# Optimized and harmonized FTIR retrieval strategy for $CH_4$ and $N_2O$ columns and profiles

Sussmann, R., Forster, F., Borsdorff, T., De Mazière, M., Vigouroux,C., Blumenstock, T., Duchatelet, P., Hannigan, J., Hase, F., Jones, N., Klyft, J., Mahieu, E., Mellqvist, J., Notholt, J., Petersen, K., Strong, K., Taylor, J.

This talk presents the outcome of the
Work Package "Optimized retrieval strategy for $CH_4$ and $N_2O$"
lead by IMK-IFU within the EC-HYMN project
(update of HYMN deliverable document D4.4, dated Oct 2009, http://...)

The HYMN-applications are:

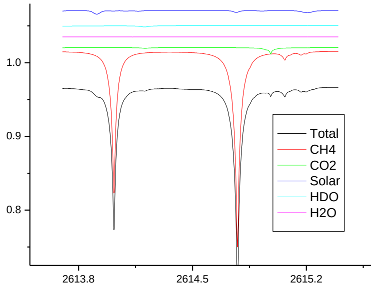
- revised historical time series of CH4 & N2O
- satellite validation
- model validation

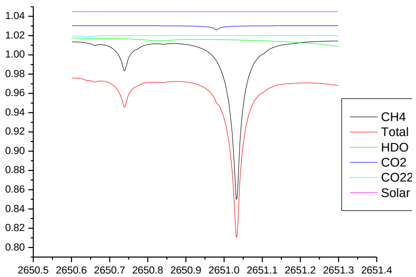
# 13 station participated to the CH4 & N2O harmonization effort

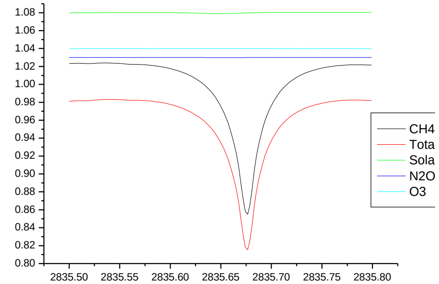
| station | latitude | longitude | station altitude | number of columns in 2003/2004 | tropopause height |
|---|---|---|---|---|---|
| Spitzbergen | 78.92 °N | 11.92 °E | 20 m | 113 | 8.95 km |
| Thule | 76.53 °N | 68.74 °W | 225 m | 177 | 8.51 km |
| Kiruna | 67.84 °N | 20.41 °E | 419 m | 338 | 9.62 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 |
| 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 |
| 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 |

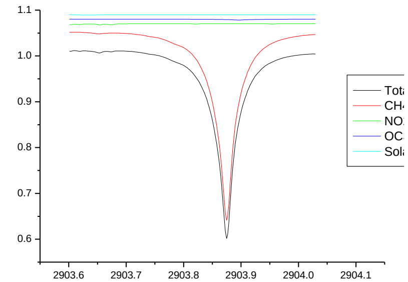
# Retrieval homogenization CH4: status April 2008

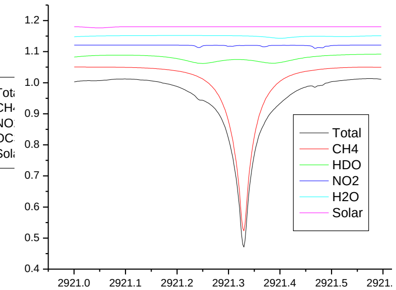
- one common micro-window set (i.e., the "UFTIR set")



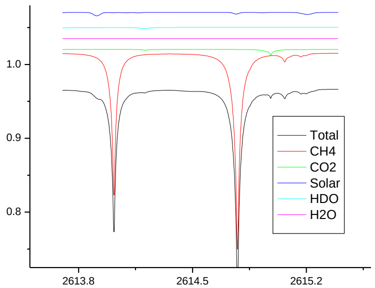



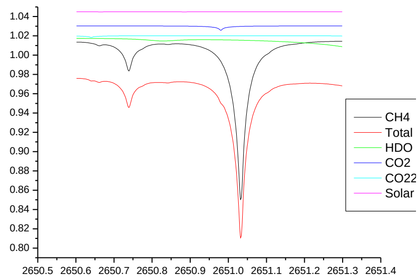


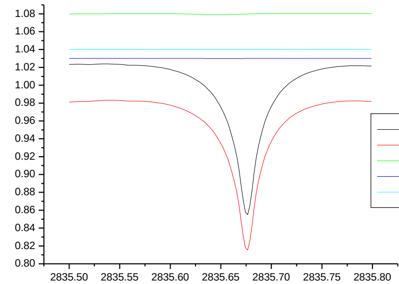

- harmonized treatment of interfering species?
- identical spectroscopic line list for all partners ?
- one common source of pT-input profiles ?
- one consistent set of a priori profiles?
- one consistent set of regularization matrices and altitude grids?

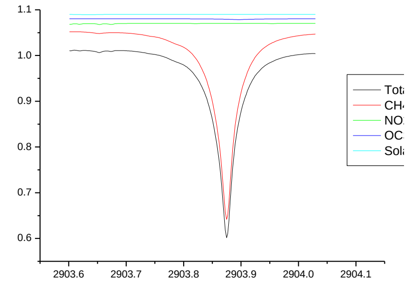
# Retrieval homogenization CH4: status May 2008

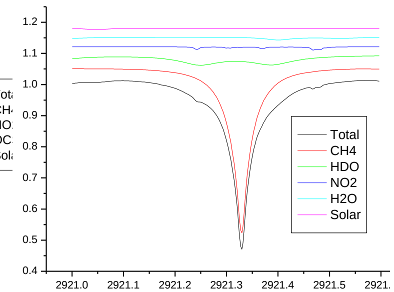
- one common micro-window set: <u>"UFTIR set"</u>






- harmonized treatment of interfering species: joint scaling of

| | | | | |
|---|---|---|---|---|
| CO2, | HDO, CO2 | - | NO2 | H2O, HDO |
| HDO | CO22 | | | NO2 |

⇒ **<u>one set of binput-files distributed</u>**

- identical spectroscopic line list for all partners ?
- one common source of pT-input profiles ?
- one consistent set of a priori profiles?
- one consistent set of regularization matrices and altitude grids?

## Retrieval homogenization CH4: status June 2008

👍 one common micro-window set: “UFTIR set”

👍 harmonized treatment of interfering species: same binput-file

👍 identical spectroscopic line list for all:

- new CH4 lab measurements at Bremen in collab. with IMK-ASF
- Frank Hase retrieved a new set of line-parameters

$\Rightarrow$ **one set of cfgl´s distributed: HITRAN 04 incl. Hase update**

👎 common source of pT-input profiles

👎 one consistent set of a priori profiles?

