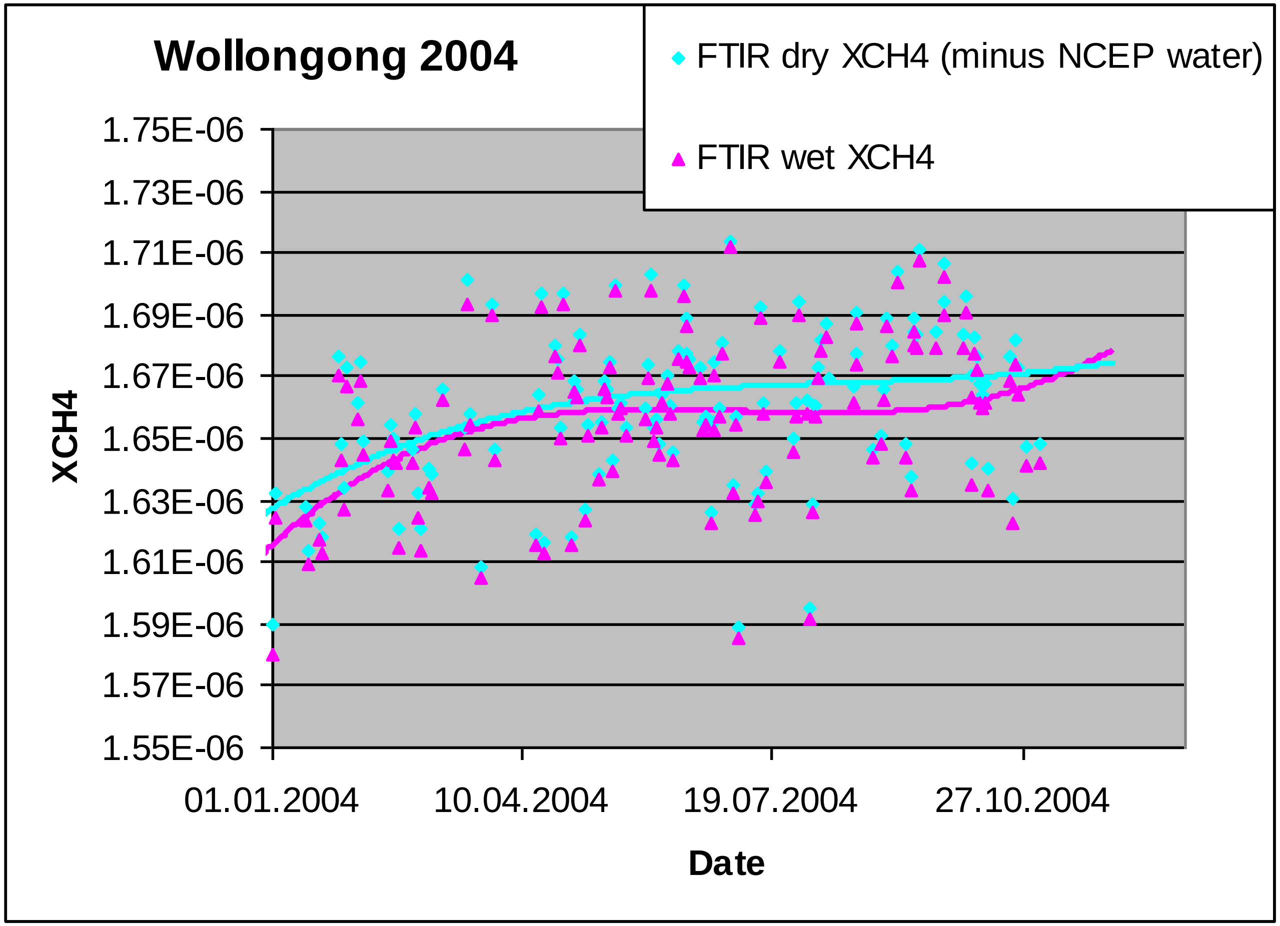
validate NCEP water columns
against
Optimized Zugspitze FTIR water vapor column retrieval (ACPD 2009, IRWG science talk)



⇒ NCEP water ok, use for all stations

Harmonizing the g.-b. MIR XCH4 validation data set: dry versus wet XCH4

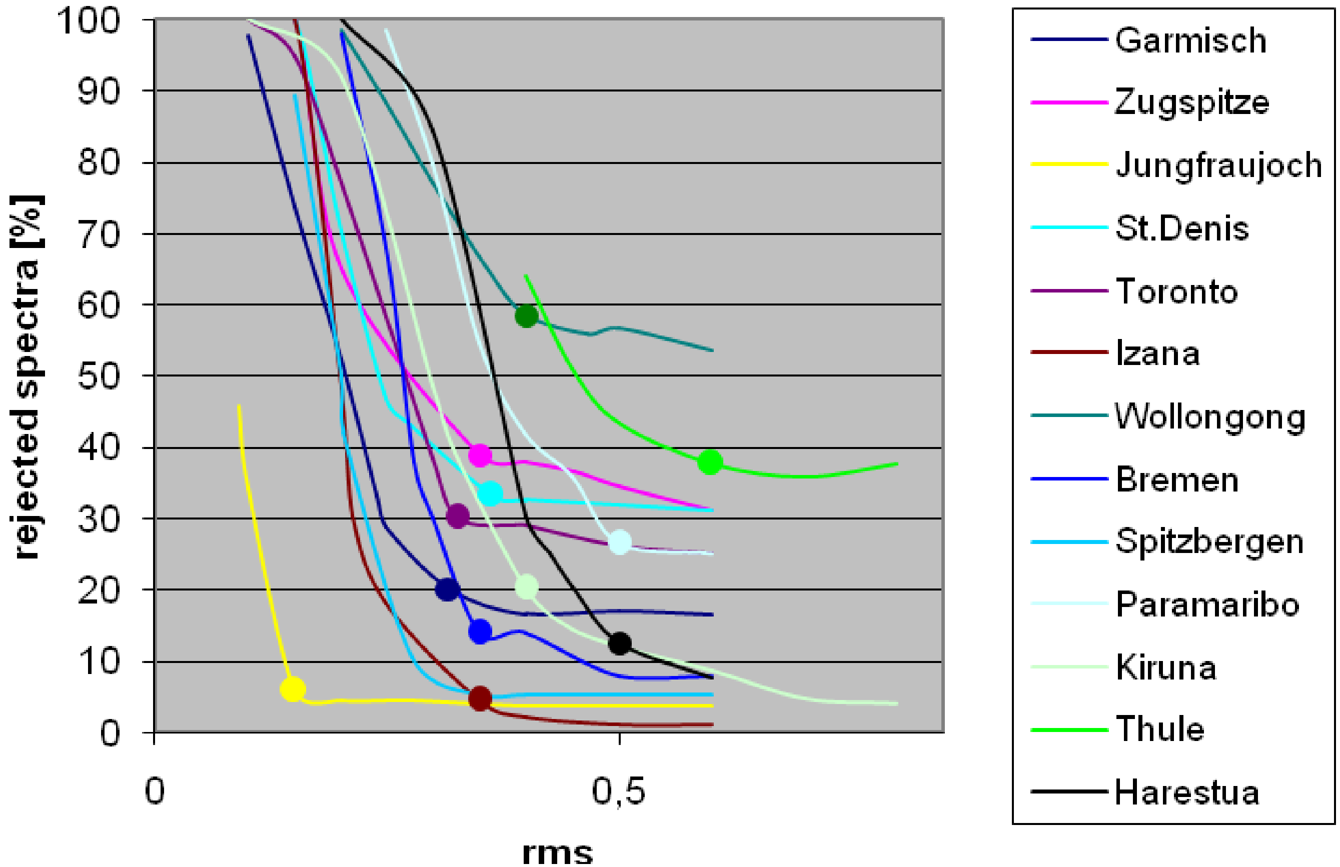
… impact on bias, annual cycle



MIR-FTS, homogenization: data selection / quality control

FTIR spectra quality (rms of the spectral fitting residuals)

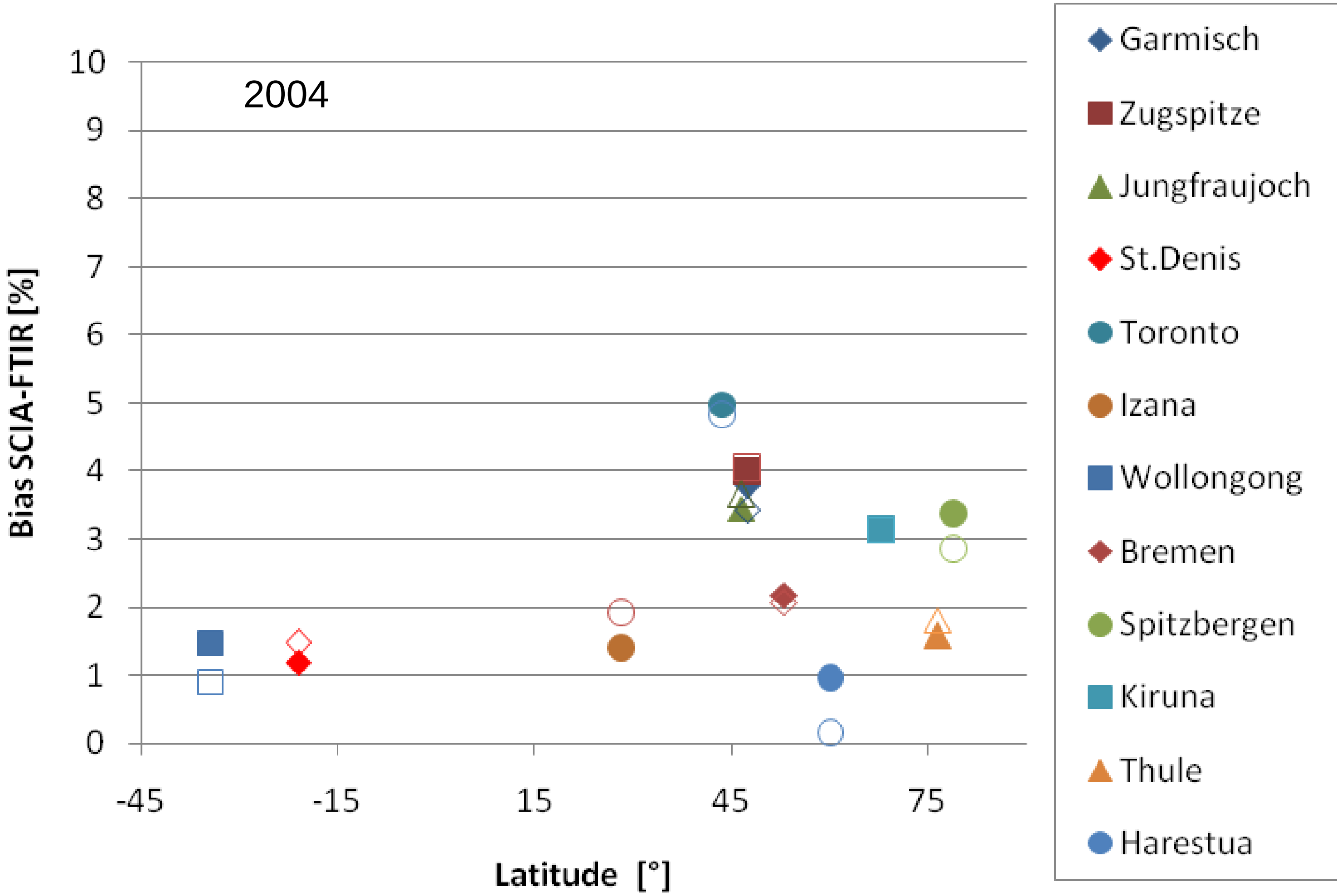
⇒ harmonized selection thresholds for all FTIR data-sets



