

Bringing FTIR measurements into GRUAN

- (1) The ground-based FTIR remote sensing technique
- (2) Generation of error estimates
- (3) Example: The **water vapour** products within the project **MUSICA**
- (4) Progress in EU FP7 project NORS
- (5) Assets of the Technique:
 - ✓ high quality,
 - ✓ profiling capability,
 - ✓ high measurement frequency
- (6) Notes & Discussion Points

M. De Mazière, M. Schneider, J. Hannigan

A ground-based solar-viewing FTIR remote-sensing installation ~\$500k

Often the observations are made at remote sites (mountains, polar regions, etc.): the whole experiment can be mounted in a standard shipping container with electricity, heating, internet connection, etc.

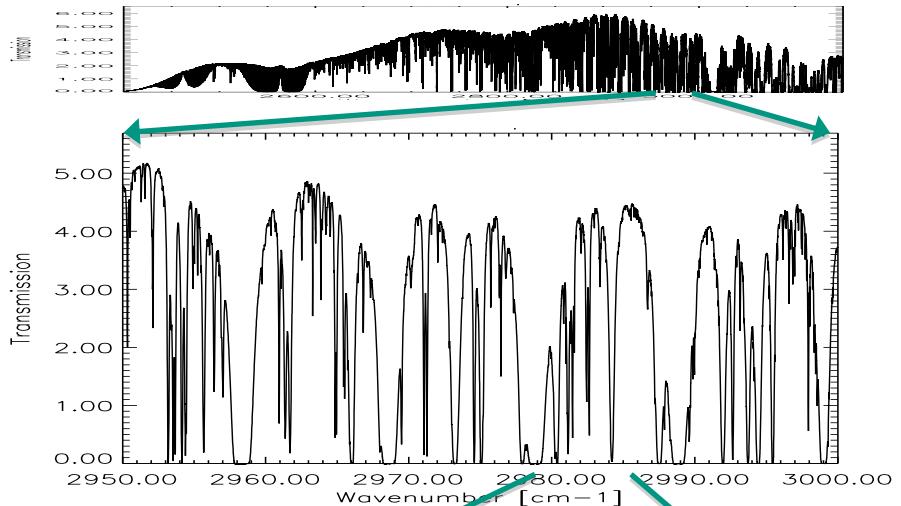
Most stations use a Bruker IFS 125HR: very high quality and commercially available. Dimensions: 200cm x 300cm; Price: ~ 300 k€

Instrument status is monitored via cell measurements (commonly manufactured)

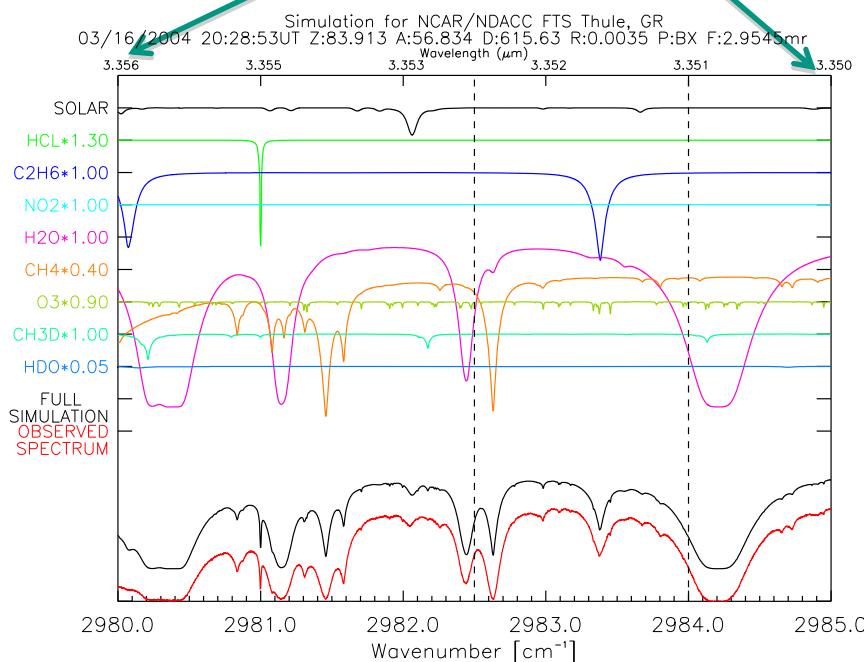
Furthermore a precise solar tracer system is required (e.g., Gisi et al. AMT 2011)