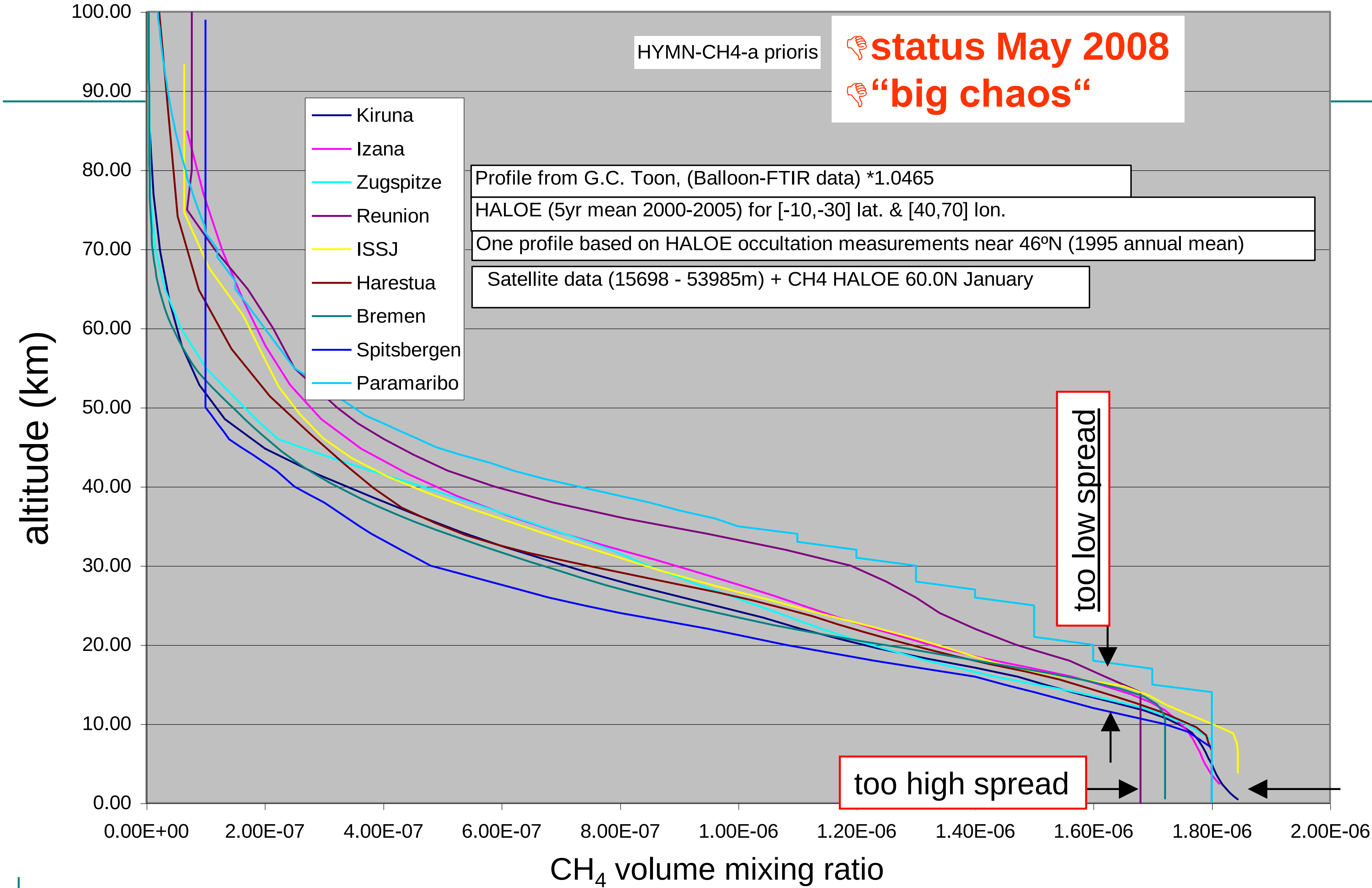
👎 one consistent set of regularization matrices and altitude grids?

## Retrieval homogenization CH4: status June 2008

- 👍 one common micro-window set: "UFTIR set"
- 👍 harmonized treatment of interfering species: same binput-file
- 👍 identical spectroscopy for all: same cfgls (HIT04 & Hase update)

- 👍 common source of pT-input profiles: NCEP

- 👎 one consistent set of a priori profiles?
- 👎 one consistent set of regularization matrices and altitude grids?

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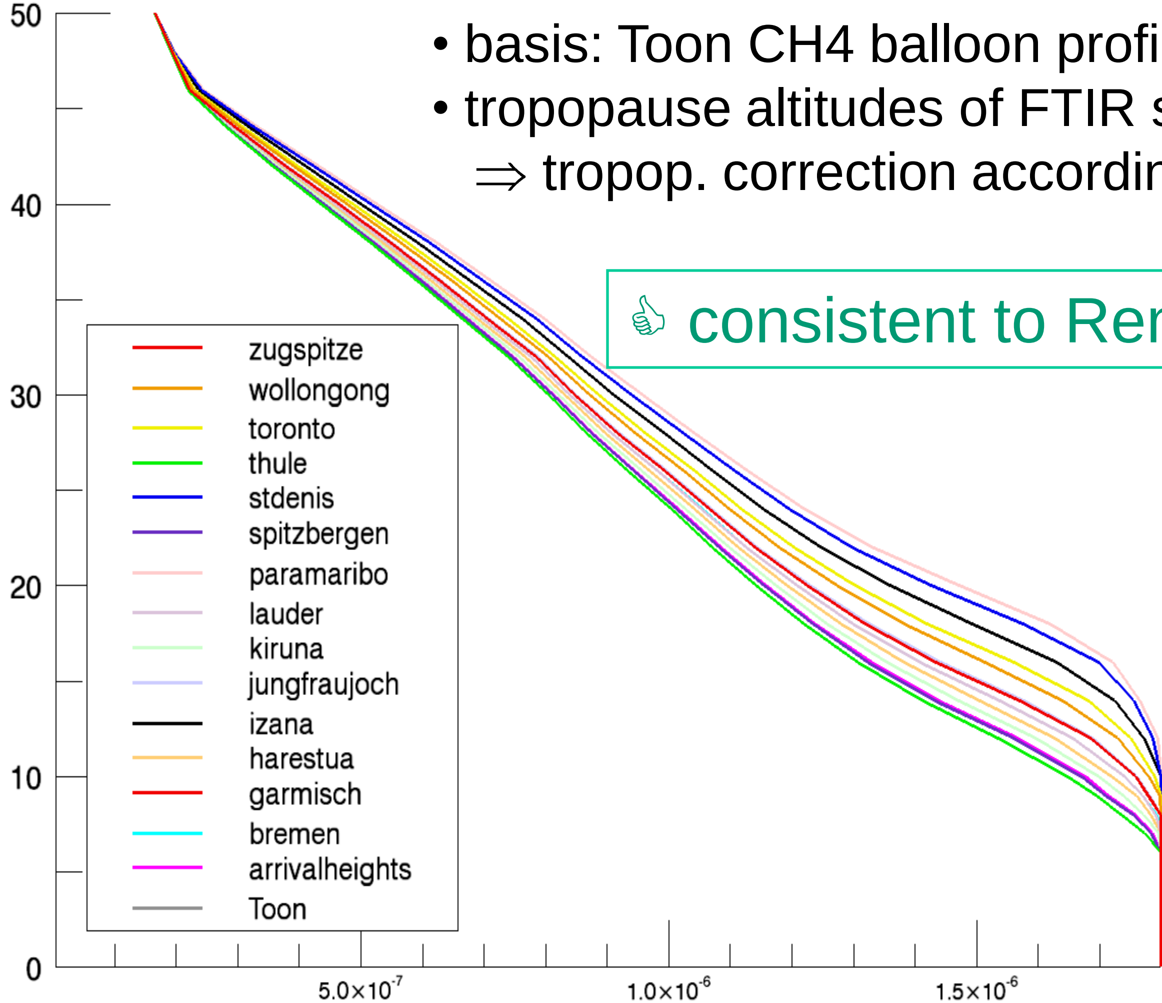
***Ralf Sussman et al.: Retrieval strategy for $CH_4$ and $N_2O$***