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)

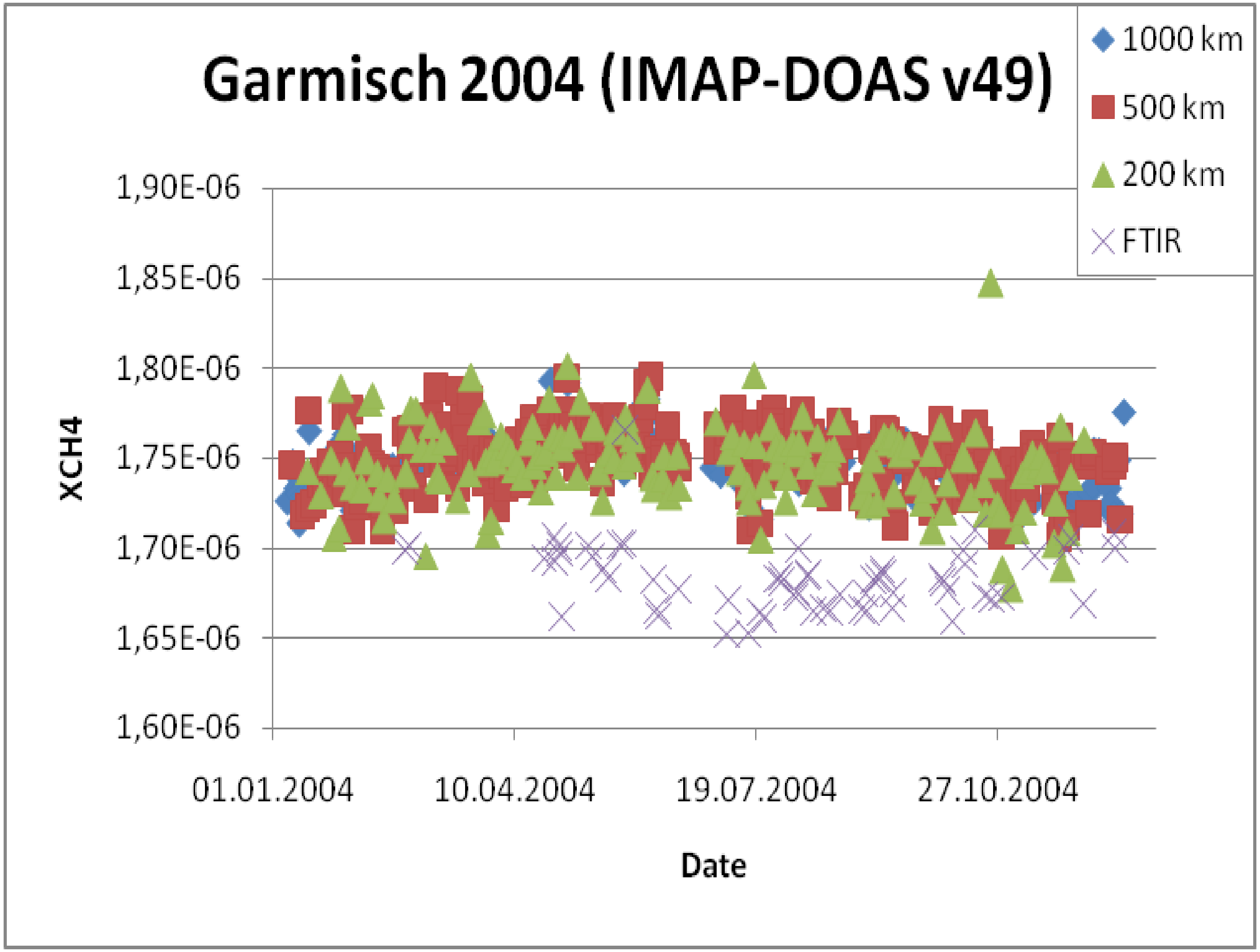
according to Rodgers and Connor (JGR, 2003)

Intercomp. results: global XCH4 biases SCIA - MIR-FTIR (same day, 500 km radius)

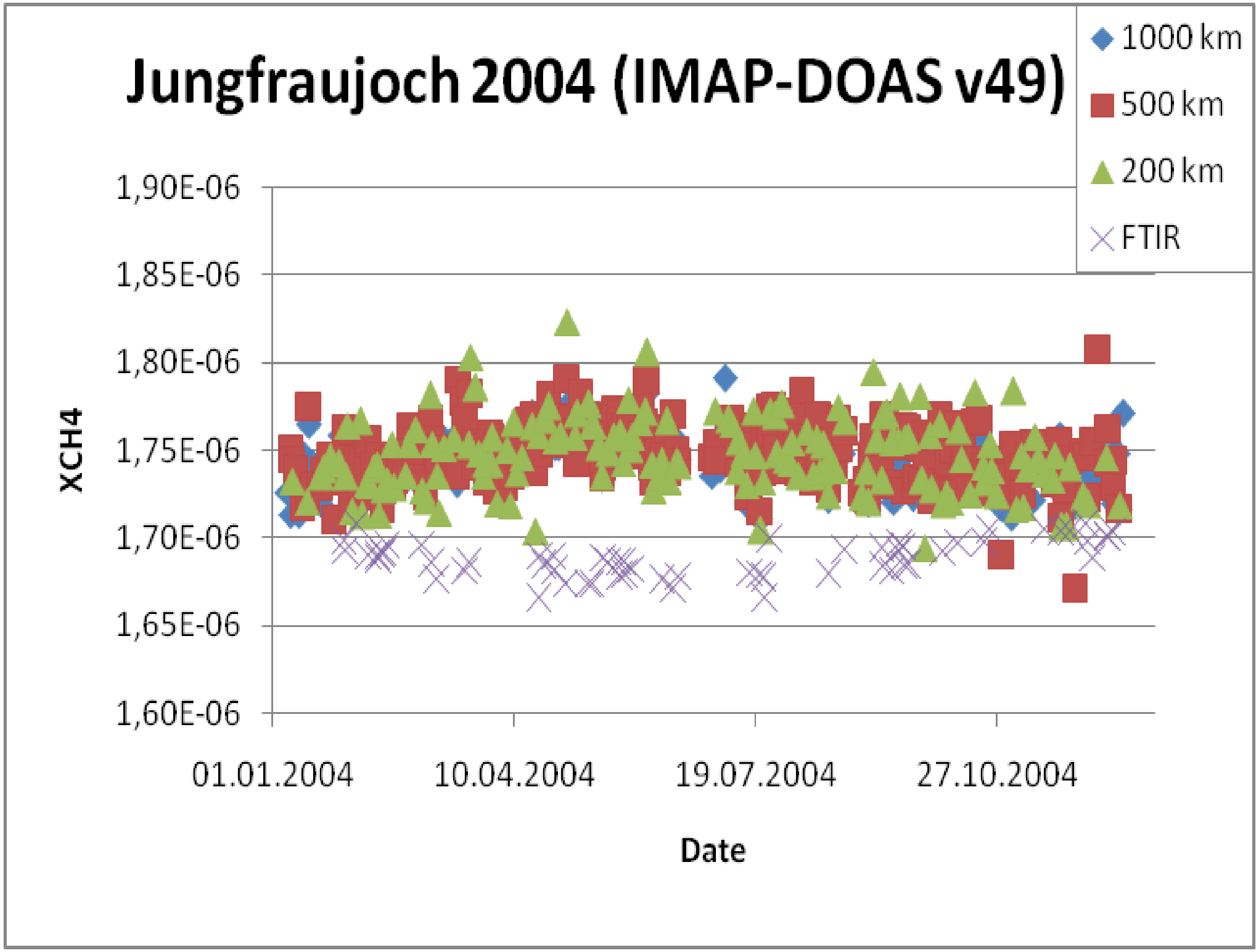


open symbols: without averaging kernel correction

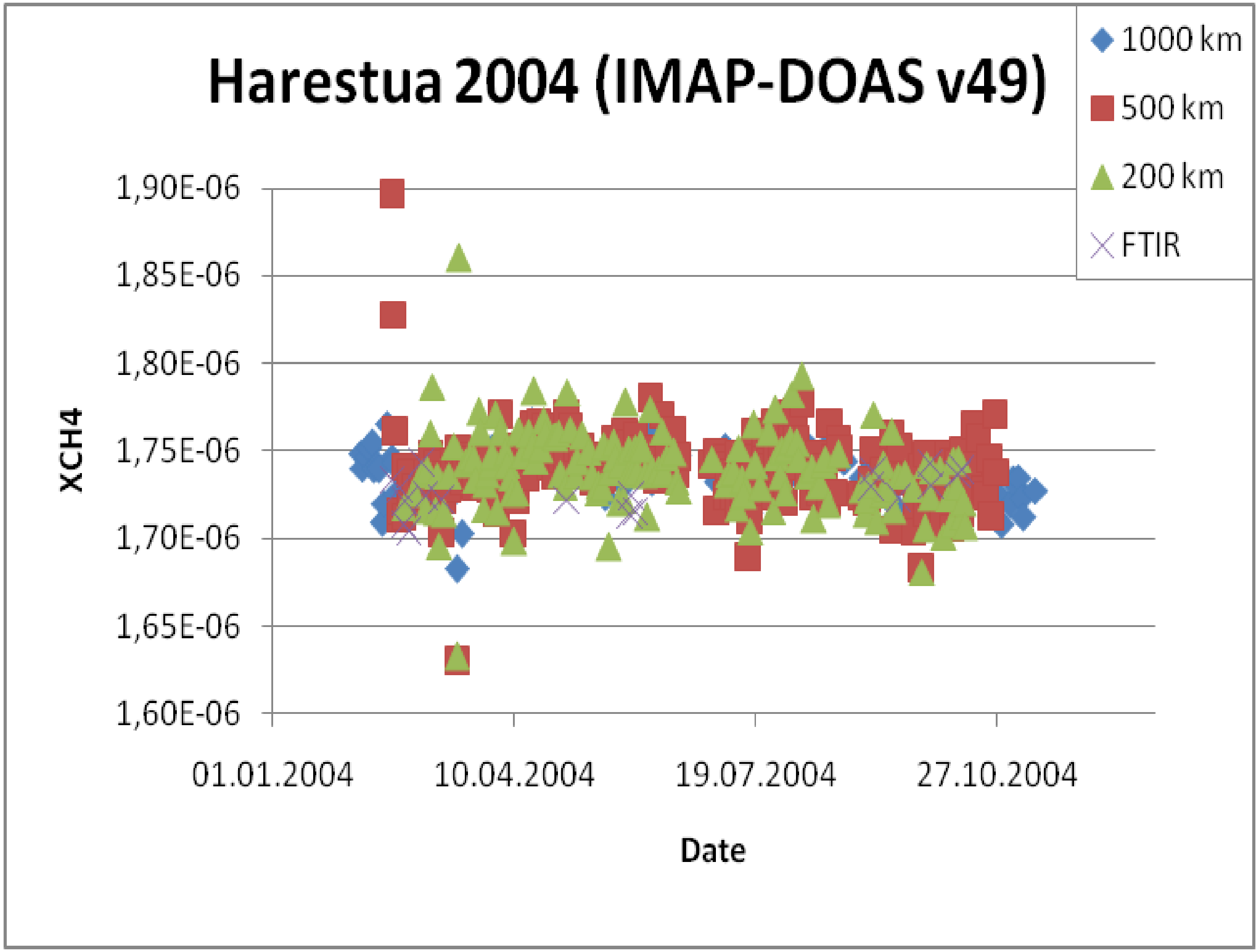
Intercomp. results: validation plots (daily means FTIR, SCIA-200, -500, -1000 km)