Gb FTIR measurements within NDACC



Simultaneous observation at high spectral resolution in wide spectral bands yield absorption signatures of many trace gases (**required**)



Spectral Resolution:

0.0035-0.002 cm⁻¹ required for profiling using pressure (Lorentz) broadening effect.

SNR:

300 – 2000 RMS

Spectral Range:

750–4500 cm⁻¹

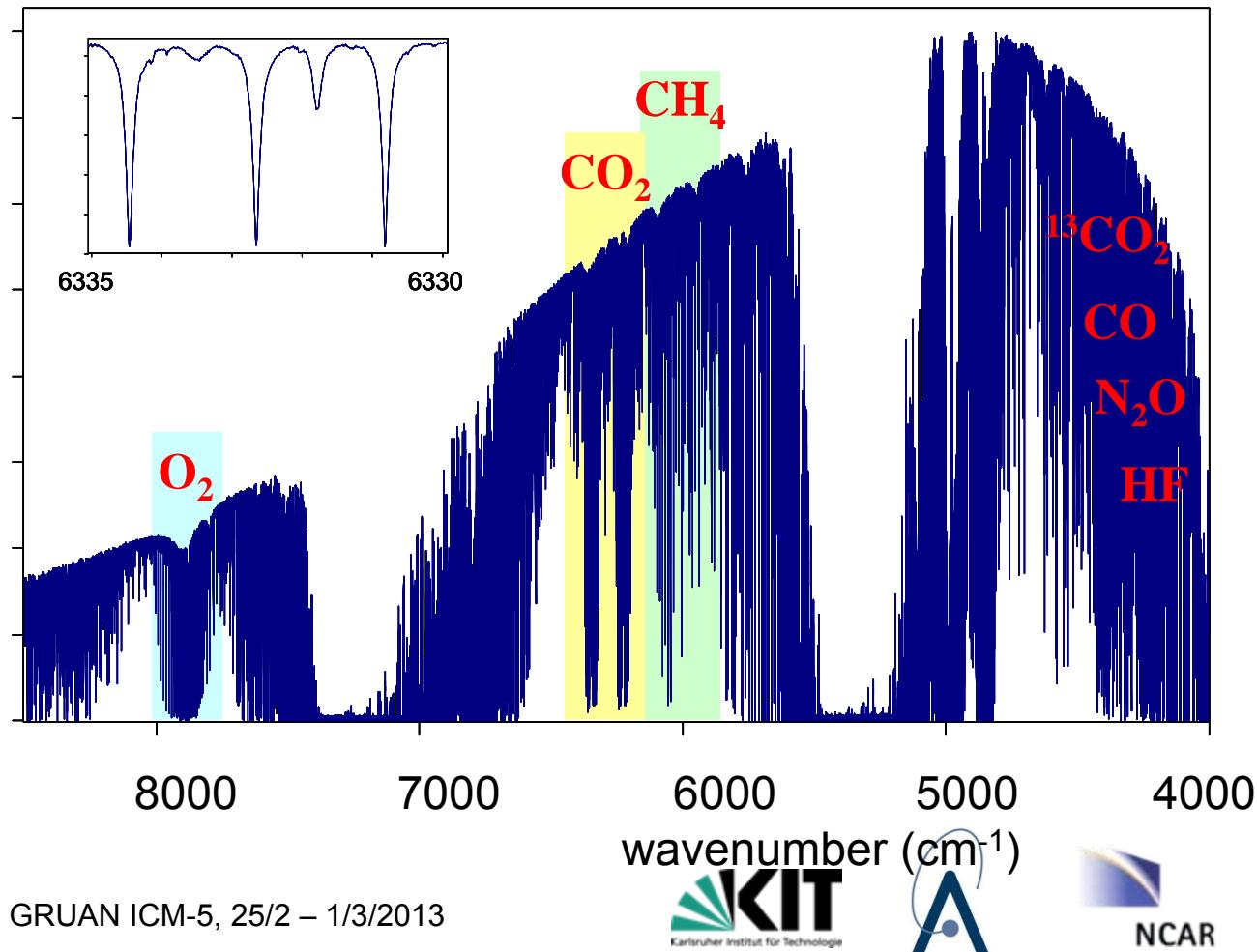
Data Rate:

Daily but many sites all daylight clear-sky time

H2O
HDO
O3
N2O
CH4
HNO3
CCl2F2
CCl3F
CHClF2
COF2
CIONO2
CIO
NO
NO2
HCl
C2H6
HF
HCN
C2H2
CO
CO2
OCS
NH3
COCl2
N2
CO2

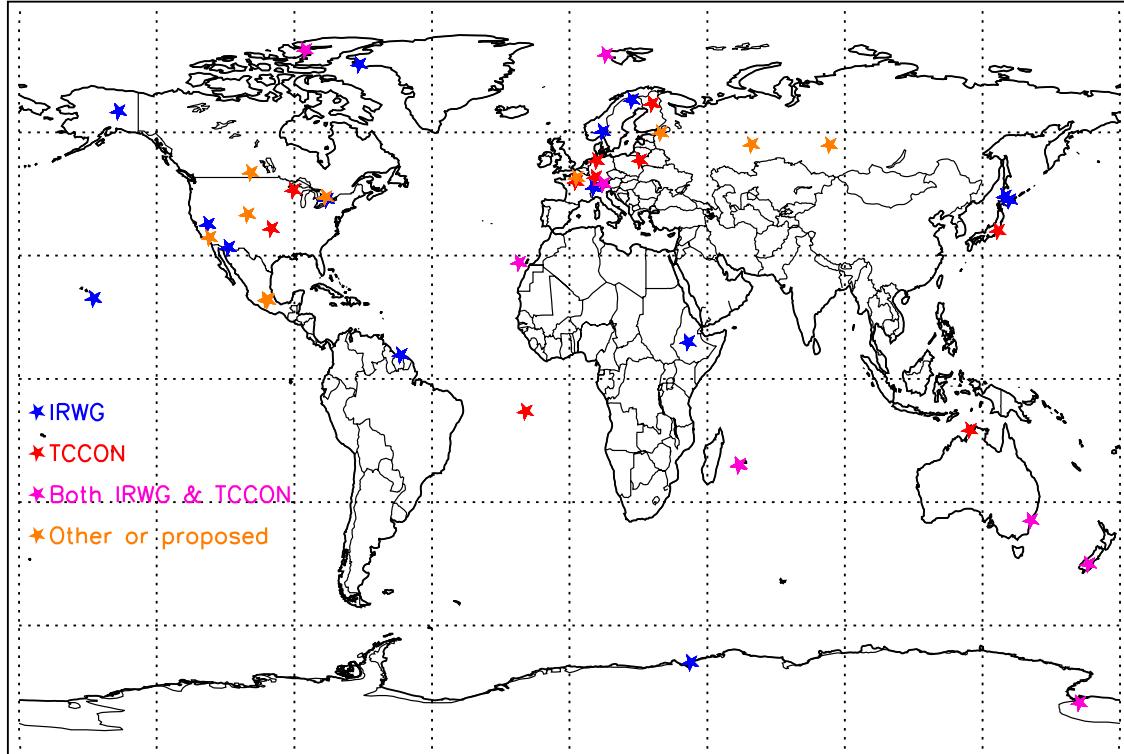
TCCON: Total Carbon Column Observing Network

- similar instruments
- similar data analysis principles
- But
 - In near-infrared
 - More prescriptive procedures for data acquisition
 - Focus on high-precision column-averaged dry-air volume mixing ratios of greenhouse gases CH₄, CO₂, N₂O, H₂O, CO
 - 1 single data processing S/W