# Retrieval homogenization CH4: status June 2008

- basis: Toon CH4 balloon profile
- tropopause altitudes of FTIR sites derived from NCEP

  ⇒ tropop. correction according to A. Meier´s thesis



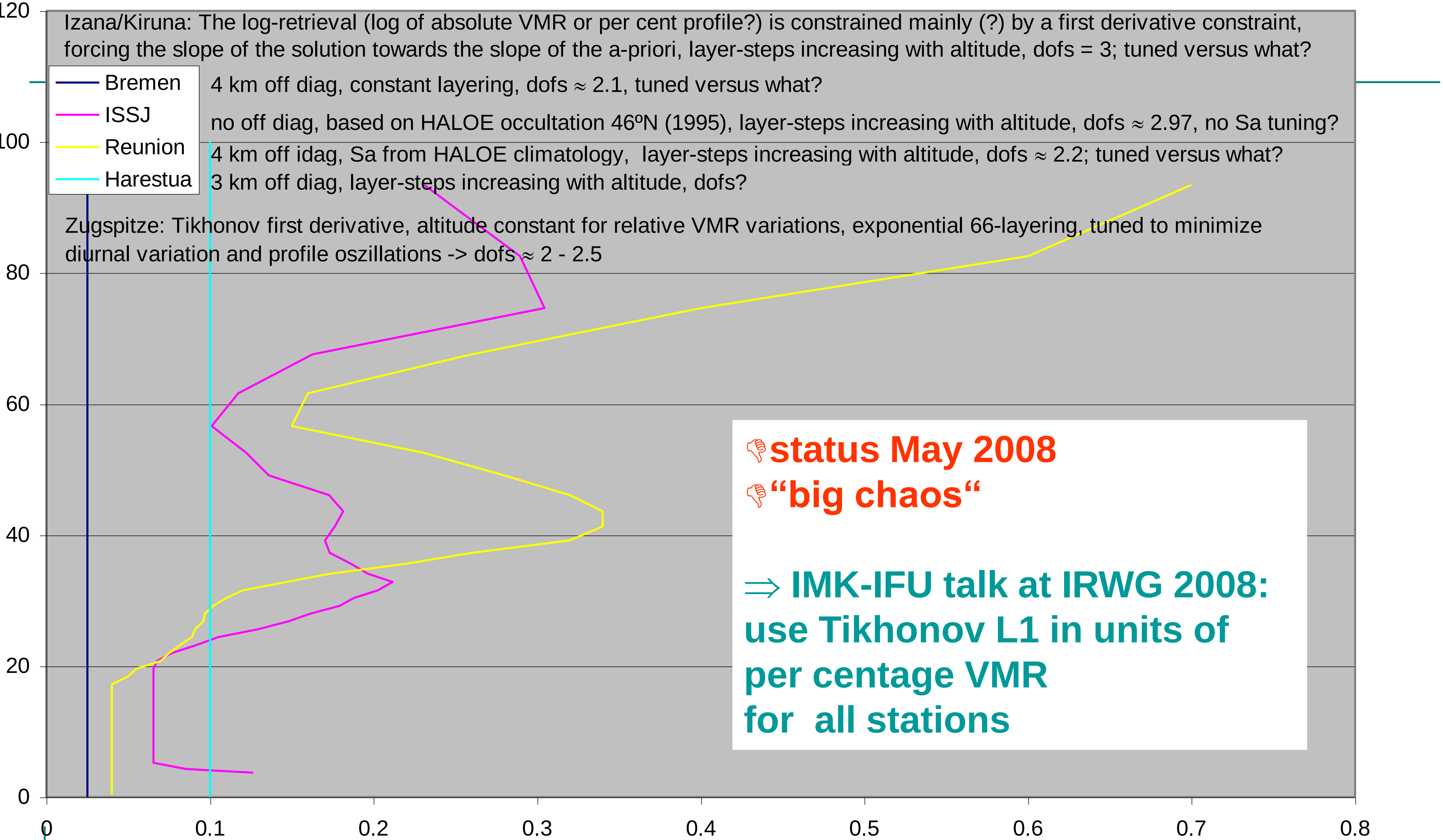

☝ consistent to Remedios climatology

# Retrieval homogenization CH4: status June 2008

- one common micro-window set: “UFTIR set”
- harmonized treatment of interfering species: same binput-file
- identical spectroscopy for all: same cfgls (HIT04 & Hase update)
- common source of pT-input profiles: NCEP
- one consistent set of a priori profiles: Toon with Meier correction

- one consistent set of regularization matrices and altitude grids?

CH4 regularization. Issue: for direct quantitative intecomparison the layering would have to be the same!

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***Ralf Sussman et al.: Retrieval strategy for $CH_4$ and $N_2O$***

# What is Tikhonov Regularization: Definition

$$\mathbf{R} = \mathbf{S}_a^{-1} = \alpha \, \mathbf{L}^T \mathbf{L} \qquad \in \Re^{n \times n}$$

with the Tikhonov regularization operator **L** and the regularization strength $\alpha$.