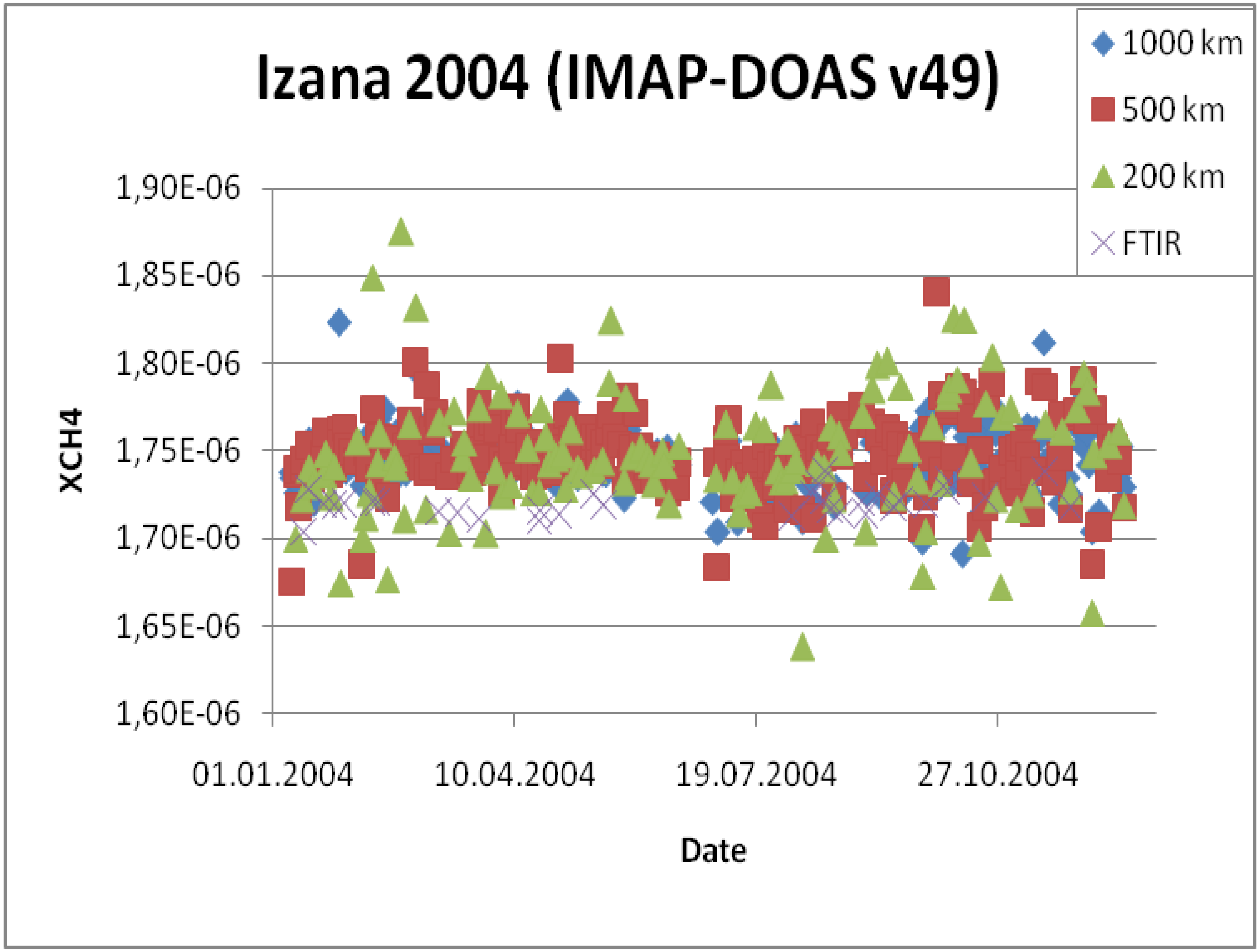
Intercomp. results: validation plots (daily means FTIR, SCIA-200, -500, -1000 km)



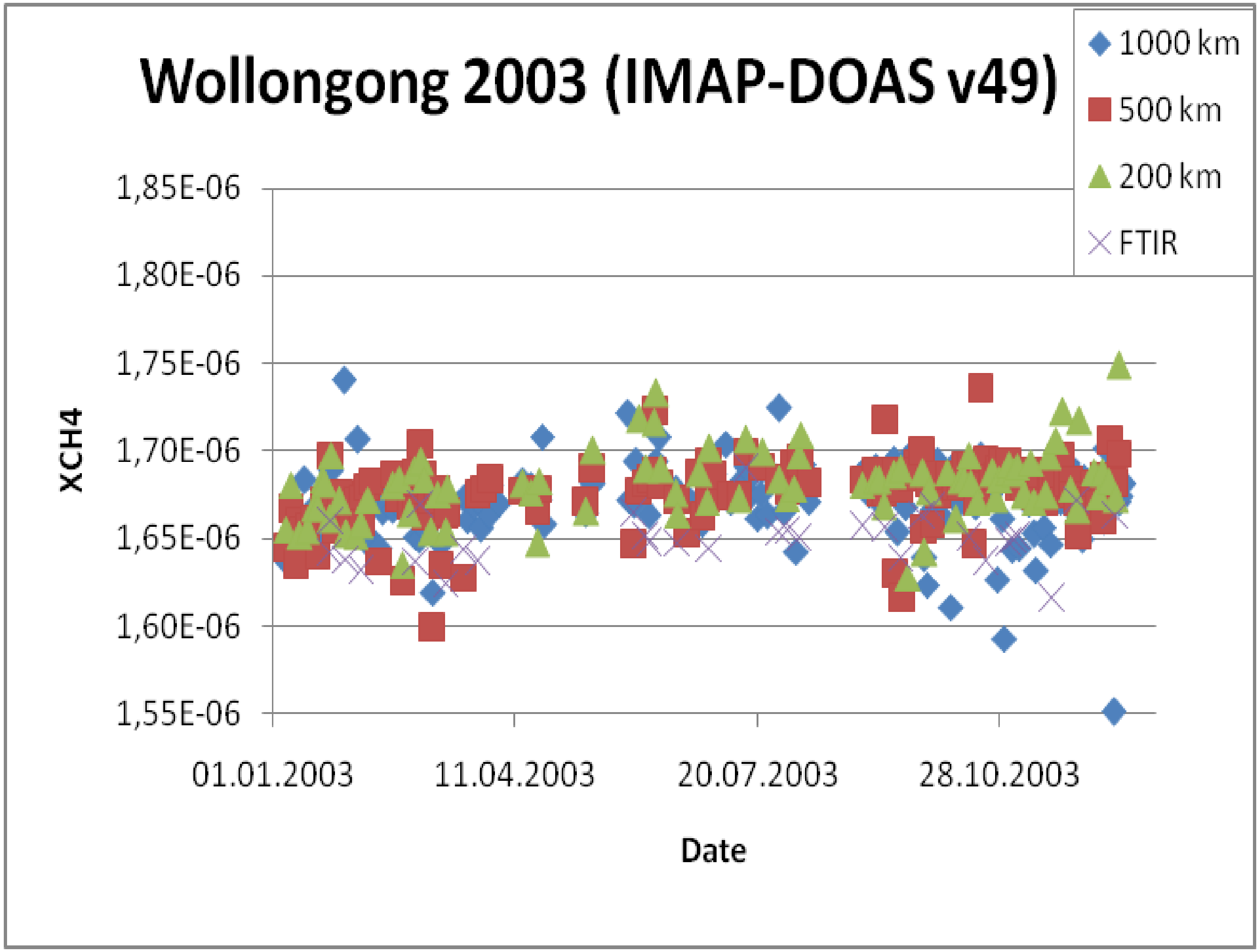
Intercomp. results: validation plots (daily means FTIR, SCIA-200, -500, -1000 km)



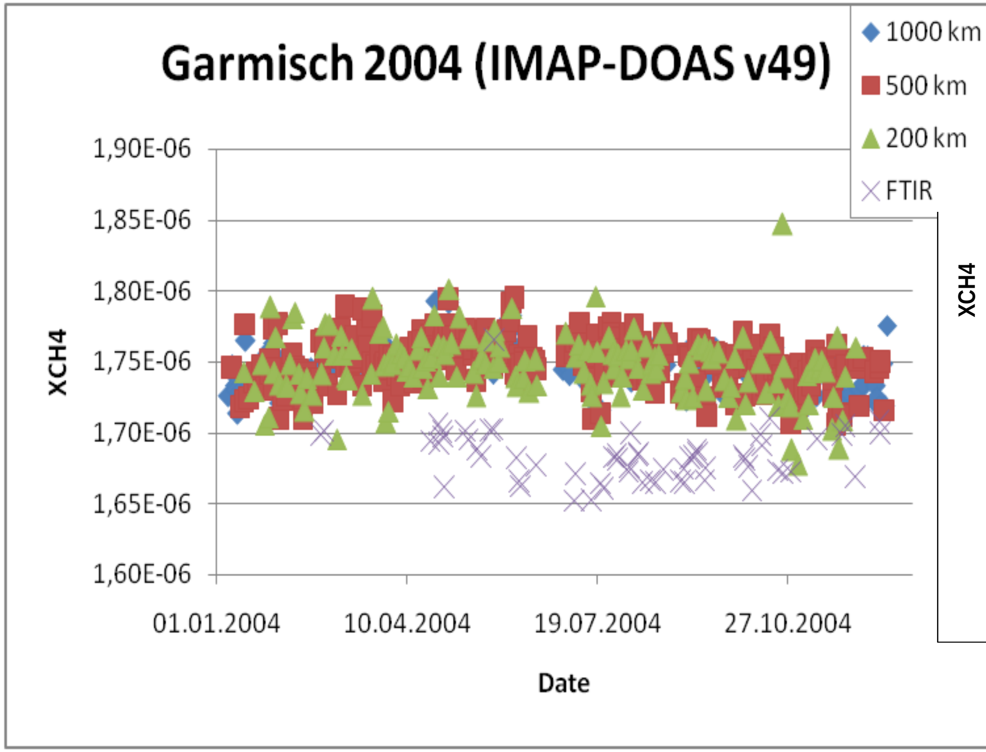
Intercomp. results: validation plots (daily means FTIR, SCIA-200, -500, -1000 km)