Global FTS Stations

Global Ground-Based FTIR Spectrometers



~Tropical

Izana	28	344
Mauna_Loa	20	204
Mexico_City	19	-99
Altzomoni	19	-99
Addis_Ababa	9	39
Paramaribo	6	305
Ascension	-8	-14
Darwin	-12	131
Reu_Maido	-21	55
Reu_St_Denis	-21	55

Arctic

Eureka	80	274
Ny_Alesund	79	12
Thule	77	291
Kiruna	68	20
Sodankyla	67	27
Poker_Flat	65	213

Antarctic

Syowa_Station	-69	40
Arrival_Heights	-79	167

Mid-Latitude

Harestua	60	11
St_Petersburg	60	30
Yekaterinburg	57	60
Tomsk	57	85
Bialystok	53	23
Bremen	53	9
Bratts_Lake	50	-104
Karlsruhe	49	8
Paris	49	2
Orleans	48	2
Garmisch	47	11
Zugspitze	47	11
Jungfraujoch	47	8
Park_Falls	46	270
Moshiri	44	142
Egbert	44	280
Rikubetsu	44	144
Toronto	44	281
Boulder	40	255
Barcroft	38	242
Lamont	37	263
Tsukuba	36	140
Table_Mtn	34	242
Kitt_Peak	32	248
Wollongong	-34	151
Lauder	-45	170

Many Common Members in TCCON & NDACC

MUSICA is a subset of NDACC groups...

Shared meetings for several years, common experience, problems & solutions

Institute	NDACC Sites	TCCON Sites	MUSICA
JPL	1	3+	
U. Wollongong	1	1	1
KIT Karl.	4	1	4
U. Bremen	4	3	1
BIRA	1	1	
NIES	1	1	1
KIT Gar.	1	1	
NIWA	2	1	2
U.T.	2	1	1
U Liege	1		1
	17	13	11

Instrumentation / Data Products

	TCCON	IRWG	MUSICA
Instrument	125HR (Bruker)	By spec. (Bruker)	By spec. (Bruker)
OPD*	45cm	250cm (max)	250cm (max)
Region**	Near-IR	mid-IR	mid-IR
Recording	DC	DC/AC	DC/AC
Bandwidth	3900-15000	700-4500	700-4500
Detectors	InGaAs/Si	InSb/MCT	InSb/MCT
Retrieval	NLLS / Scale of apriority	Full Optimal Est	Full Optimal Est
Species	CO ₂ (CH ₄ , N ₂ O, CO)	10 primary +	H ₂ O
Product	Column/DAMF	Column/Profile	Column/Profile

*Low resolution instruments (~1 cm) are being developed (ie lower cost)

*Possible MIR/NIR Instrument has been proposed

L1 (spectra) → L2 (columns ; vertical profiles)

Requires forward model:

➤ radiative transfer model of sunlight through the atmosphere including absorption, emission and scattering processes.

Solar absorption => direct absorption is dominant

➤ Spectroscopic data of atmospheric constituents

+ inverse model:

For vertical profile retrieval : ill-posed problem

⇒ NLLS fitting + Regularisation or Optimal Estimation Method

Actual status in NDACC: 2 standard algorithms (inter-compared)

Actual status in TCCON: 1 single algorithm and central data processing verification

Linearize the estimate of the measurement about the apriori state

$$\vec{y}(\nu) = \vec{F}(\vec{x}, \vec{b}) + \frac{\partial \vec{F}}{\partial \vec{x}} (\vec{x} - \vec{x}_0) + \varepsilon$$

Compute the sensitivity of the measurement to the state

$$\mathbf{K}_x = \frac{\partial \vec{y}}{\partial \vec{x}} = \frac{\partial \vec{F}(\vec{x})}{\partial \vec{x}}$$

\mathbf{D}_y – contribution function = $\frac{\partial}{\partial \vec{y}}$ of the inverse model

$$\mathbf{D}_y = (\mathbf{S}_a^{-1} + \mathbf{K}_x^T \mathbf{S}_\varepsilon^{-1} \mathbf{K}_x)^{-1} \mathbf{K}_x^T \mathbf{S}_\varepsilon^{-1}$$