## What is Tikhonov Regularization: you already know Tikhonov $L_0$ !

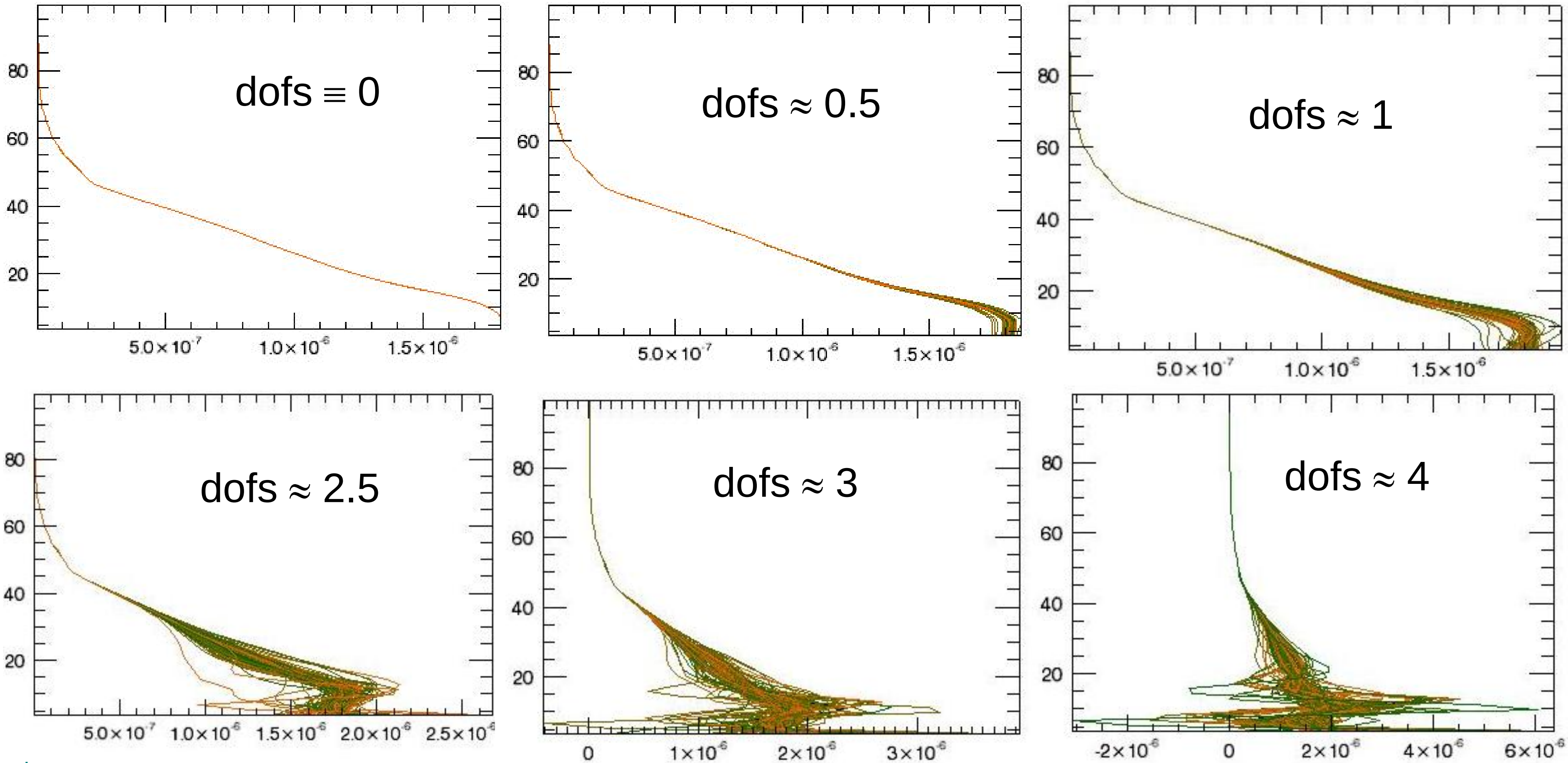
$$\mathbf{R} = \alpha\,\mathbf{L}_0^{\,T}\mathbf{L}_0 = \quad \alpha \times \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & \ddots & \ddots & \vdots \\ 0 & \ddots & 1 & \ddots & 0 \\ \vdots & \ddots & \ddots & 1 & 0 \\ 0 & \cdots & 0 & 0 & 1 \end{pmatrix} \in \Re^{n\times n}$$

In this case R = $S_a$

i.e., **Tikhonov $L_0$ is mathematically identical to a diagonal, altitude constant $S_a$**

- $L_0$ constrains the absolute values of the profile vector
- ⇒ risk that retrieval under-estimates natural columns variability

## FTIR regularization: Traditional diagonal $S_a$ - altitude-constant % VMR variabilities e.g., Rodgers and Connor, JGR, 2003



## What is Tikhonov $L_1$: it constrains the derivative of the profile with resp. to alt.

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

with regularization strength $\alpha$.

Case $\alpha \to \infty$ any change in profile shape totally is forbidden, any altitude constant change fully allowed: *dofs* $\to 1$.
Case $\alpha \to 0$ is a totally unconstrained profile retrieval with *dofs* $\to n$ = number of model layers (oscillations)

**☝ $L_1$ constrains only the profile shape and any altitude constant change is fully allowed** (2)

# What is Tikhonov : have to decide on physical units for profile regularization

Possible profile units:

- absolute VMR (default in PROFFIT)
- per centage VMR (default in SFIT 2)
- log VMR  (option in PROFFIT and, since recently, option in SFIT 2)
- number density
- partial column

Examples for $L_1$:

- regularization in units of absolute VMR favors shifting of VMR profiles to higher/lower VMR´s
- regularization in units of %-VMR favors scaling of VMR profiles
- …

## IMK-IFU pledger: Tikhonov $L_1$ on the %-VMR-scale is probably the most robust standard procedure very well applicable to all species

Arguments

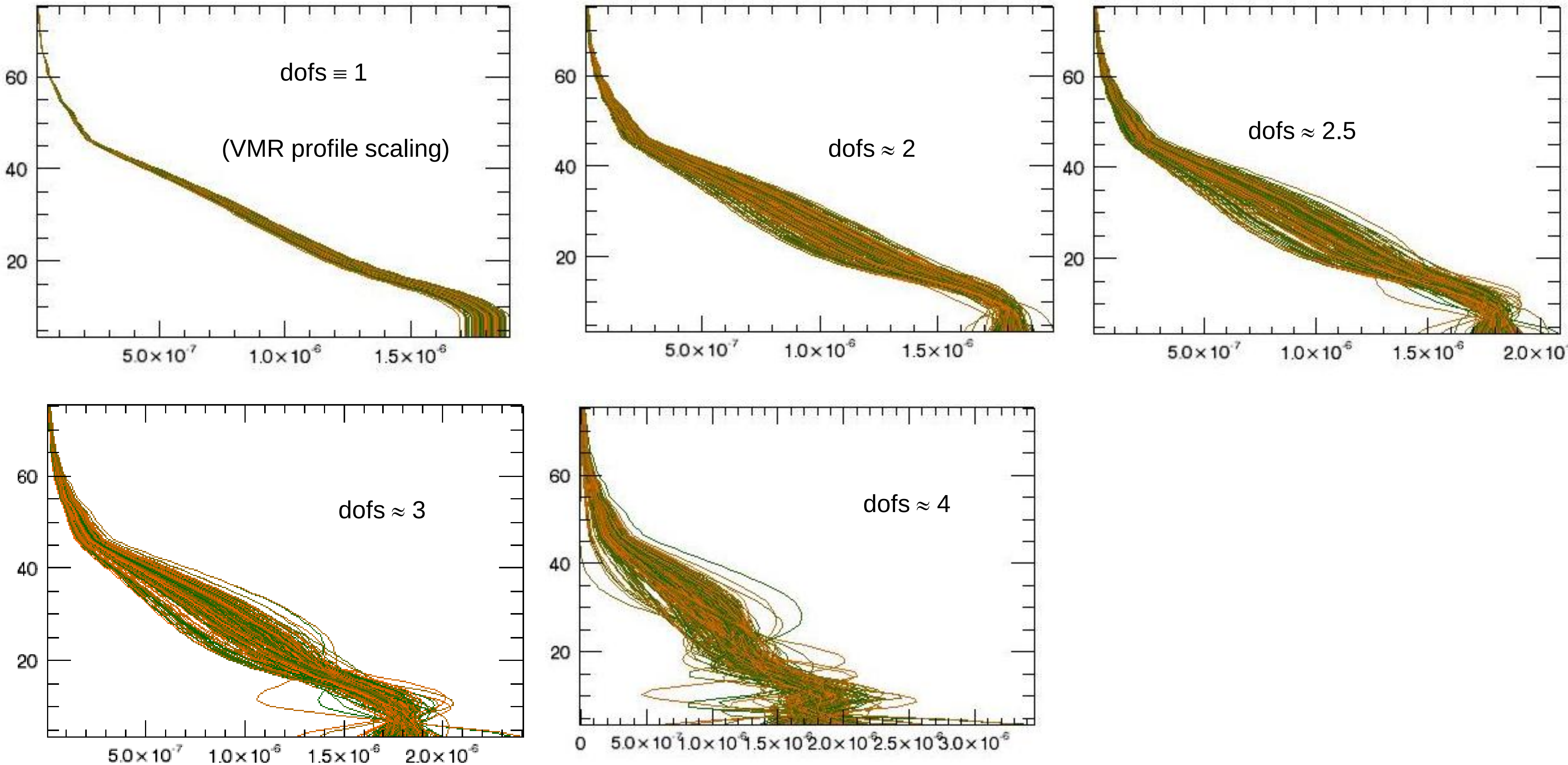
• VMR profile scaling ($L_1$ with $\alpha \rightarrow \infty$, *dofs*≡1) is one of the best-tested retrieval approaches (SFIT 1, WFM-DOAS, …)