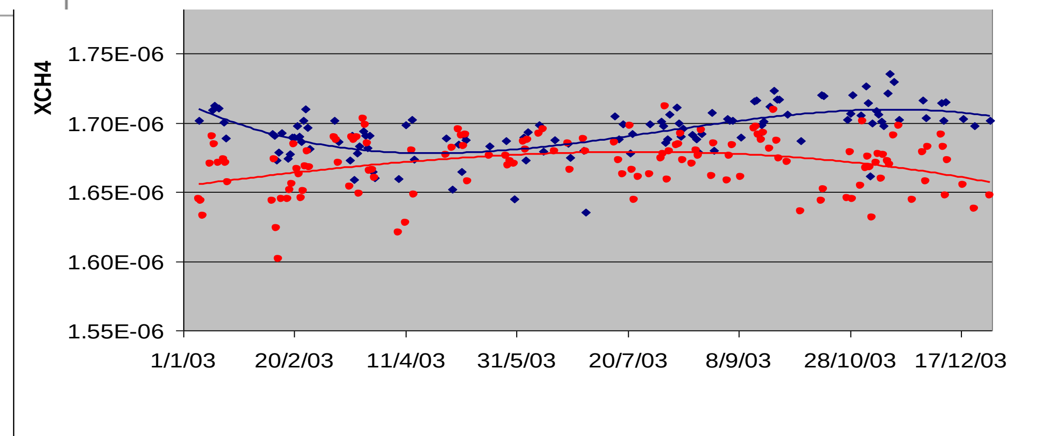
Intercomp. results: validation plots (daily means FTIR, SCIA-200, -500, -1000 km)



Does SCIA just reflect dynamical prior, i.e., is not able to retrieve the ≈1 % CH4 changes above clean sites?



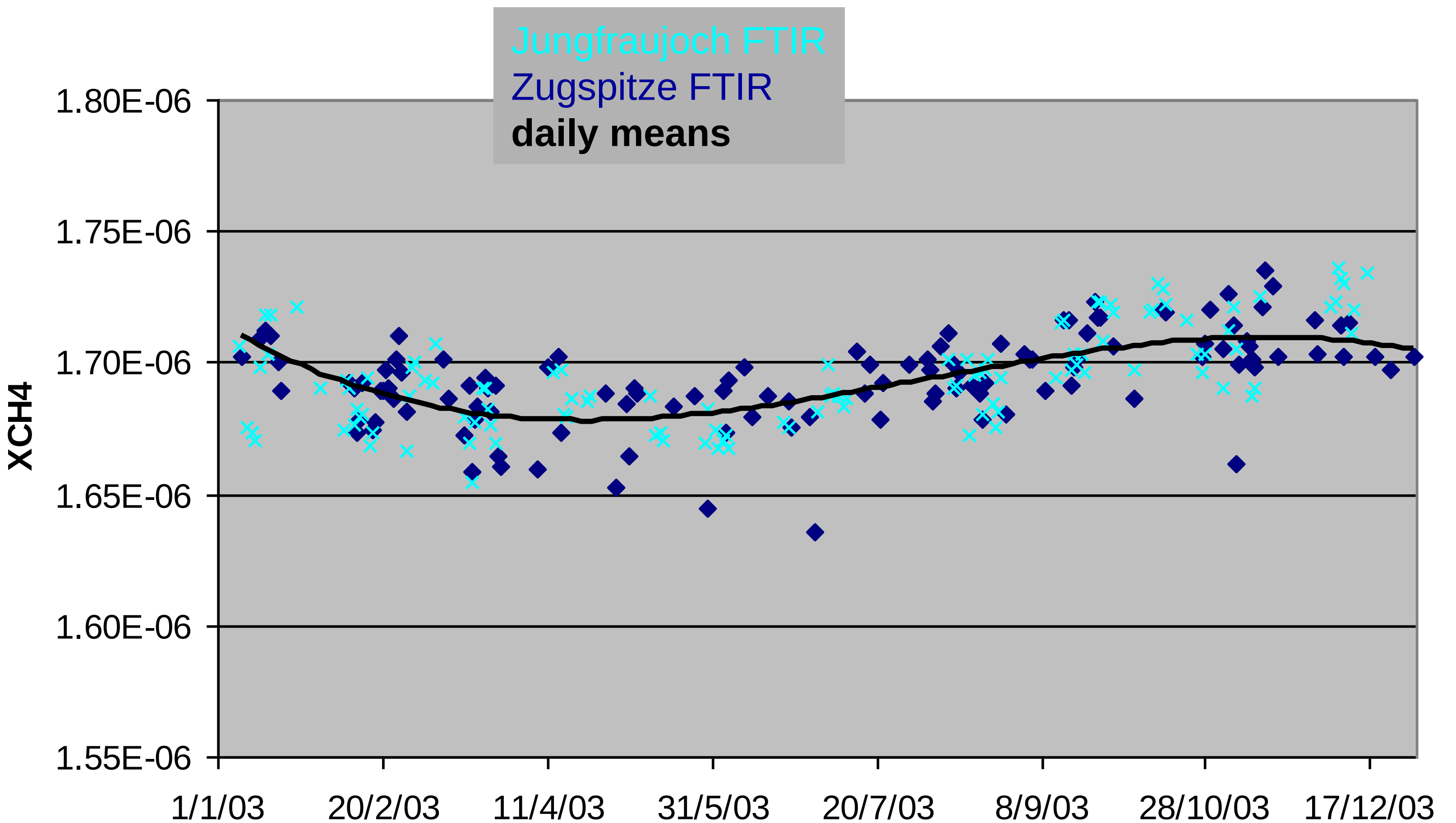
Red: XCH4 calculated from fixed a priori profile taking daily pT-profiles and tropopause altitudes into account



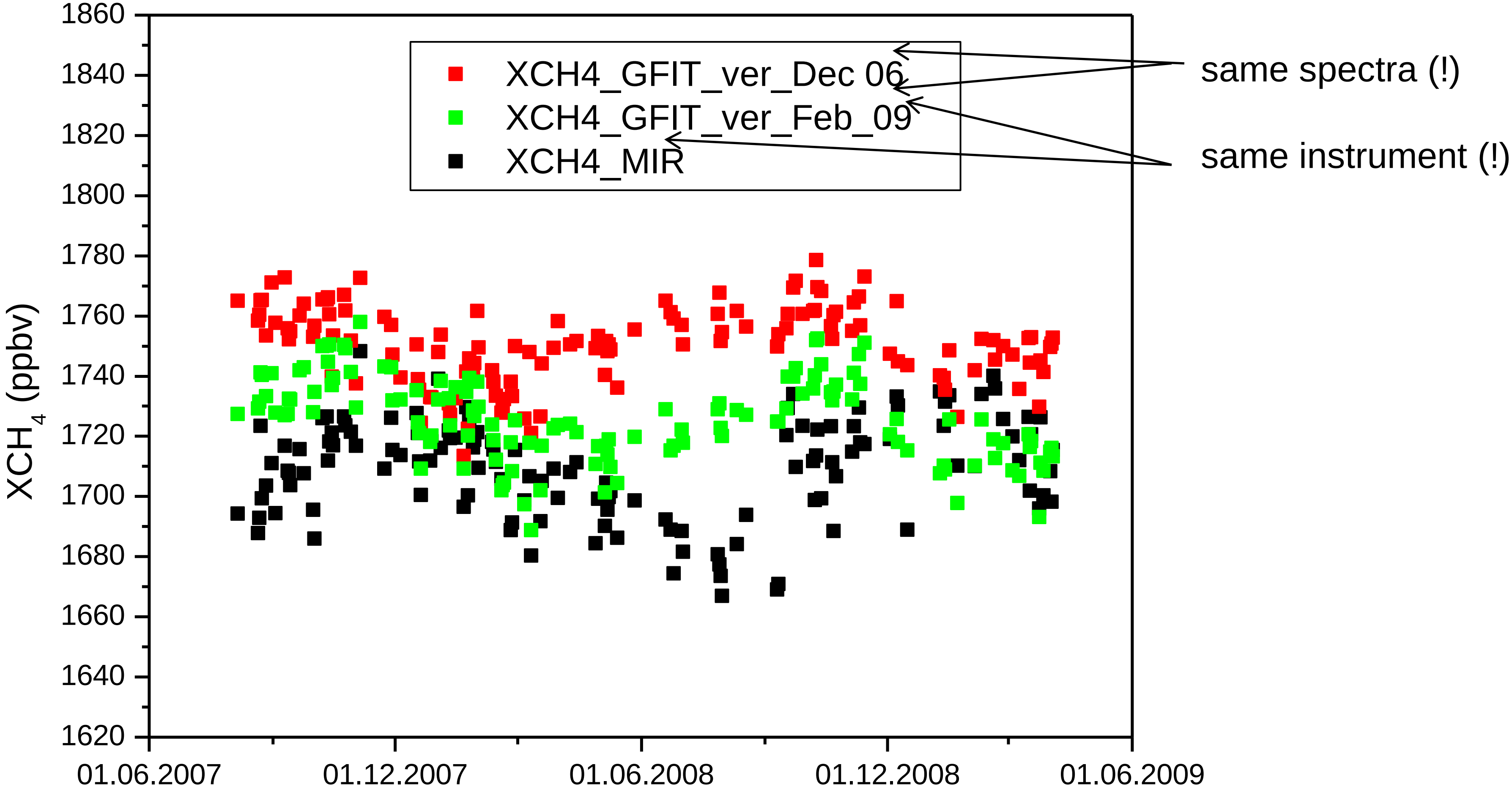
… probably not: WFM-DOAS uses 1 fixed a priori profile

