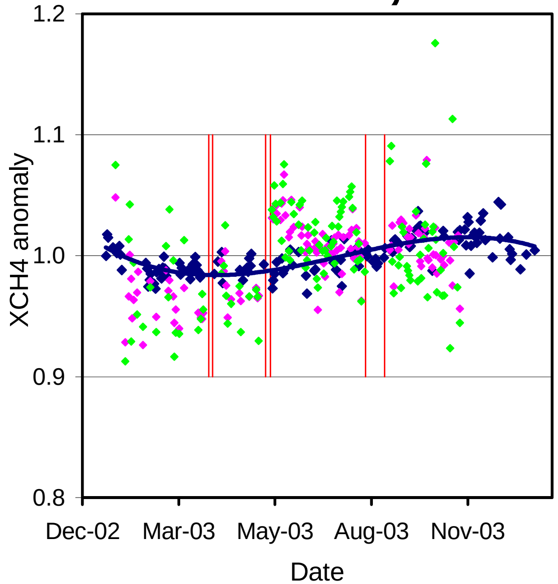
Optimizing precision of columnar methane retrievals

Ralf Sussmann, Frank Forster, Tobias Borsdorff, Markus Rettinger

Motivation:

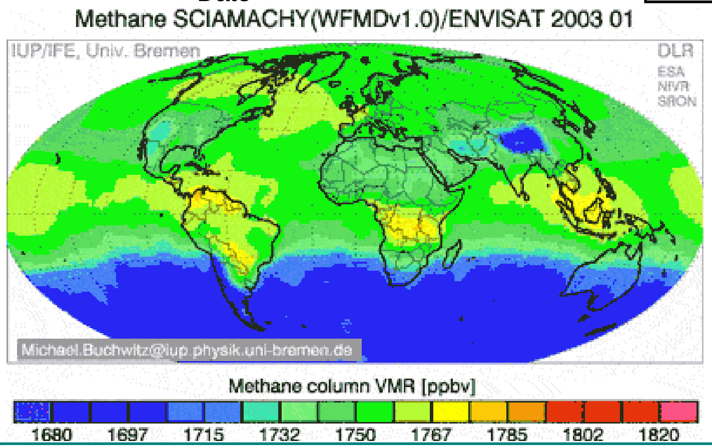
- investigate prior impact on column precision / response to true variability: complementary but related to TCCON
- ENVISAT/SCIAMACHY XCH4 validation with Zugspitze FTIR in 2005 had quantified strong time-dependent biases due to icing problems in channel 8
- newest SCIA IMAP-DOAS (ver. 49) XCH4 retrievals (cannel 6) have been significantly improved
- repeat SCIA validation with an optimized set of MIR-NDACC-FTIRs (HYMN project)
- point to a riddle in the annual cycle found by MIR-FTIR versus SCIAMACHY



SCIA 2005

Sussmann, Stremme, Buchwitz, de Beek, ACP, 2005

SCIA 2008



from “ESA kids“ website

MIR-FTIR XCH4 precision: Specific questions addressed in this talk

MIR-FTIR retrieval of CH_4 within the EC-HYMN project:

2613.70 - 2615.40
2650.60 - 2651.30
2835.50 - 2835.80
2903.60 - 2904.03
2921.00 - 2921.60

HITRAN 2004

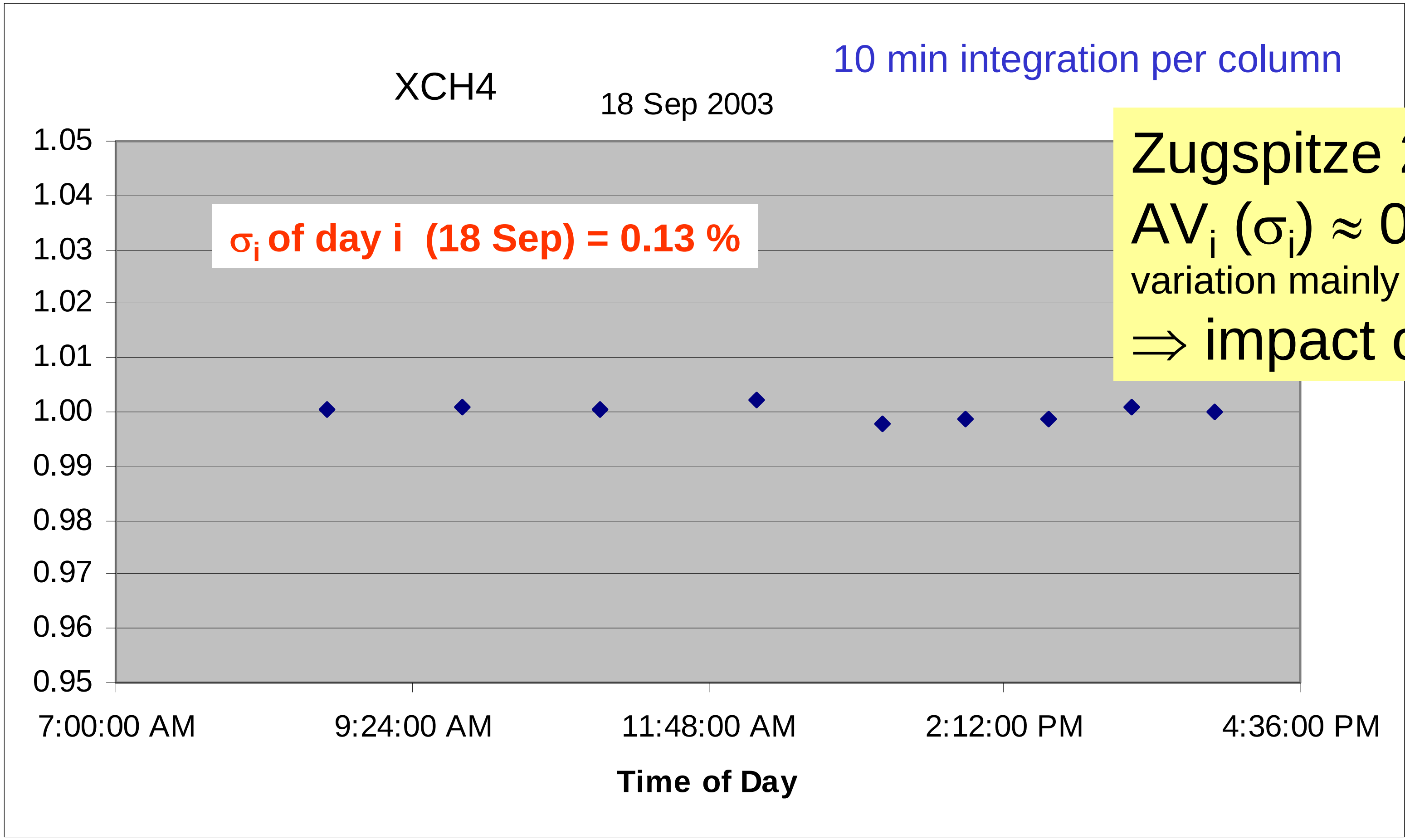
XCH4 calculated via daily local pT-profiles (fasmas)