• VMR profile scaling is more realistic than VMR profile shifting (i.e., $L_1$ on absolute VMR scale) : avoids neg. VMR´s

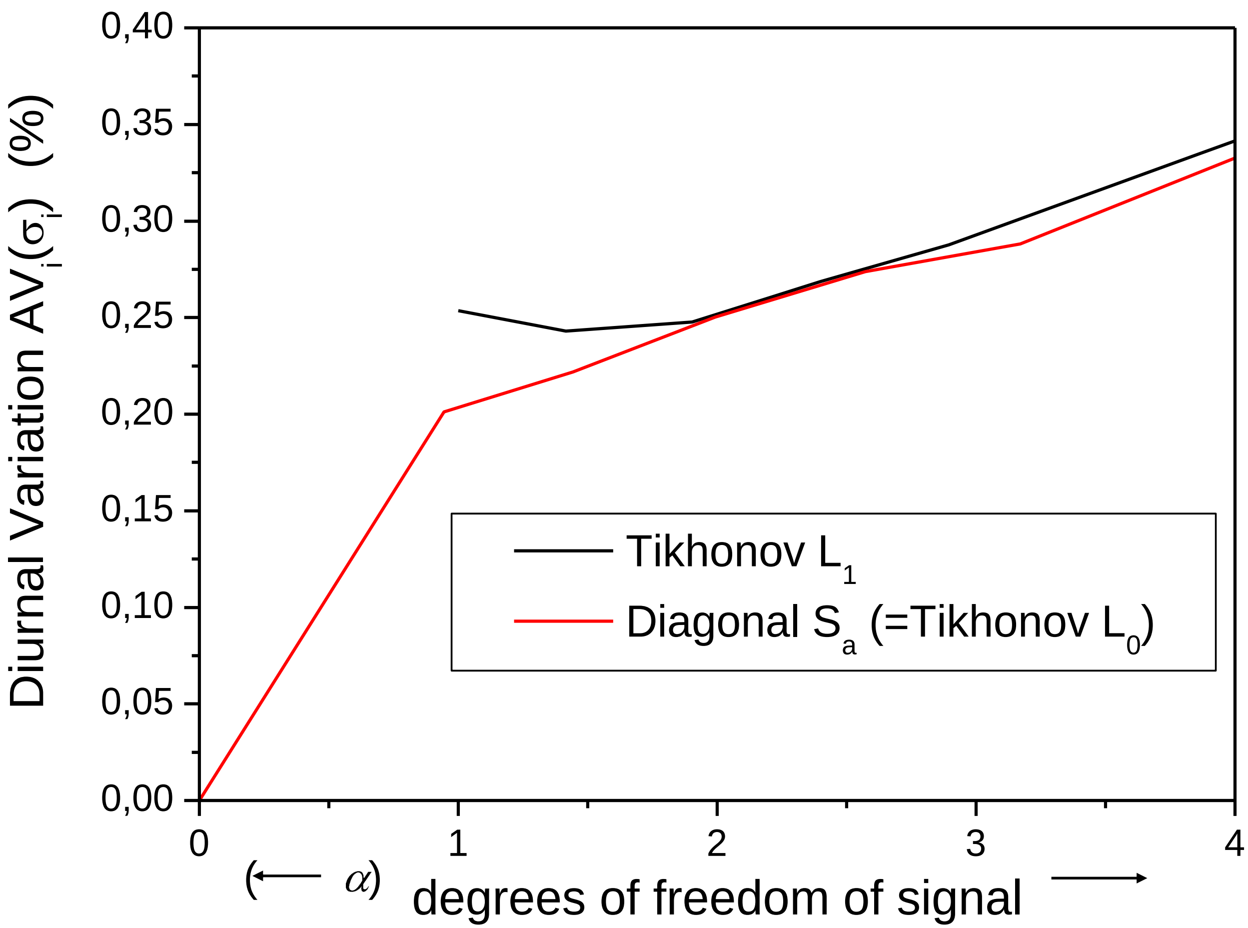
• starting from high $\alpha$ , $\alpha$ can be empirically reduced (*dofs* increased) to allow for some additional flexibility in the profile to account for true profile variations and/or cloud impact on the spectra ⇒ to get even more precise columns than by profile scaling