XCH4 annual cycles: Different MIR instruments and differing ray tracing algo´s

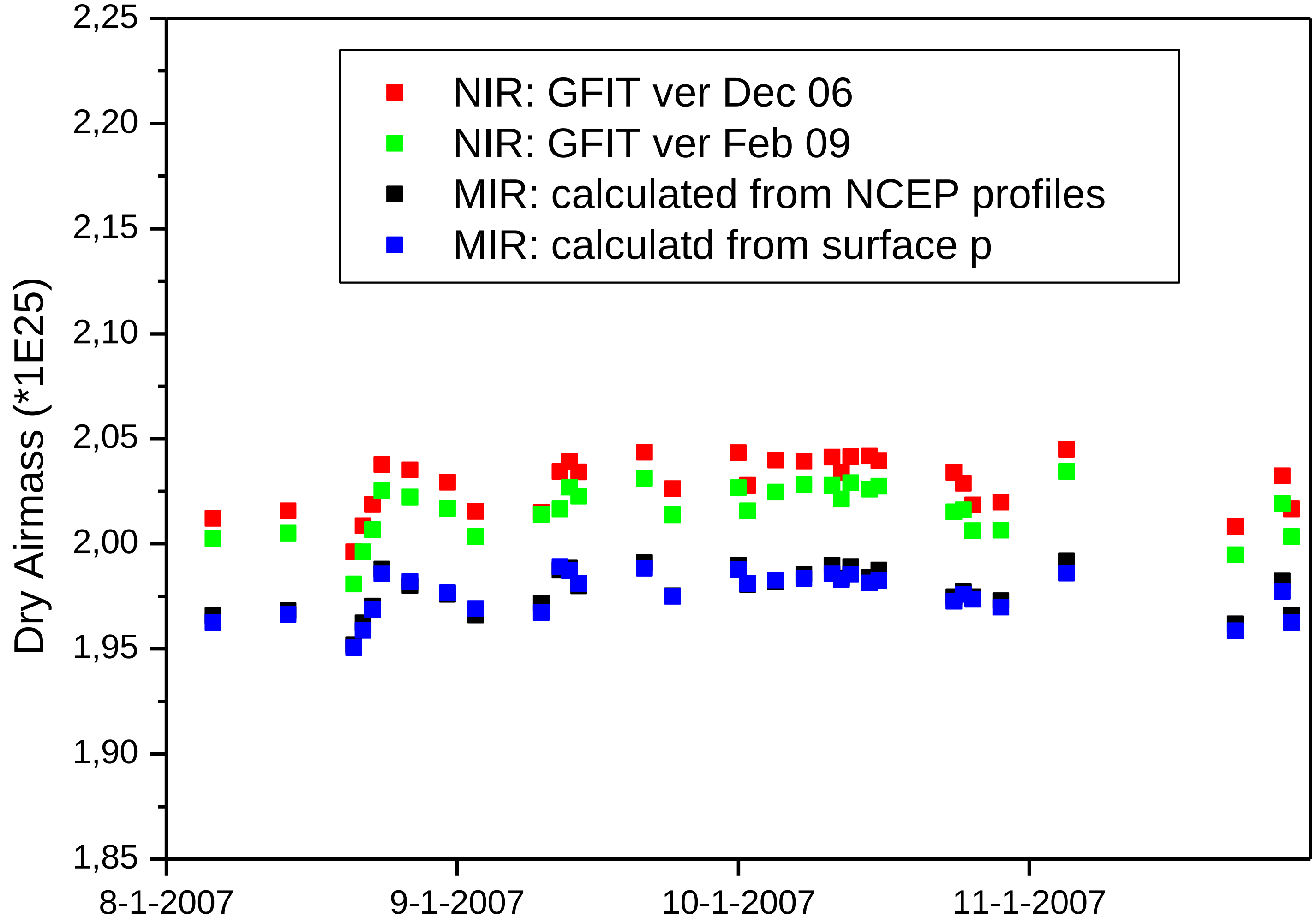
…. impact on annual cycles? No. ☺



Annual cycles: g.-b. XCH4 MIR versus NIR



Annual cycles: trust in dry airmass derived from O2, NCEP and *p* measurements

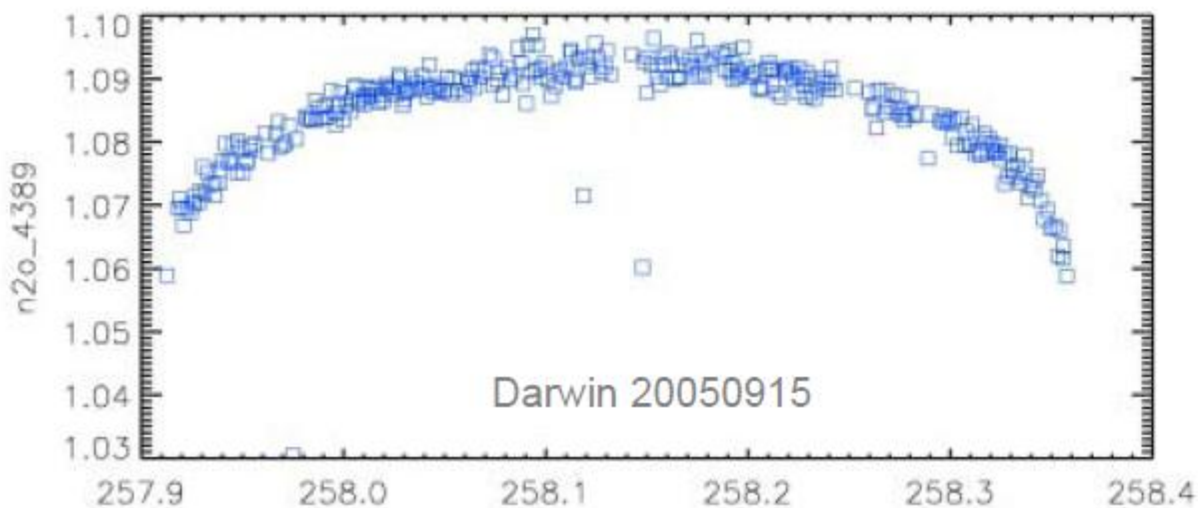


Annual cycles: airmass-dependent artifacts – taken from Geoff´s 2006 talk

Retrievals of gases known to have tiny diurnal variations, e.g. O_2, CO_2 (winter), CH_4, N_2O, often exhibit airmass-dependent artifacts.

These are often termed a “smile” (column increases with airmass) or a “frown” (column decreases with airmass) due to their shape when plotted versus time of day.

taken from
Geoff´s 2006 talk

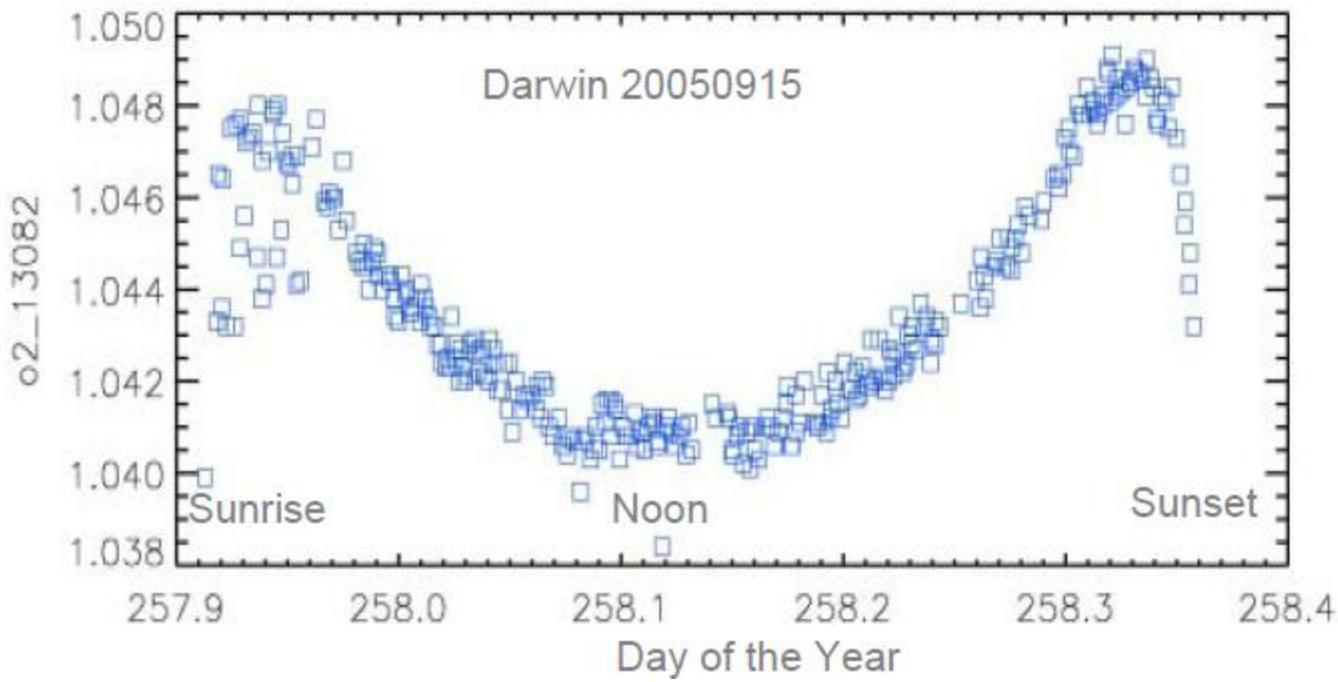


Annual cycles: airmass-dependent artifacts – taken from Geoff´s 2006 talk

These artifacts are often quite small (<1%) and can only be seen in data of the highest quality. But they can be an annoyance (e.g. can be aliased into the seasonal variation) and indicate a serious underlying problem.

They are also a very sensitive indicator of spectroscopic deficiencies, assuming that the atmospheric model and ray-tracing are correct.