MIR-FTIR XCH4 precision: Specific questions addressed in this talk

Precision (diurnal variation) of (MIR-)FTIR XCH4 measurements
$\Rightarrow$ impact of regularization scheme used?

Day-to-day variability detected by (MIR-)FTIR XCH4 measurements
$\Rightarrow$ impact of regularization scheme used?

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



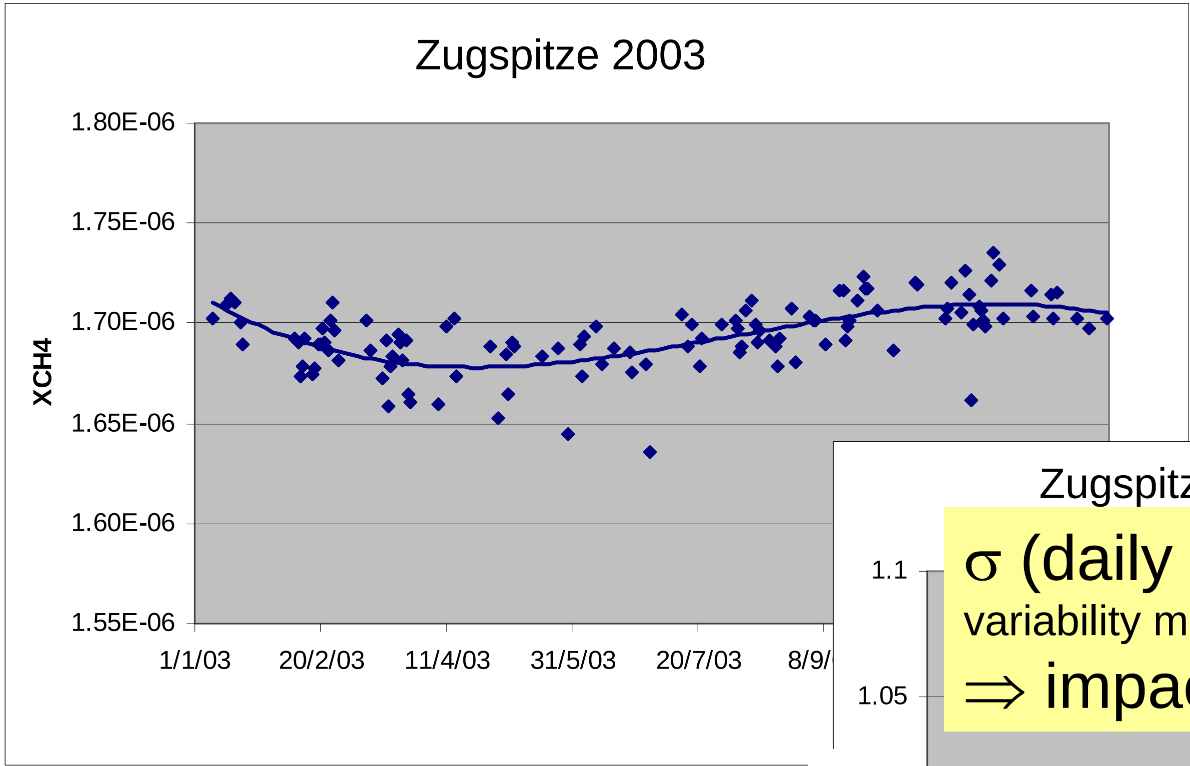
Zugspitze 2003:

AV_i (σ_i) ≈ 0.5 %

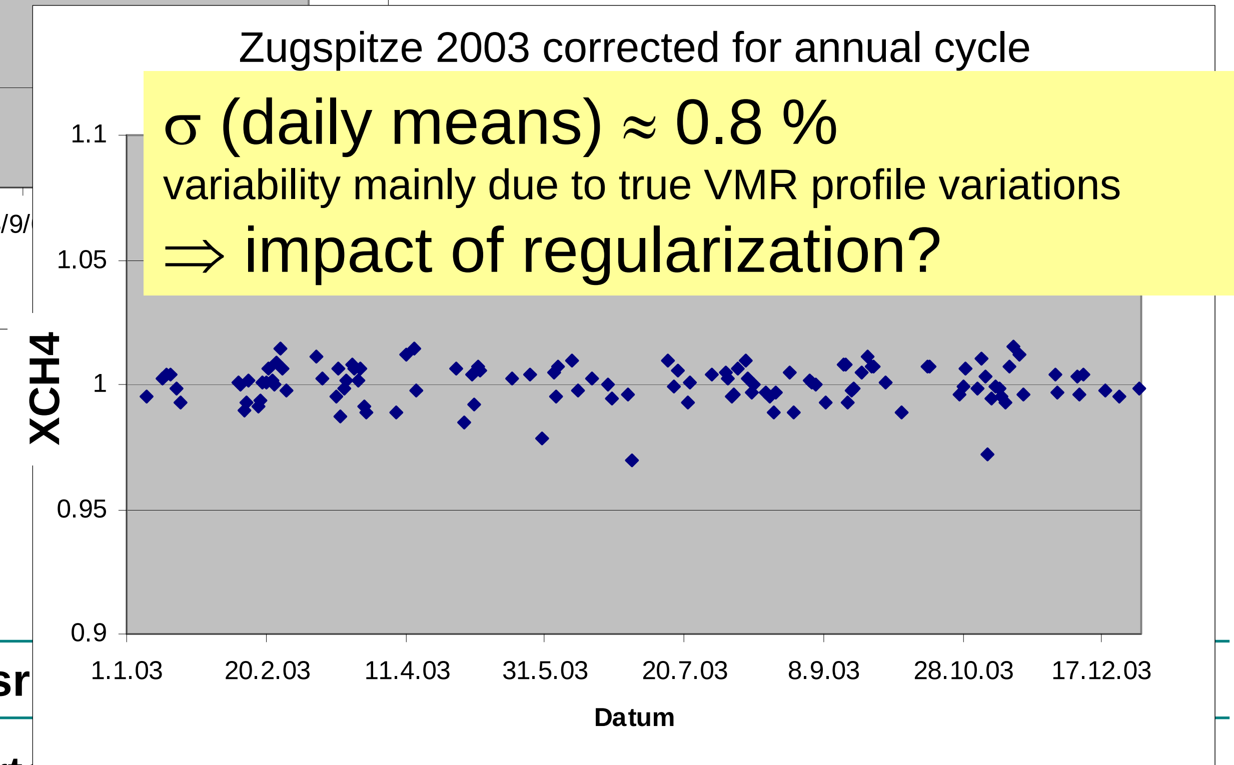
variation mainly due to clouds

⇒ impact of regularization?

MIR-FTIR XCH4 day-to-day variability: impact of regularization?



Zugspitze FTIR 2003
daily means



σ (daily means) ≈ 0.8 %
variability mainly due to true VMR profile variations
⇒ impact of regularization?

• because of CH_4 spectroscopy problems OE (realistic $\mathbf{S}_e$ and climatological $\mathbf{S}_a$, e.g., *dofs* ≈ 3) leads to profile oscillations

• to avoid oscillations stronger regularization is required

• for this purpose, sometimes the (diagonal) variances of an OE $\mathbf{S}_a$ are reduced empirically, but this leads to a significant forcing towards the a priori

• as a consequence, this leads to a significant under-estimation of true columns variability, e.g., for *dofs* ≈ 2 one may find ≈ 50 % under-estimation of day-to-day-variability

Optimize MIR-FTIR XCH4 precision: Tikhonov first derivative regularization L_1

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

with regularization strength α.

Case $\alpha \to \infty$ is a VMR-profile scaling retrieval with *dofs* $\to 1$.
Case $\alpha \to 0$ is a totally unconstrained profile retrieval with *dofs* $\to n$ = number of model layers

We derive an analytic relation between α and *dofs* by putting eq. 1 into eq. 3.28 of Rodgers (2000):

$$dofs = trace(\mathbf{A}) = trace\left((\mathbf{K}_x^T \mathbf{S}_\varepsilon^{-1} \mathbf{K}_x + \alpha\, \mathbf{L}_1^T \mathbf{L}_1)^{-1} \mathbf{K}_x^T \mathbf{S}_\varepsilon^{-1} \mathbf{K}_x\right) \qquad (2)$$

MIR-FTIR XCH4 precision / diurnal variation: why optimize via Tikhonov L_1 ?

• profile scaling (L_1 with $\alpha \rightarrow \infty$, *dofs*≡1) is known to be a good starter for getting reasonable CH_4 columns

• starting from that α can be empirically reduced (*dofs* increased) to allow for some additional flexibility in the profile to account for true profile variations and/or cloud impact on the spectra
$\Rightarrow$ to get even more precise columns than by profile scaling

• whatever the *dofs* (α) is, there is *per definitionem* never any under-estimation of true profile-scaling-type variability using L_1

XCH4 retrieval: as to which quantity optimize L_1 regularization strenght α ?

- „the colleagues use *dofs* = 3, therefore we tune α in a way to achieve *dofs* = 3"

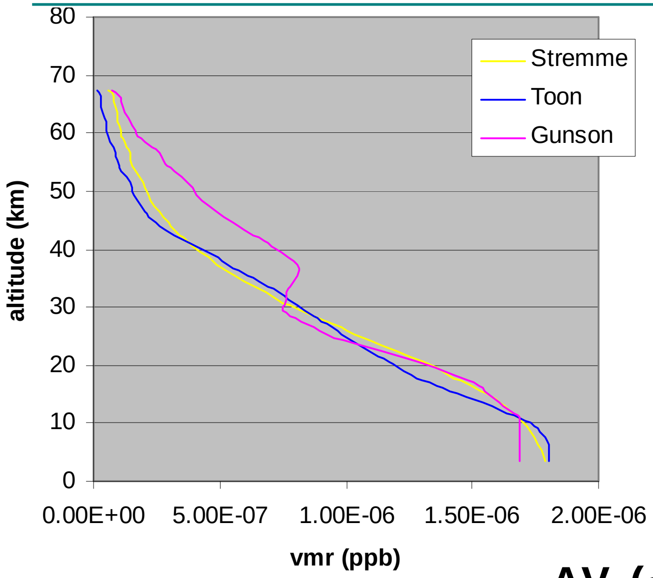
or better:

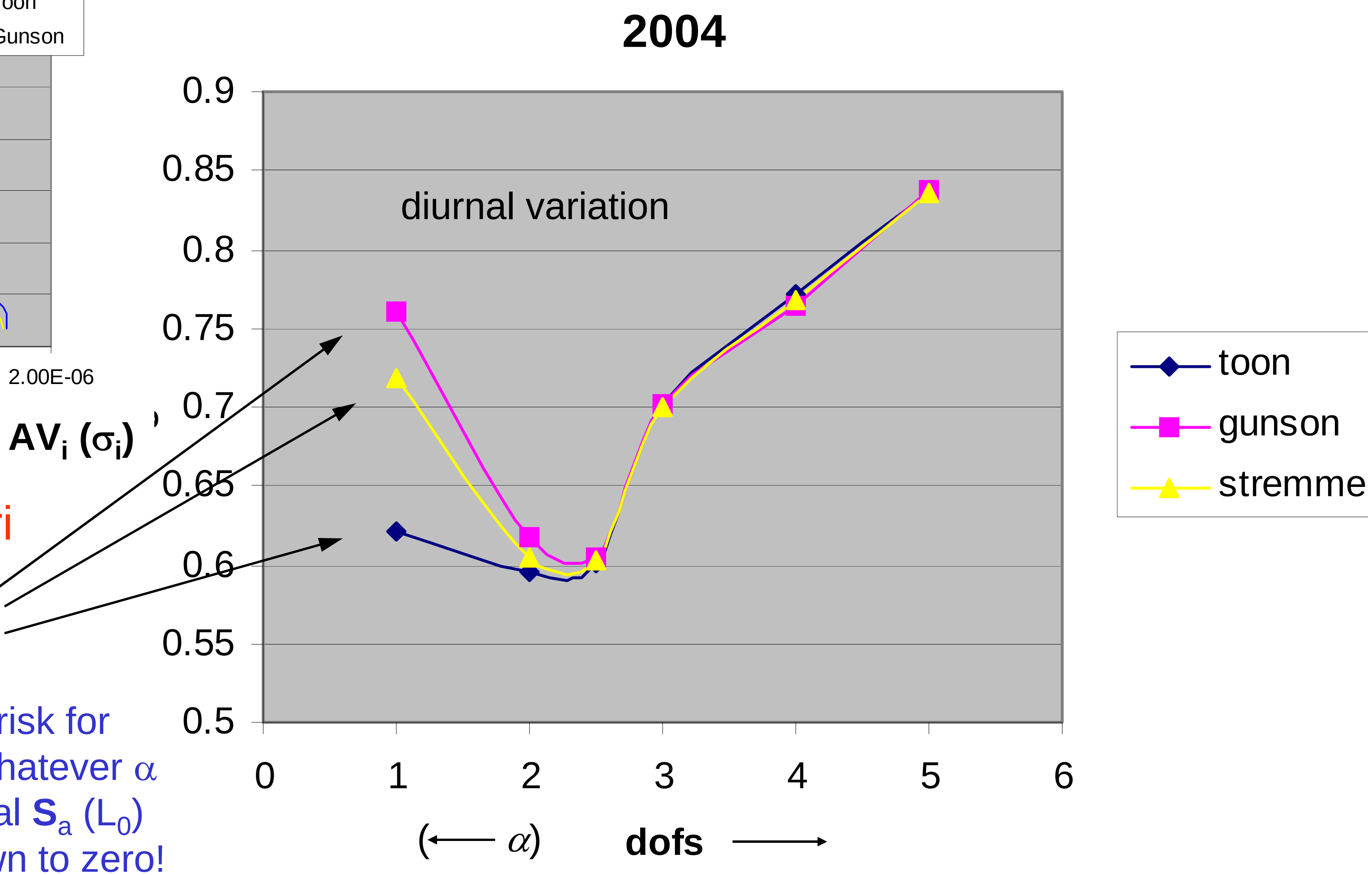
- elbow plot "residual-rms versus α"
- reduce α until first profile oscillations occur
- tune α for optimum trade off between smoothing errors and retrieval noise (Steck, Appl. Opt., 2002)

or (this talk):

- tune α for minimum XCH4 diurnal variation
- tune α for minimum XCH4 day-to-day variability