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

# Tikhonov $L_1$ : how find optimum regularization strenght $\alpha$ ?

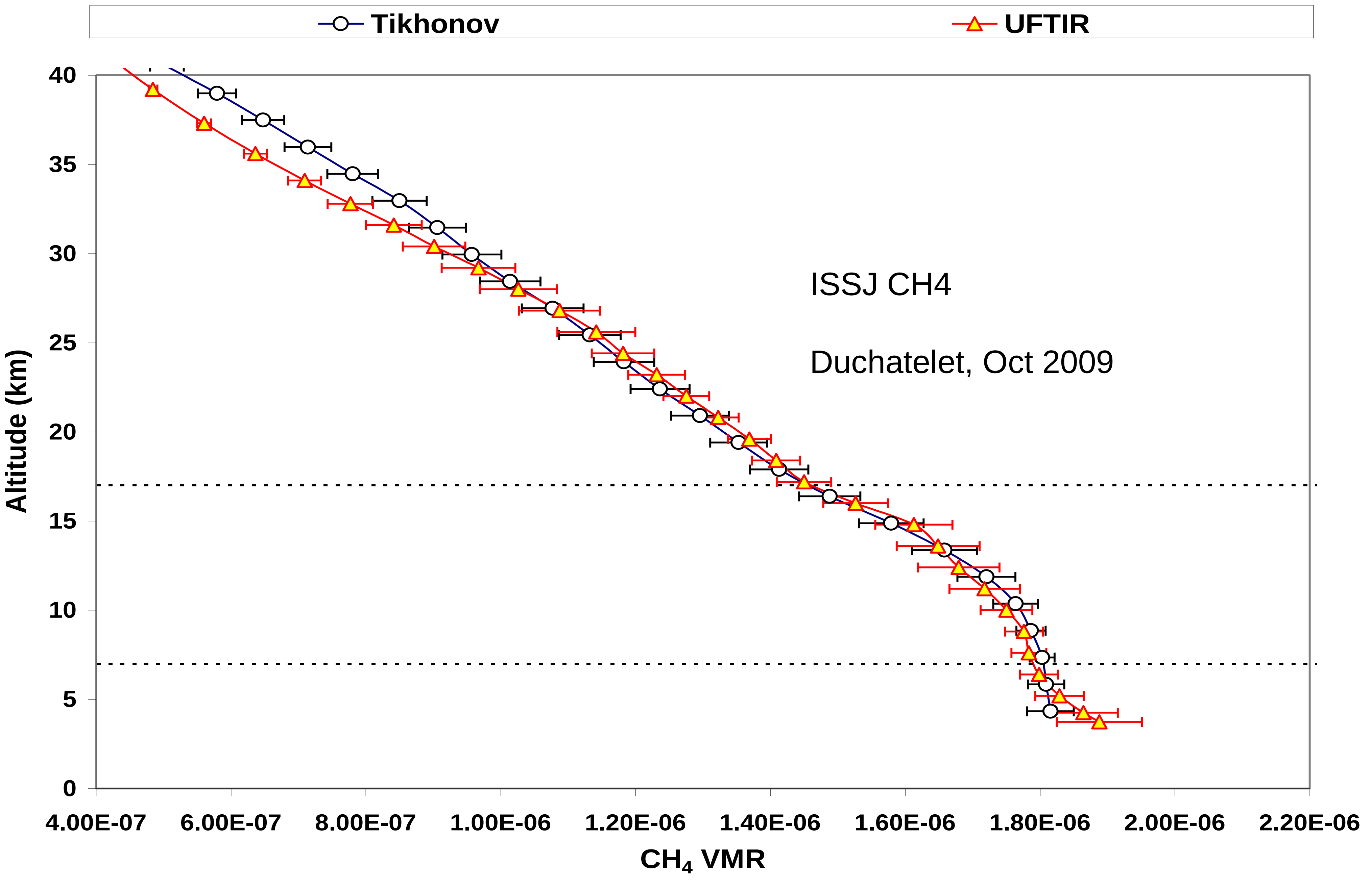


## $L_0$ versus $L_1$: diurnal variation as a function of α (dofs) - $L_1$ more robust




⇒$L_1$ is robust even for low dofs

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



Tikhonov
UFTIR
ISSJ CH4
Duchatelet, Oct 2009
Altitude (km)
0
5
10
15
20
25
30
35
40
4.00E-07
6.00E-07
8.00E-07
1.00E-06
1.20E-06
1.40E-06
1.60E-06
1.80E-06
2.00E-06
2.20E-06
$CH_4$ VMR

# Tikhonov vs UFTIR: main facts

| | Tikhonov | UFTIR |
|---|---|---|
| **Mean DOFS** | 2.73 | 3.03 |
| **Residuals** | No significant difference | |
| **$CH_4$ Tot Col** | No significant difference | |
| **$CH_4$ VMR** | No oscillations | Still oscillates |
| **$CH_4$ Part Col** | ~10% bias | |

**Values obtained for one year of observations @ Jungfraujoch (~300 spectra)**

Had to decide at Garmisch HYMN meeting in Oct 2009 how to proceed:

a) all use same Tikhonov-Regularization ("%-VMR-L1") & äquidistant altitude grid (IMK-IFU)

versus

b) freedom in regularization matrices & grids ("UFTIR strategy", BIRA)

Decided for HYMN (CH4 & N2O):

obligatory use of Tikhonov ("%-VMR-$L_1$") but freedom in regularization strength and altitude grid

## So, finally, a word about altitude grids has become necessary…: Status Nov 2008

Tikhonov matrices shown in this talk were for altitude-constant grid only.

“Freedom“ in layering means:

- we had to recalculate the Tikhonov matrices for each group individually

*coded by Frank Hase*

```
do i = 1,nl - 2
    Bmat(i,i) = 1.0d0
    Bmat(i,i+1) = -1.0d0
end do
! Setup matrix D
Dmat = 0.0d0
do i = 1,nl - 1
    Dmat(i,i) = 1.0d0 / ((altvec(i+1) - altvec(i)) * (altvec(i+1) - altvec(i)))
end do
! Calculate BT * D * B
```

L1 operator (annotating the Bmat lines)

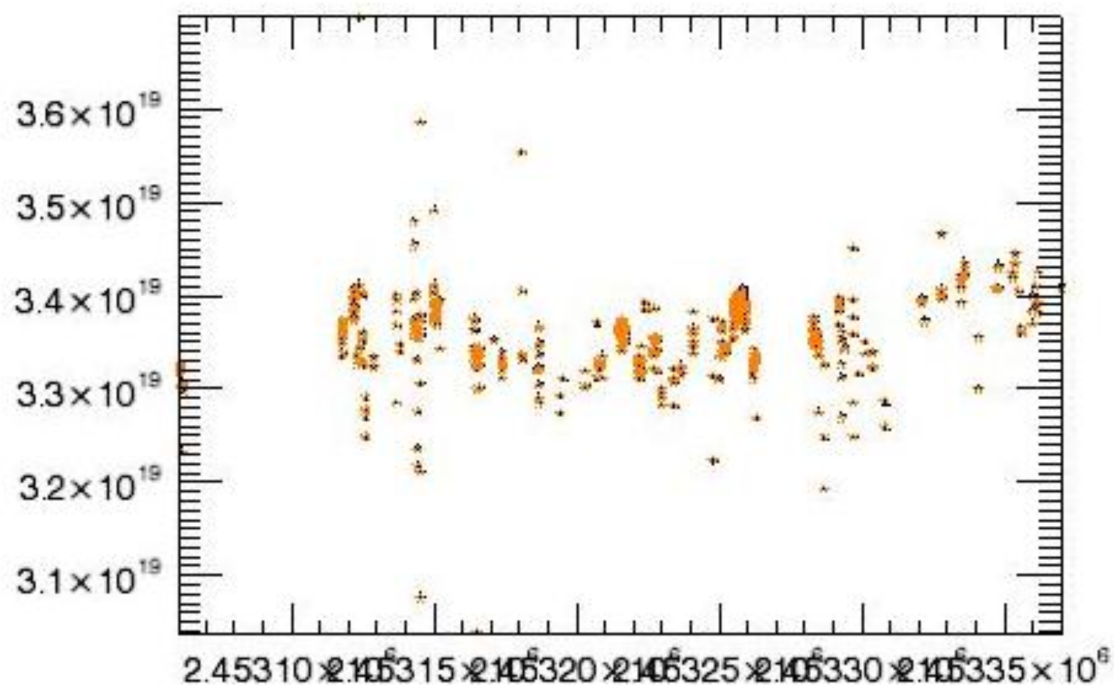
transfer matrix “square root of layer thickness“ (annotating the Dmat(i,i) line)

- elegant and simple altitude-constant formulation of Tikhonov matrices got lost

# So, finally, a word about altitude grids has become necessary…: Status Nov 2008

- it is possible with sufficient accuracy:

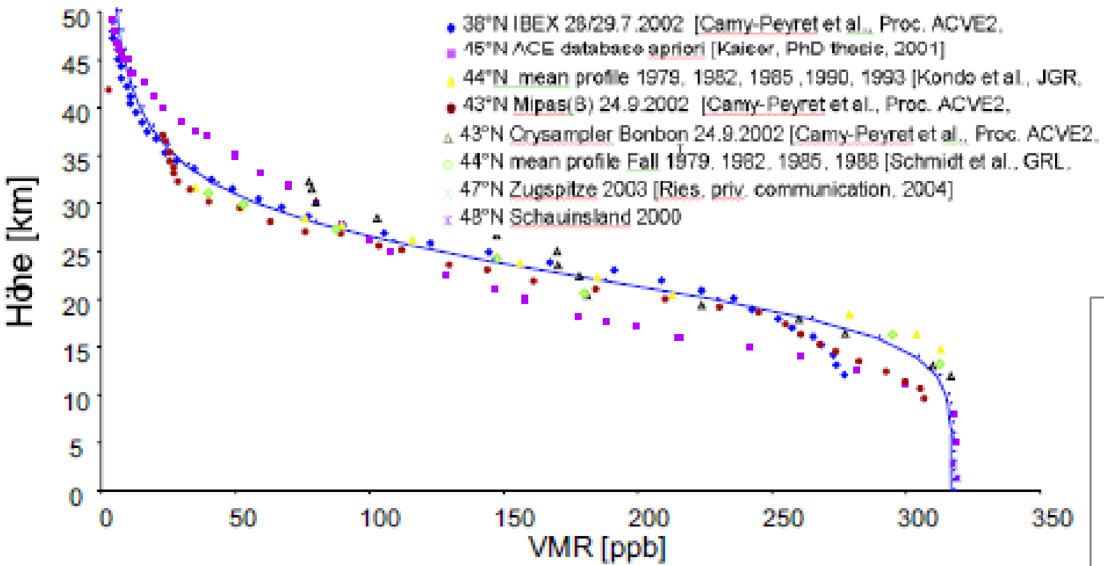
Zugspitze 2004 columns differ only by 0.02 % between an equidistant and an exponential layering – after recalculation of the L1 matrix



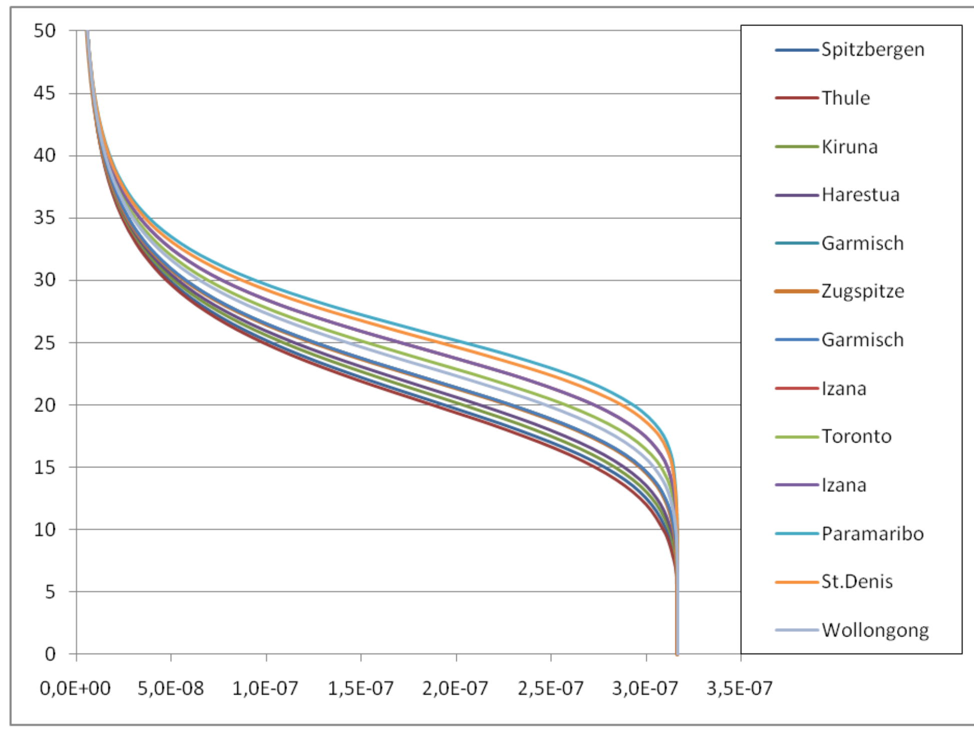
# Retrieval homogenization N2O: microwindows and fitted interf. species

```
2481.3000 2482.6000    4   0.00    0    0      IP
    N2O       0 9500
    CH4       0 9500
    CO2       0 9500
    H2O       0 9500
 2526.4000 2528.2000    3   0.00    0    0      IP
    N2O       0 9500
    CO2       0 9500
    CH4       0 9500
 2537.8500 2538.8000    3   0.00    0    0      IP
    N2O       0 9500
    HDO       0 9500
    CH4       0 9500
 2540.1000 2540.6000    1   0.00    0    0      IP
    N2O       0 9500
```

# Retrieval homogenization N2O: prior




## Same Tikhonov $L_1$ (%-VMR scale) as for CH4




- basis: Stremme mid-lat. N2O profile
- tropopause altitudes of FTIR sites derived from NCEP

  ⇒ tropop. correction according to A. Meier´s thesis

# $CH_4$ & $N_2O$ retrieval strategy: some reference

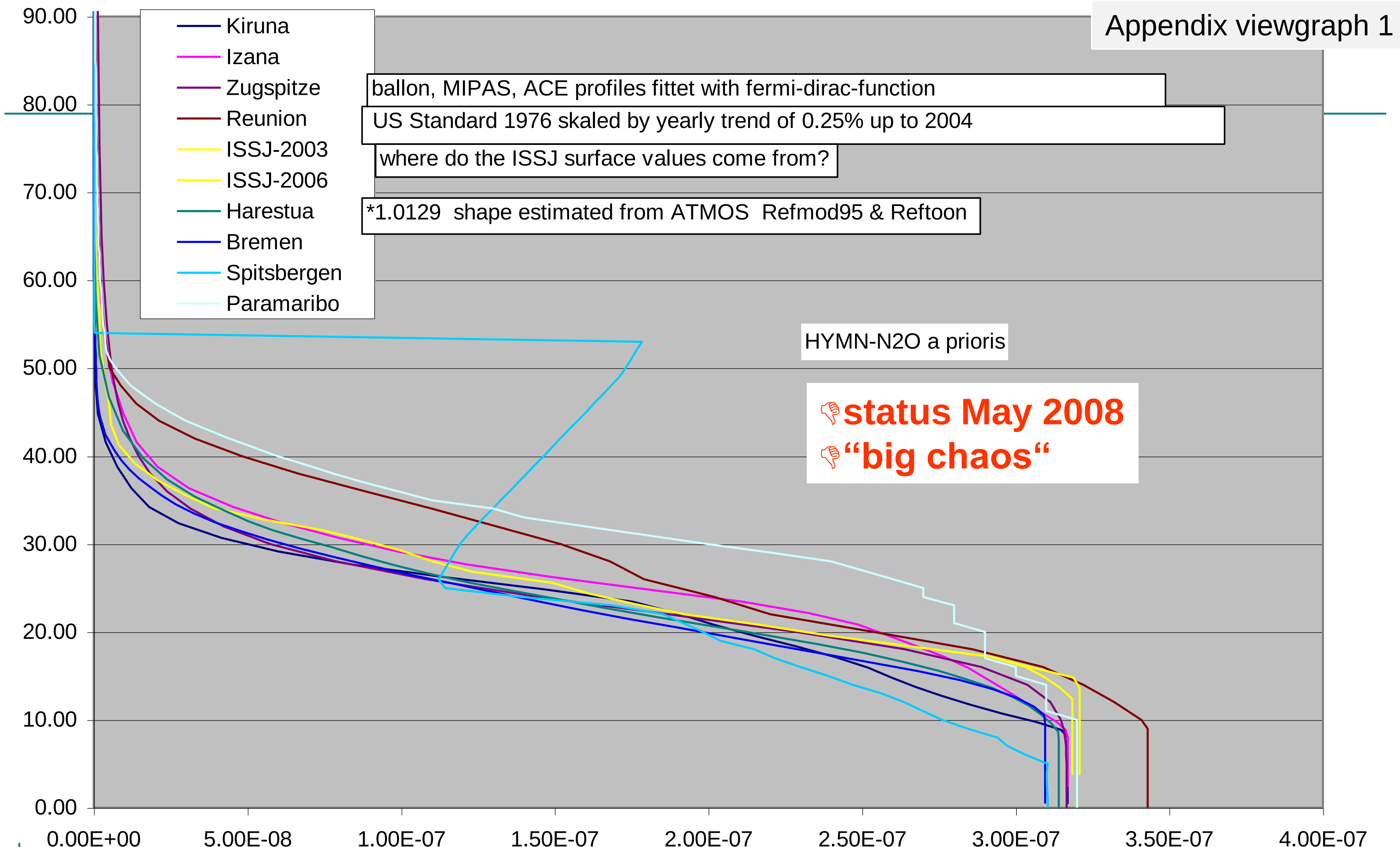
Description of strategy:

Sussmann et al., D4.4 document on HYMN retrieval strategy: http:\\... type “HYMN” to google

Sussmann, R., F. Forster, T. Borsdorff, B. Dils, M. De Mazière, C. Vigouroux, T. Blumenstock, M. Buchwitz,J.P. Burrows, P. Duchatelet, C. Frankenberg, J. Hannigan, F. Hase, N. Jones, J.Klyft, E. Mahieu, J. Mellqvist, J. Notholt, K. Petersen, O. Schneising, K. Strong, J. Taylor: A novel Tikhonov-based approach for harmonized high-accuracy retrieval of methane columns and profiles from NDACC FTIR network measurements. Application to global validation of ENVISAT/SCIAMACHY biases, Geophysical Research Abstracts, Vol. 11, EGU2009-7869-2, 2009, http://meetingorganizer.copernicus.org/EGU2009/EGU2009-7869-2.pdf, EGU General Assembly 2009 (Talk).

Why we did that effort:

Sussmann., R., Forster, F., Borsdorff, T., Dils, B., De Mazière, M., Vigouroux, C., Blumenstock, T., Buchwitz, M., Burrows, J.P., Duchatelet, P., Frankenberg, C., Hannigan, J., Hase, F., Jones, N., Klyft, J., Mahieu, E., Mellqvist, J., Notholt, J., Petersen, K., Schneising, O., Strong, K., Taylor, J.: Satellite validation of column-averaged methane on global scale: ground-based data from 13 FTIR stations versus last generation ENVISAT/SCHIAMACHY retrievals,
ACP or AMT in preparation 2009.

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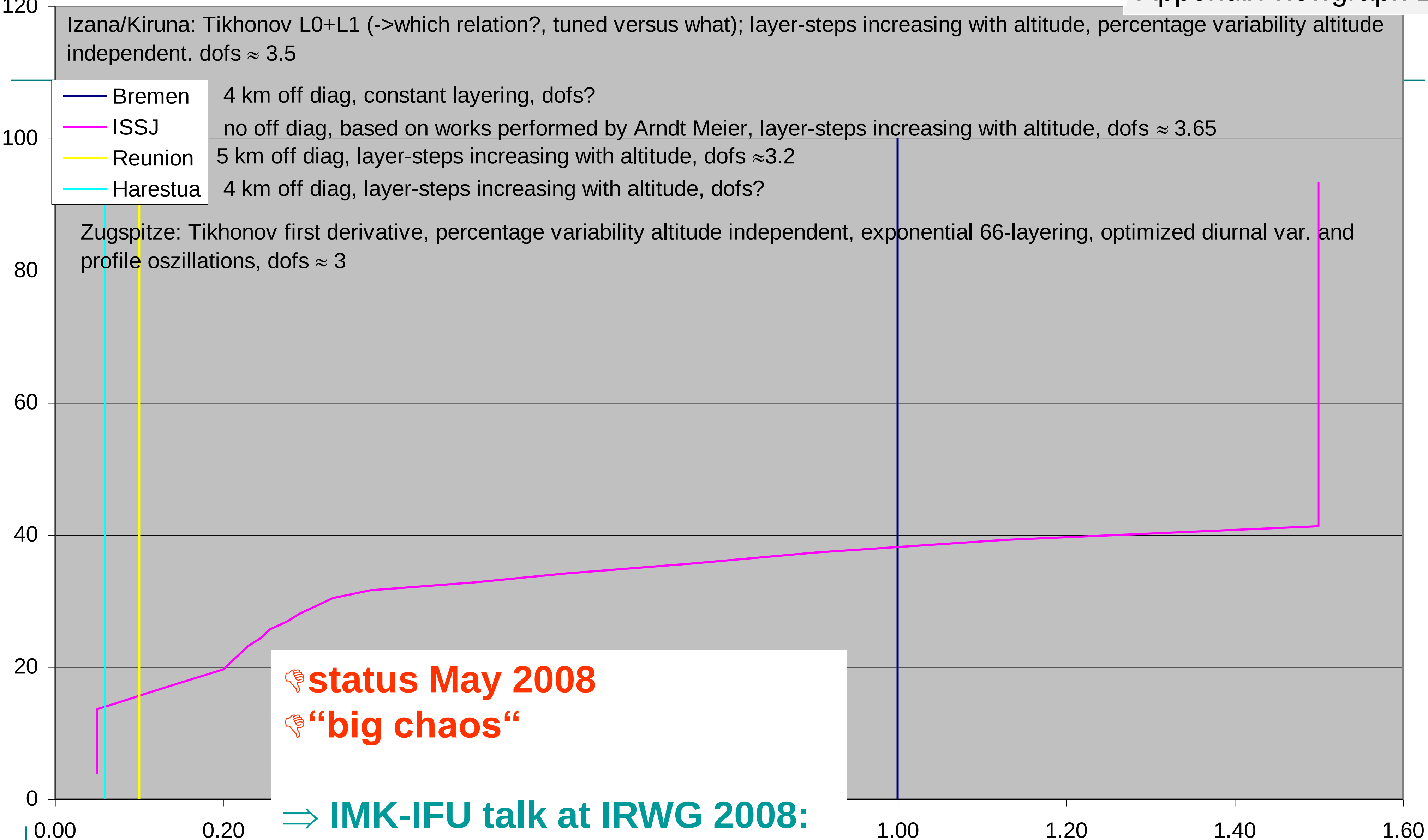
N2O regularization. Issue: for direct quantitative intercomparison the layering would have to be the same




**status May 2008**

**"big chaos"**

**⇒ IMK-IFU talk at IRWG 2008: use Tikhonov L1 in units of per centage VMR for all stations**