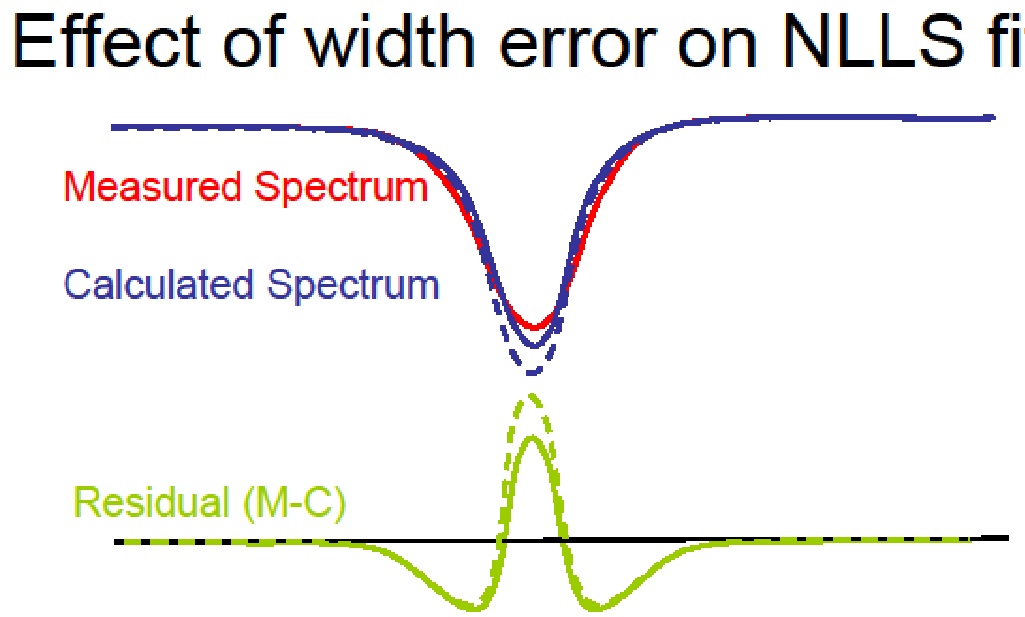
taken from
Geoff´s 2006 talk



Annual cycles: airmass-dependent artifacts – taken from Geoff´s 2006 talk

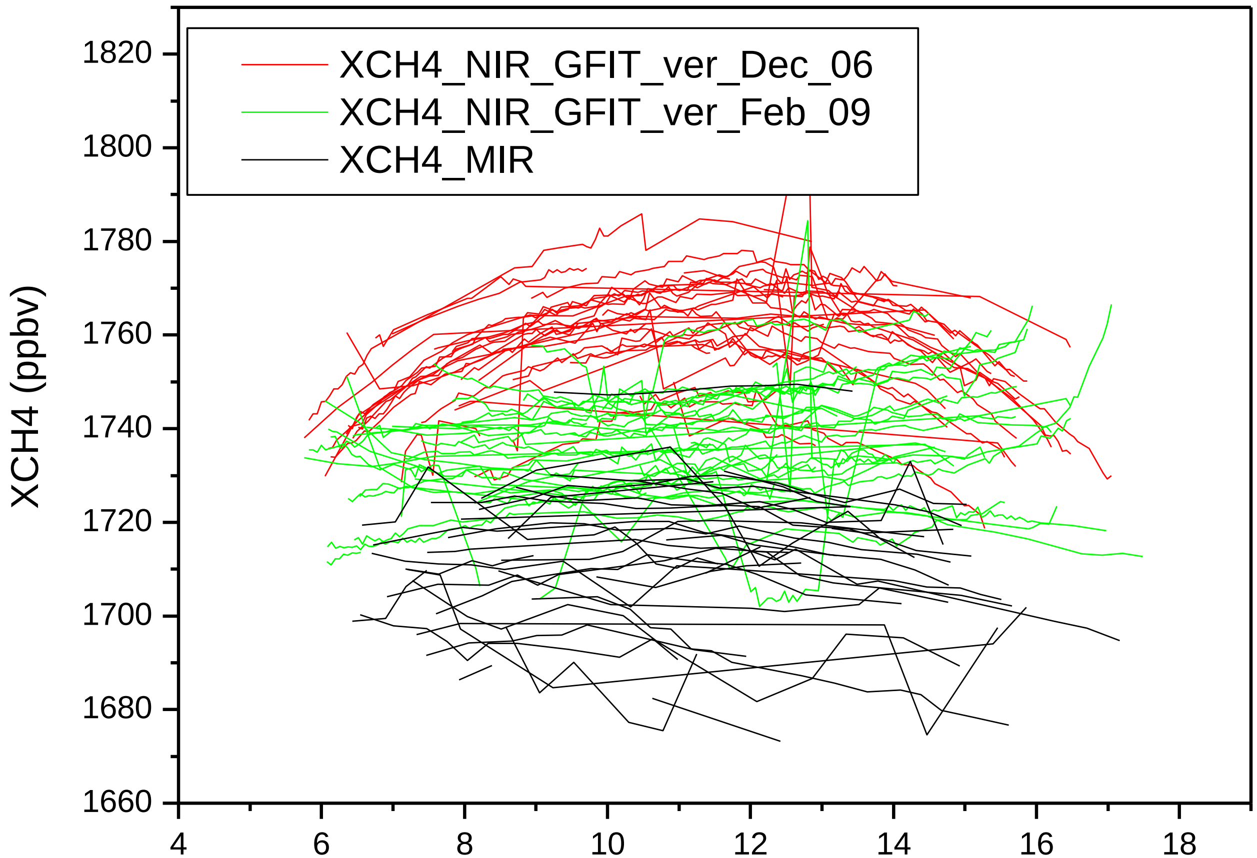
"Unfortunately, virtually all modern retrieval algorithms use NLLS methods, which do not match equivalent widths. Since NLLS methods minimize the square of the residuals, and since the largest residuals typically arise at line center, NLLS methods try harder to fit the line center than elsewhere on the line profile."

taken from Geoff´s 2006 talk

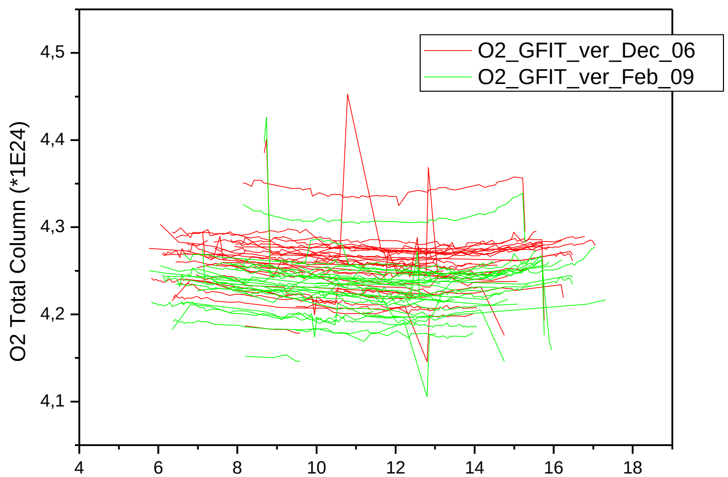


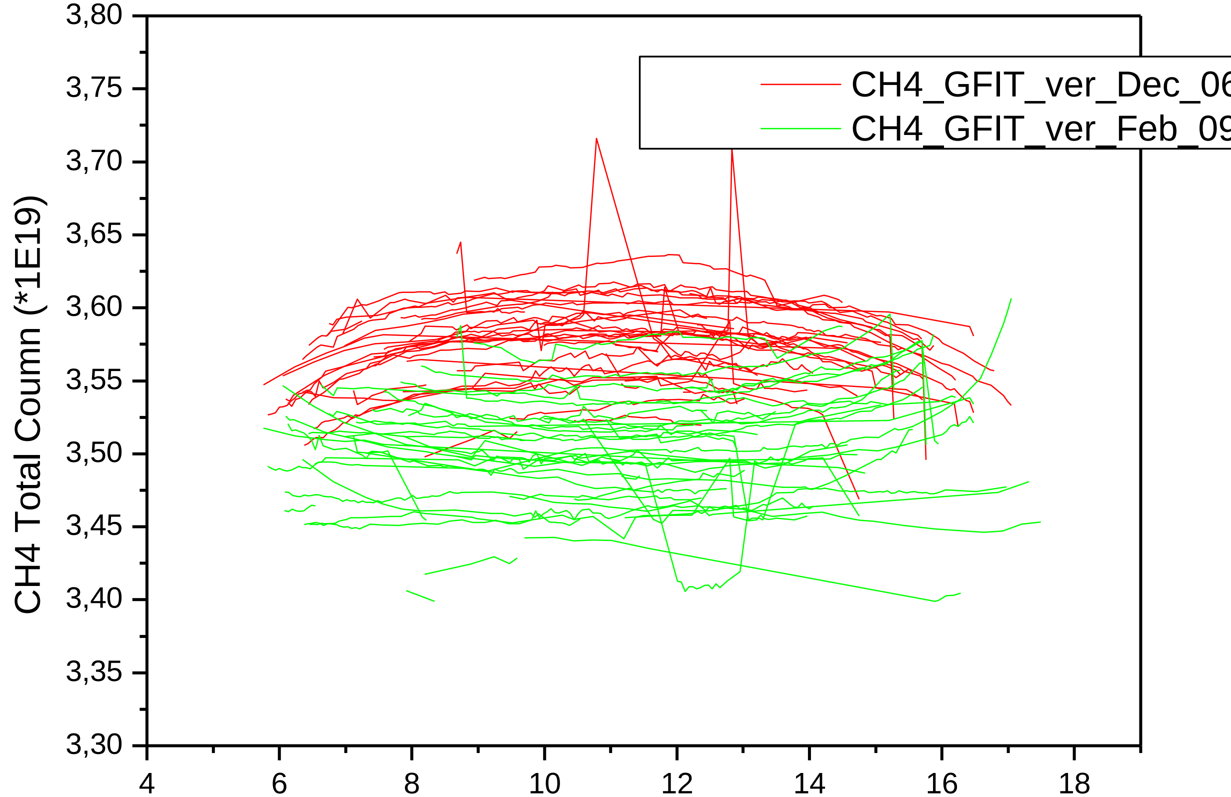
EW-matching retrieval (dashed line). NLLS retrieval (solid)
Area under NLLS residual curve is -ve
Calculated Spectrum has smaller EW than measured spectrum
Retrieved column is therefore under-estimated.