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

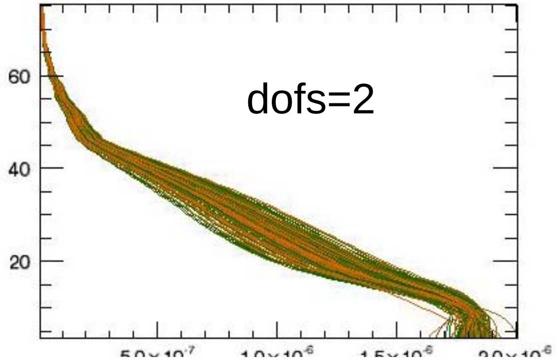


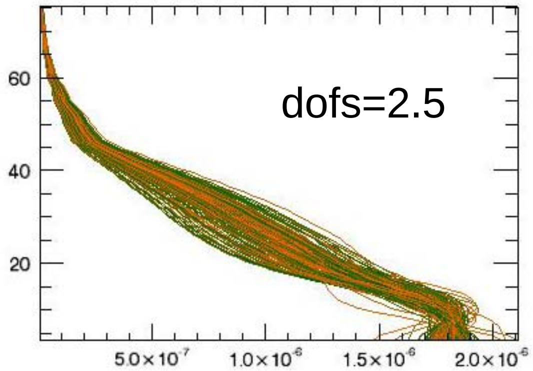


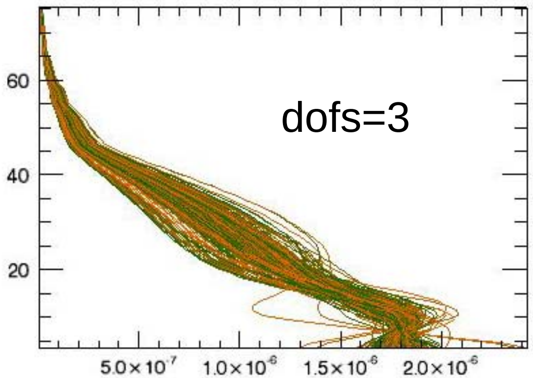
note strong a priori impact for profile scaling (dofs = 1)

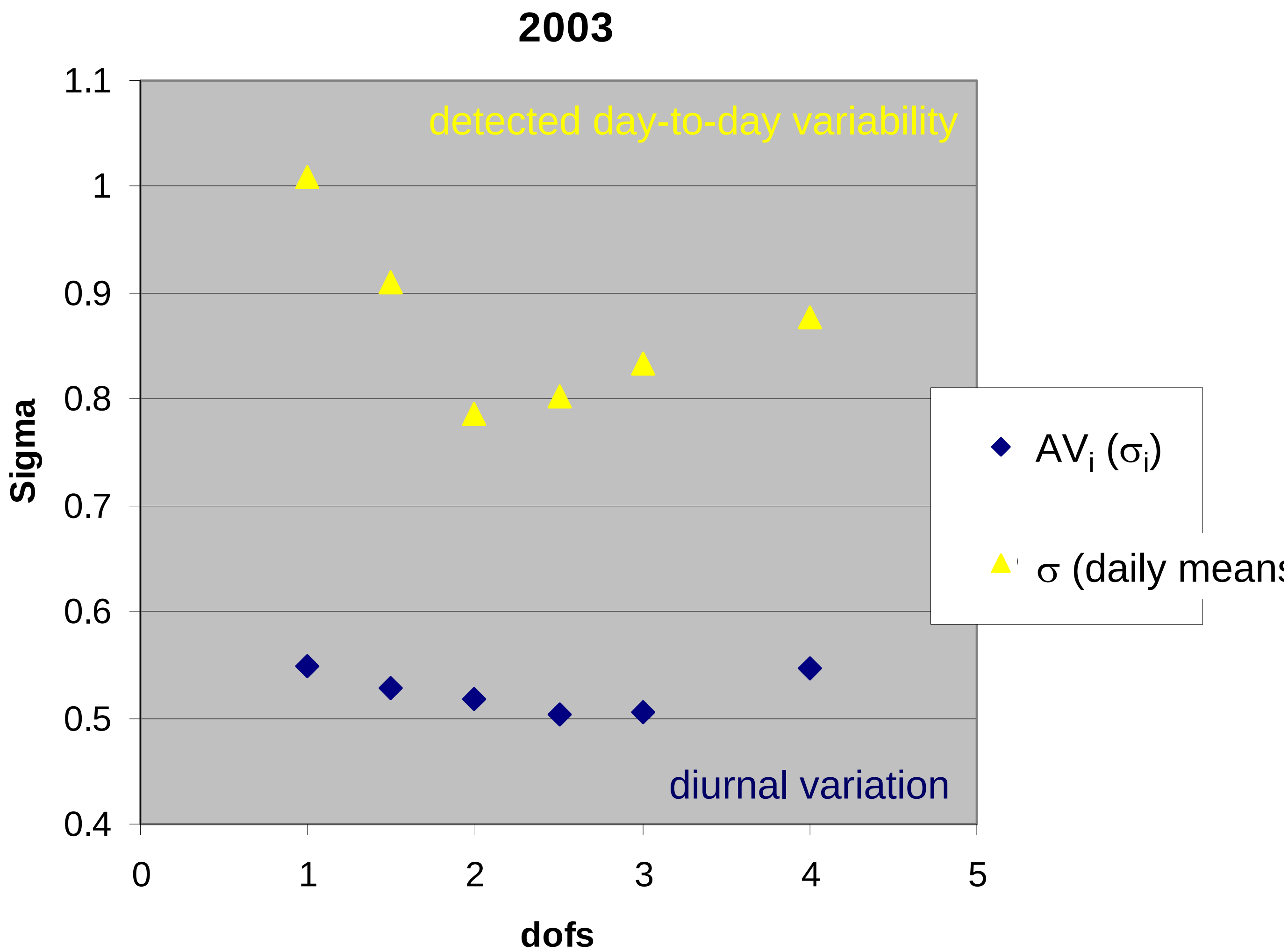
⇒ using L_1 there is no big risk for producing nonsense σ´s whatever α you use; but with a diagonal $\mathbf{S}_a$ (L_0) you could produce σ´s down to zero!

Minimize: diurnal variation, detected day-to-day variability, and profile ozillations

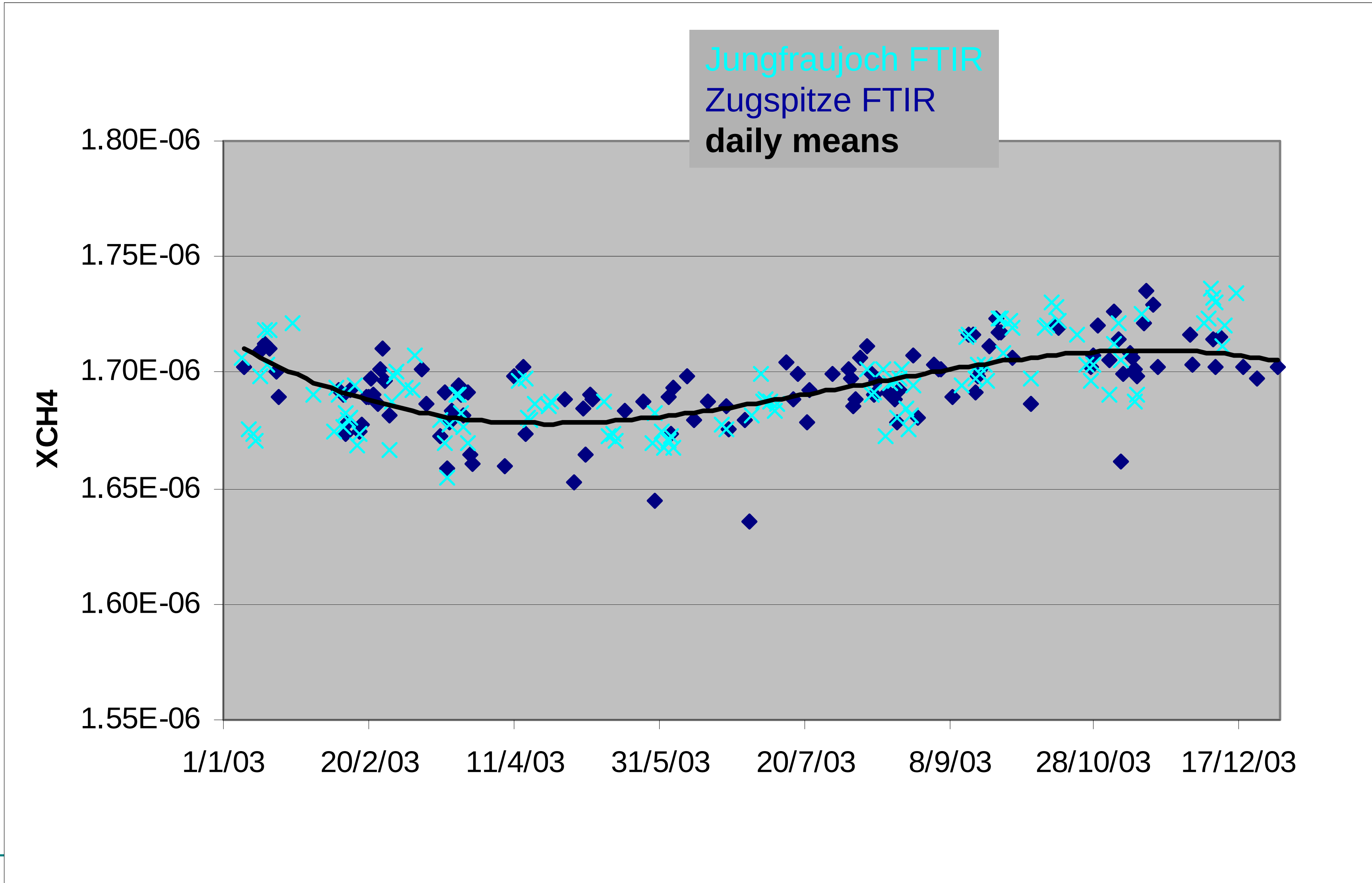




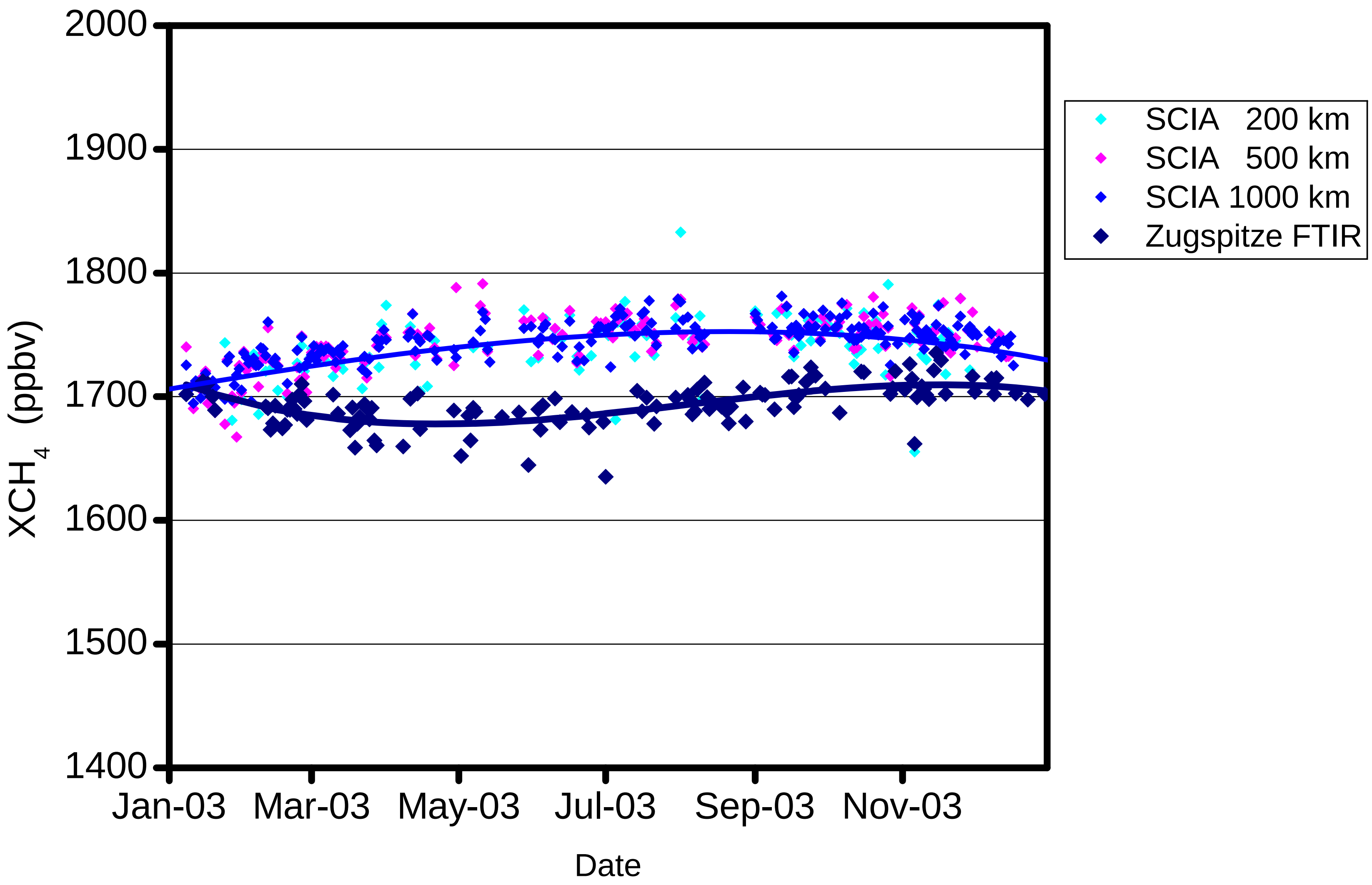




XCH4 daily means: Zugspitze versus Jungfraujoch

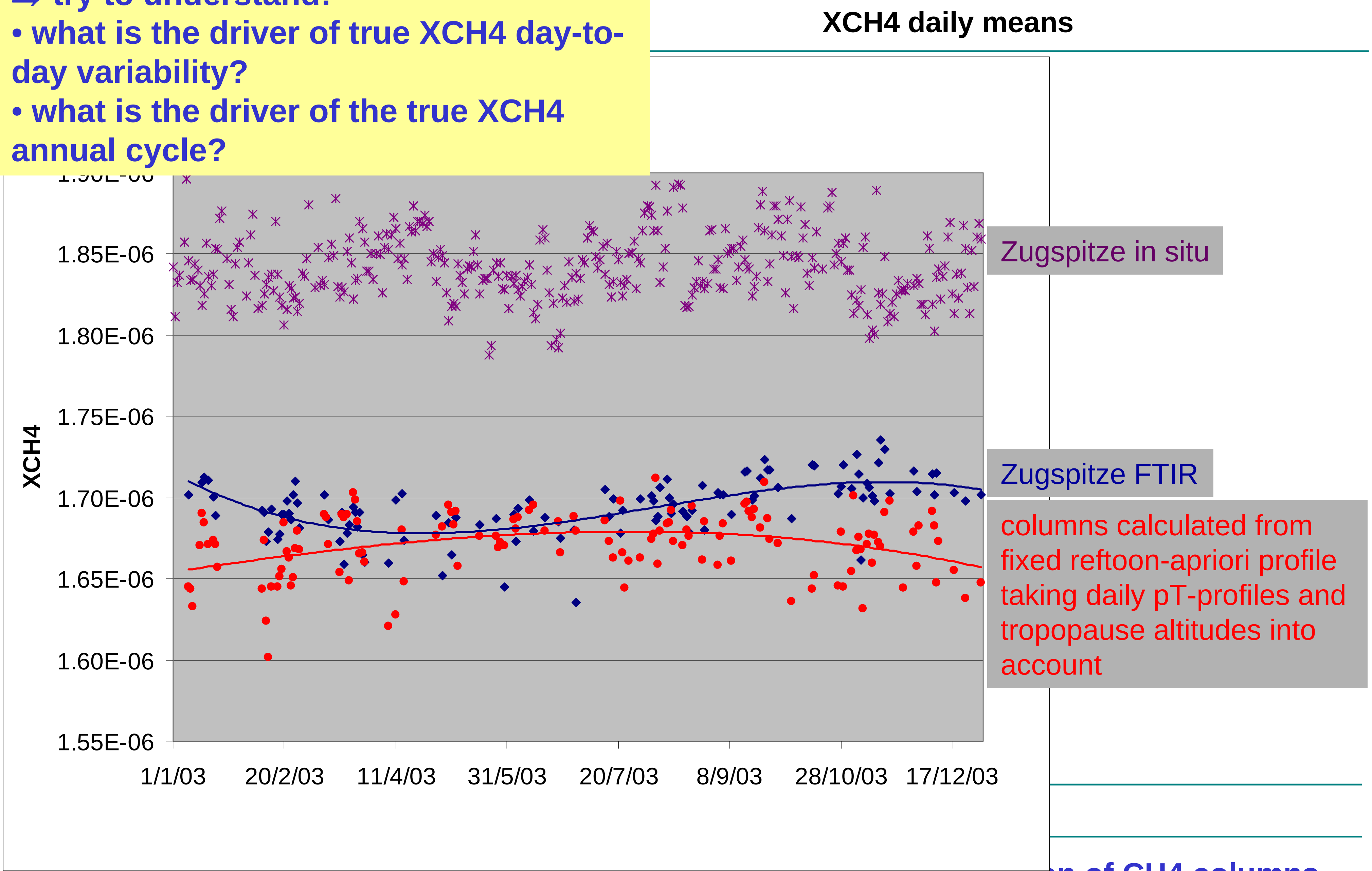


XCH4 daily means: Zugspitze FTIR versus SCIA



⇒ **try to understand:**

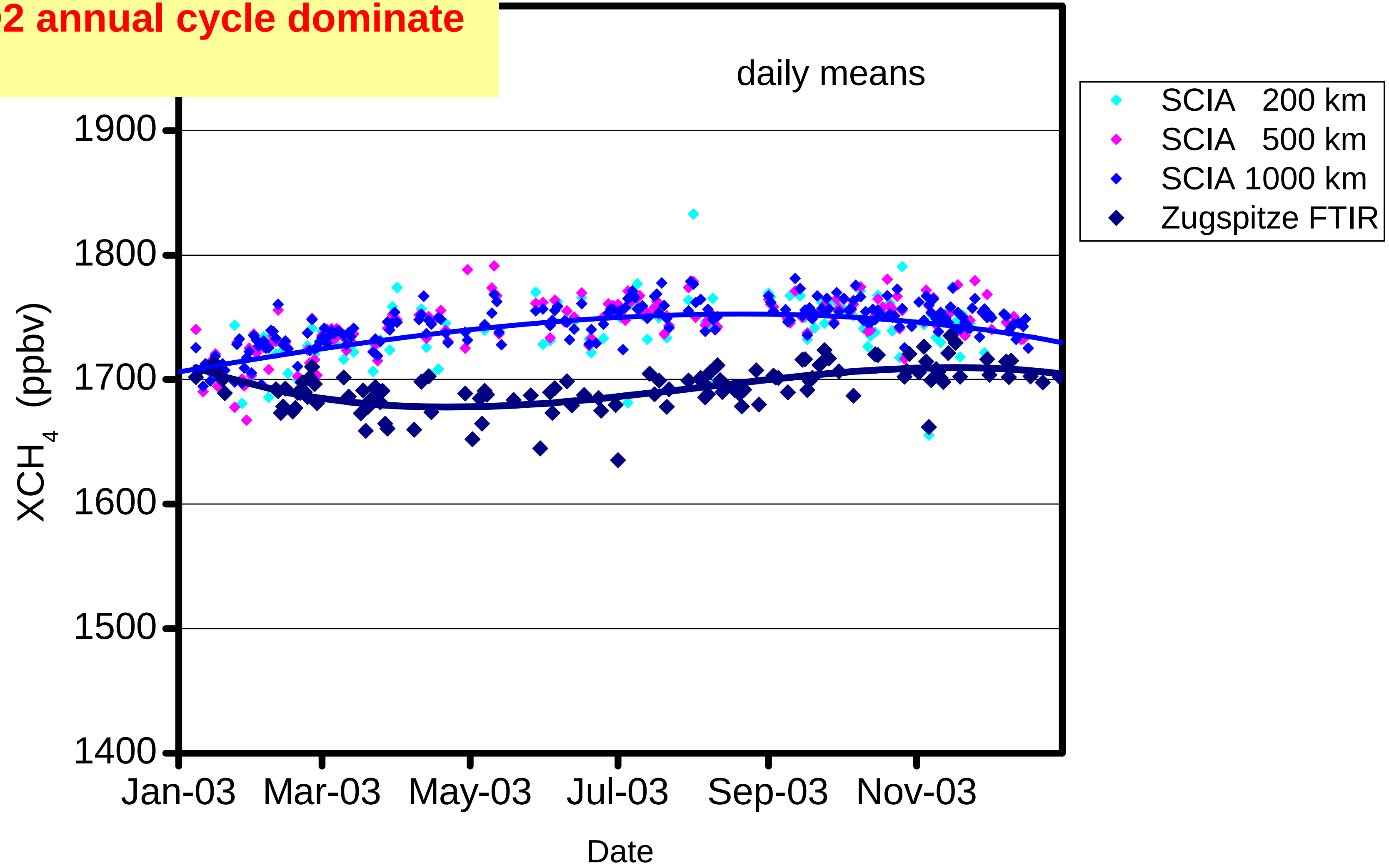
- **what is the driver of true XCH4 day-to-day variability?**
- **what is the driver of the true XCH4 annual cycle?**



⇒ **Riddle: do we (FTIR) have a zenith angle problem with XCH4?**

or does the CO2 annual cycle dominate SCIA XCH4?

XCH4 Zugspitze FTIR versus SCIA



Summary and conclusions

• since there are problems with CH_4 spectroscopy, often stronger regularization is applied to avoid profile oscillations ($\Rightarrow$ lower *dofs* than OE-derived *dofs*)

• in this case classical OE-based regularization leads to a forcing towards a priori and thereby significant under estimation of true colmns variability (e.g., day-to-day variability)

• this can be avoided by using a Tikhonov L_1 (or related) regularization scheme

• in tuning L_1 regularization stength, there is both a minimum in diurnal variation and day-to-day variability around *dofs* $\approx$2-3

• this regularization setting is assumed to yield the best measure for true day-to-day variability

• there is a riddle as to the phase of the annual cycle of XCH_4 derived from MIR-FTIR versus ENVISAT/SCIAMACHY we are currently investigating

• the strategy of tuning Tikhonov L_1 to minimum diurnal variation might be tested for NIR retrievals (TCCON) and be applied to future validation of GOSAT XCH_4

Acknowledgments
Christian Frankenberg, Pierre Duchatelet, Emmanuel Mahieu
EC-HYMN project, BMBF/DLR-SATVAL-A project