XCH4 diurnal variation: g.-b. MIR versus NIR



Diurnal variation O2 and CH4: old GFIT versus newest version GFIT

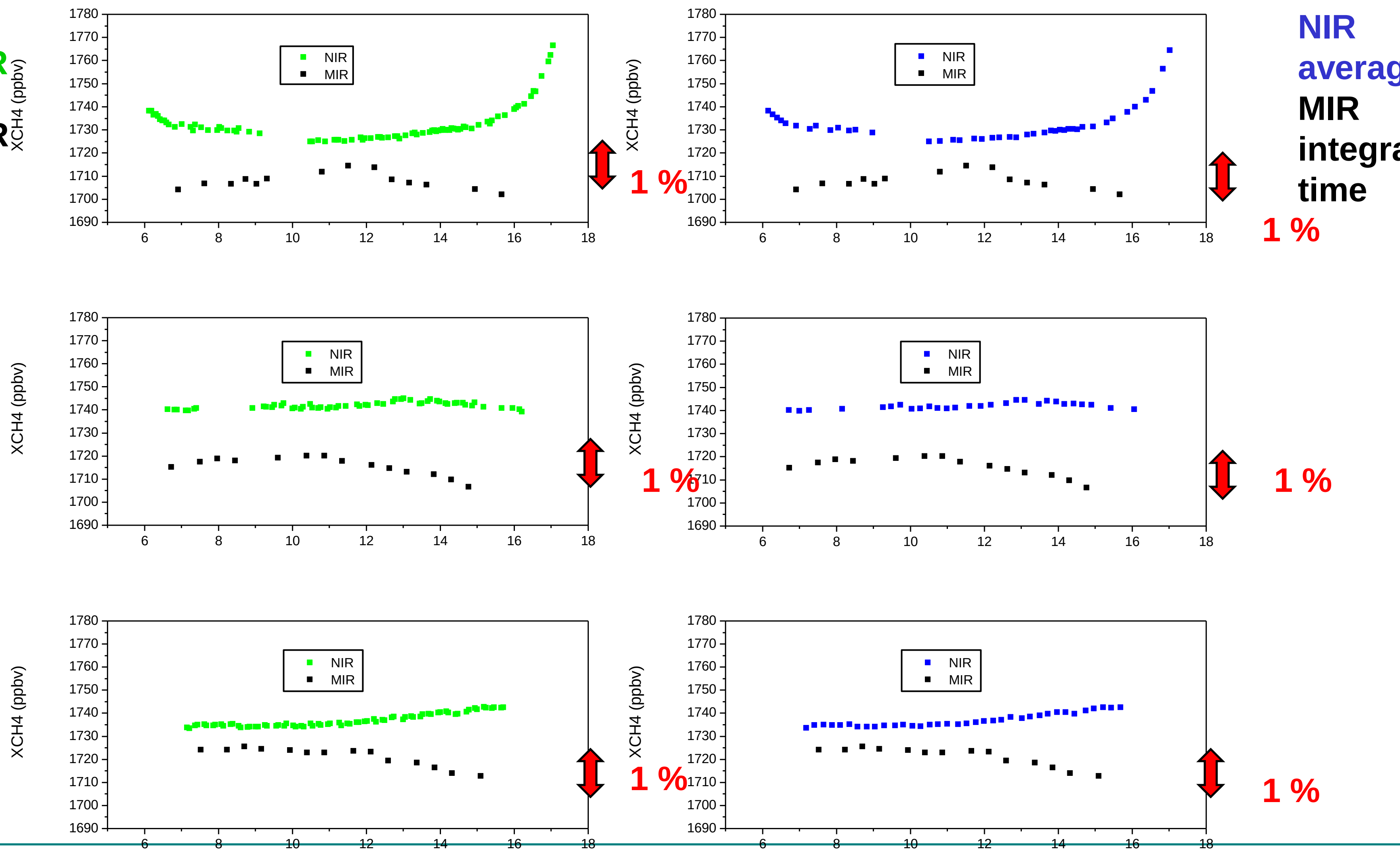




Diurnal cycles: measured in alternating NIR-MIR mode with Garmisch FTS

NIR

MIR



NIR averaged to MIR integration time

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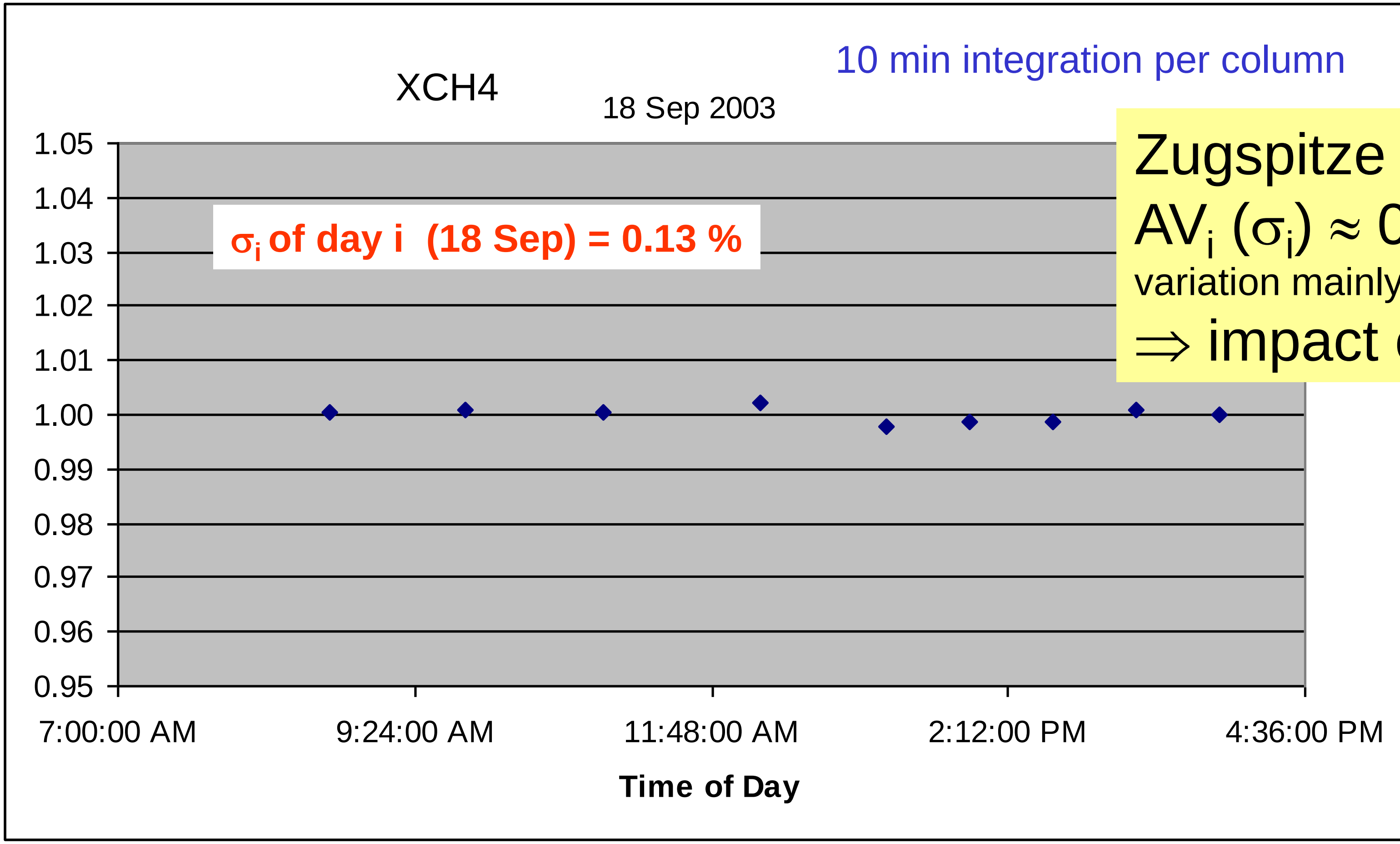
Sussmann et al.: *Validation of SCIA & GOSAT XCH4 by NDACC & TCCON FTS*

MIR-FTIR XCH4 precision/diurnal variation: impact of regularization?



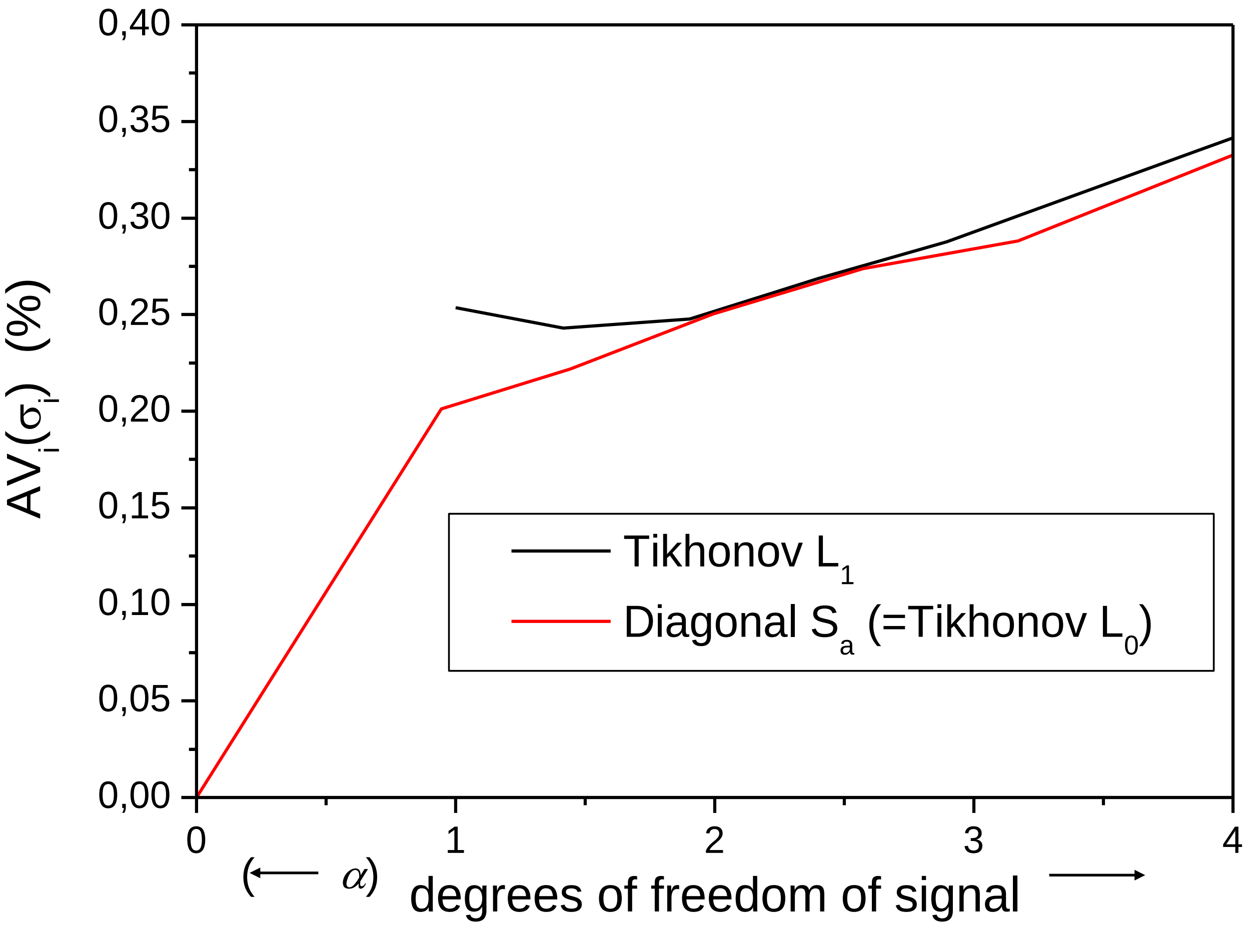
Zugspitze 2003:

$AV_i(\sigma_i) \approx 0.5$ %

variation mainly due to clouds

$\Rightarrow$ impact of regularization?

L_1 as a function of α (dofs): minimize diurnal variation averaged over all days

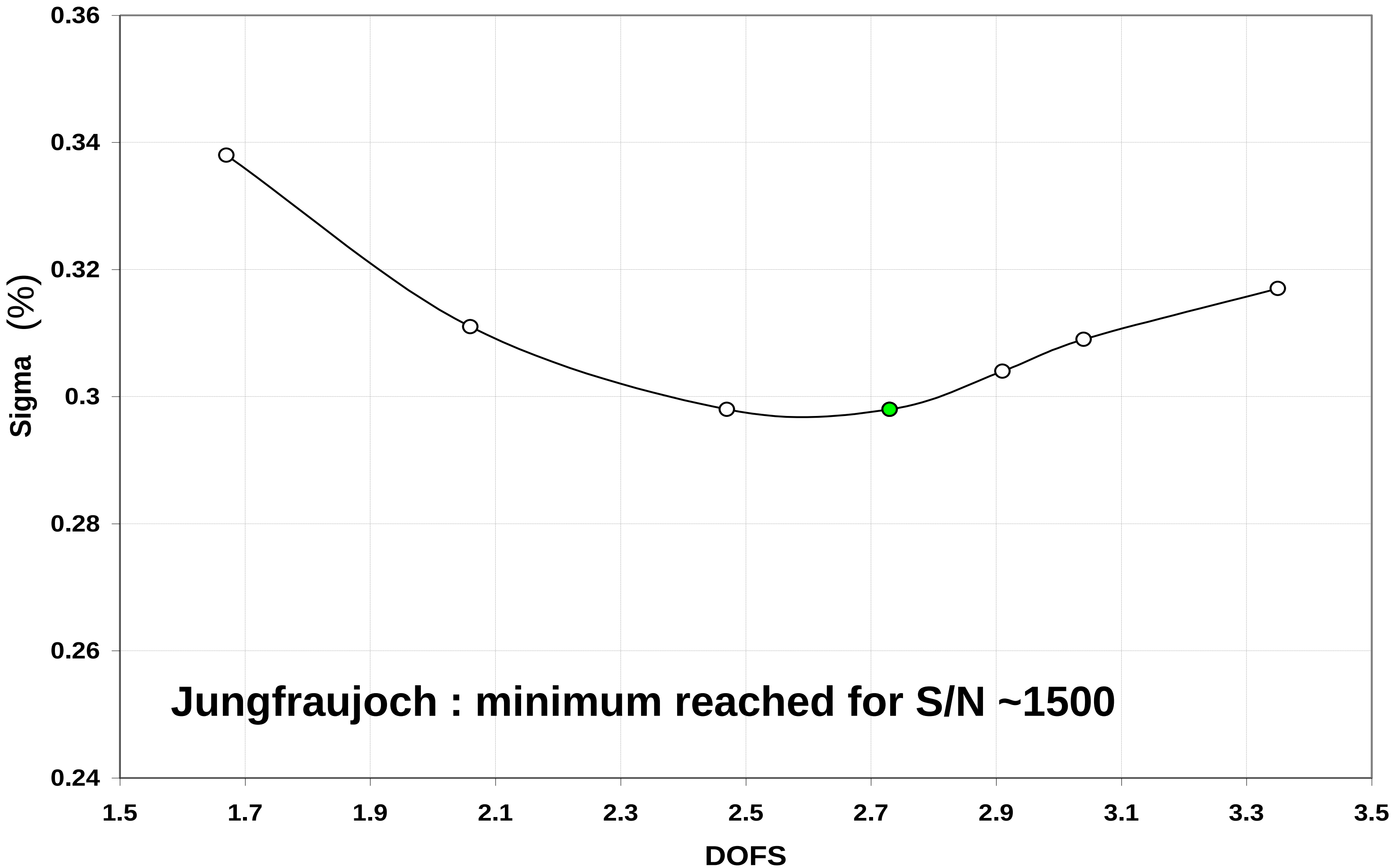


⇒L_1 is robust even for low dofs

⇒with diagonal $\mathbf{S}_a$ (L_0) you can understimate true variability with σ´s down to zero

Zugspitze result reproduced at ISSJ:

Tikhonov L_1 retrievals optimization: intra-day CH_4 column variability vs mean DOFS



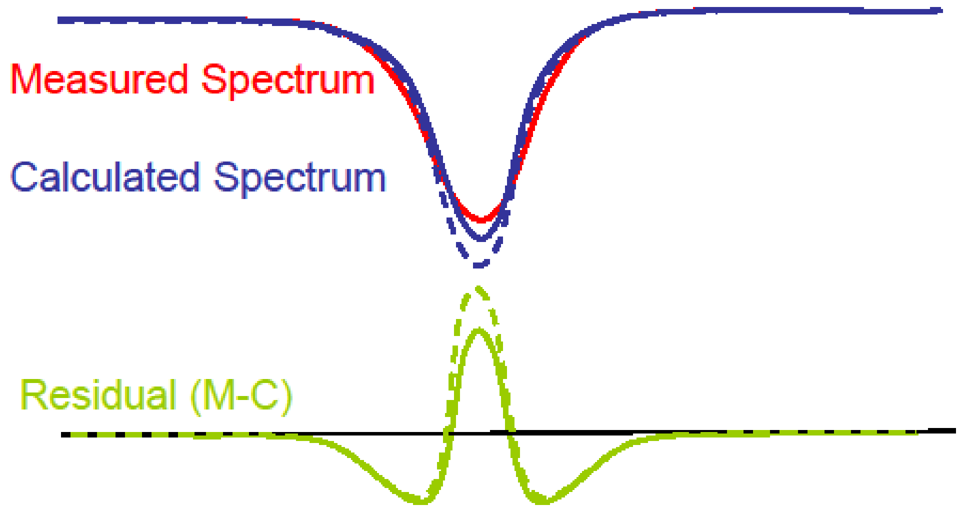
Duchatelet, Oct 2009

MIR-FTIR CH4 precision: why does Tikhonov L_1 reduce cloud-induced scatter?

"Unfortunately, virtually all modern retrieval algorithms use NLLS methods, which do not match equivalent widths. Since NLLS methods minimize the square of the residuals, and since the largest residuals typically arise at line center, NLLS methods try harder to fit the line center than elsewhere on the line profile."

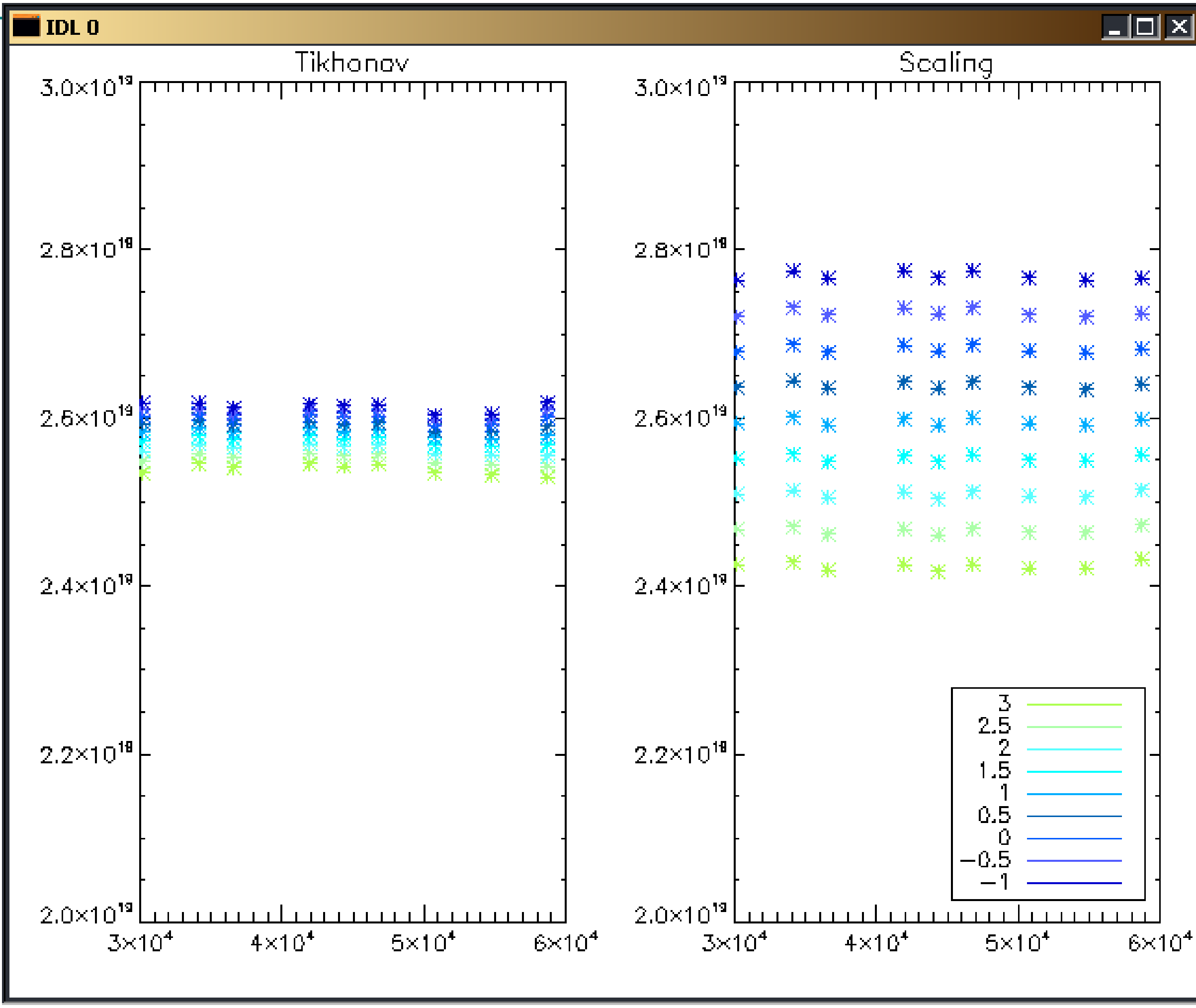
taken from Geoff´s 2006 talk

Effect of width error on NLLS fit



EW-matching retrieval (dashed line). NLLS retrieval (solid)
Area under NLLS residual curve is -ve
Calculated Spectrum has smaller EW than measured spectrum
Retrieved column is therefore under-estimated.

MIR-FTS CH4 precision: Tikhonov L_1 better integrates line area than VMR-scaling



time of day

time of day

… certainly at the cost of somewhat unphysical profile shapes at the presence of clouds, but never mind if interested in columns

different effective apodization parameters set fix in forward model

Global validation of SCIAMACHY XCH4 by NDACC FTS – what can we learn for GOSAT validation by TCCON FTS?

Summary

• based on HYMN CH4 profile retrievals our global SCIA validation study with 12 MIR-FTS stations has lead to a maturated XCH4 retrieval from MIR-FTS which can be used to validate both TCCON-FTS and GOSAT

• XCH4 annual cycles above clean sites with ≈1 % amplitude differ on the 1 % level between SCIA MACHY & g.-b. MIR-FTS & g.-b. NIR-FTS (⇒ GOSAT?)

• GFIT-O2 compares very well to dry airmass derived from NCEP or in situ *p*

• CH4 smiles are reduced with GFIT ver Feb 09 compared to GFIT ver Dec 06

• still both CH4 MIR and newest version GFIT shows > ≈1 % "smiles" on some days

• although "precision" of g.-b. NIR FTS is better, g.-b. MIR is astonishingly good

• CH4 profile retrieval with SFIT 2 (Tikhonov L_1 on %-VMR scale) helps to reduce cloud-induced scatter by up to a factor of ≈3 %

MIR-FTIR regularization: Tikhonov first derivative regularization L_1

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

with regularization strength α.

MIR-FTIR regularization: Suggested Tikhonov first-derivative (L_1) regularization

… applied to profiles given in units of %-VMR changes rel. to a priori profile