Iterate to better estimates of the state with

$$\vec{x}_{i+1} = \vec{x}_a + \mathbf{D}_y [\vec{y} - \vec{F}(\vec{x}_i) + \mathbf{K}_i (\vec{x}_i - \vec{x}_a)]$$

To converge to below the noise level

$$|\mathbf{K}_i (\vec{x}_{i+1} - \vec{x}_i)| \leq \sqrt{\vec{S}_\varepsilon}$$

y	= measurement
f()	= forward model
x	= state vector
b	= parameters required by fm
ε	= experimental errors
S_a	= covariance of a priori
S_ε	= covariance of measurement
\mathbf{K}_x	= sensitivity to measurement of fm
\mathbf{K}_b	= sensitivity to param. b of fm
\hat{x}	= best estimate for x

Where the Averaging Kernel is the sensitivity of the retrieved state to the real state:

$$\mathbf{A} = \frac{\partial \vec{x}}{\partial \vec{x}} = \mathbf{D}_y \mathbf{K}_x$$

Error in \hat{x} is divided into manageable parts

$$\begin{aligned}\hat{\vec{x}} - \vec{x} = & (\mathbf{A} - \mathbf{I}_n)(\vec{x} - \vec{x}_a) && - \text{Smoothing} \\ & + \mathbf{D}_y \mathbf{K}_b (\vec{b} - \hat{\vec{b}}) && - \text{Model parameters} \quad \text{Model error is neglected} \\ & + \mathbf{D}_y \varepsilon && - \text{Measurement}\end{aligned}$$

K_b - Sensitivity of forward model to parameter b

$$\mathbf{K}_b = \frac{\partial \vec{y}}{\partial b} = [\vec{F}(\vec{x}, \vec{b} + \Delta \vec{b}) - \vec{F}(\vec{x}, \vec{b})] / \Delta \vec{b}$$

S_b is the uncertainty covariance matrix in X due to S_{par} the uncertainty in parameter b : maybe random or systematic or both. Measurement uncertainty is random

$$\mathbf{S}_b = \mathbf{D}_y \mathbf{K}_b \mathbf{S}_{par} \mathbf{K}_b^T \mathbf{D}_y^T$$

$$\mathbf{S}_m = \mathbf{D}_y \mathbf{S}_\varepsilon \mathbf{D}_y^T$$

Finally determine Random and Systematic components separately

$$\mathbf{S}_{rand} = \sum \mathbf{S}_{bi} + \mathbf{S}_m$$

$$\mathbf{S}_{syst} = \sum \mathbf{S}_{syst,i}$$

Provide averaging kernel $A \Rightarrow$ smoothing error

Error sources:

- Measurement noise
- background slope
- background curvature
- differential wavenumber shift
- single wavenumber shift
- independent wavenumber shift
- empirical apodization function
- empirical phase function
- solar line shift
- solar line strength
- simple phase error
- zero level offset
- interfering species
- channel parameters
- temperature profile
- target gas absorption line(s) *intensity*
- target gas absorption line(s) *air broadened line half-width*
- retrieved gas absorption line(s) *intensity*
- retrieved gas absorption line(s) *air broadened line half-width*
- other possible line parameters:
 - self broadening
 - lower state energy
 - temperature dependence exponent
 - pressure shift
 - Galatry Beta
 - line mixing parameters
 - S-DV parameters
- solar pointing

- The sensitivity of \hat{x} on a given b_i is minimized by early choices in the retrieval process (eg spectral region).
 - *This is made homogeneous across the network by recent efforts to use identical retrieval parameters at all sites.*
- The best estimate of S_{bi} may be
 - Site and instrument dependent
 - Needs to be physically based,
 - May require some testing to determine,
 - *Procedure to evaluate it needs to be 'homogeneous' across all sites.*
- Error analysis homogenization effort in progress (recent NDACC/NORS Error Analysis Workshop NCAR Jan 2013)

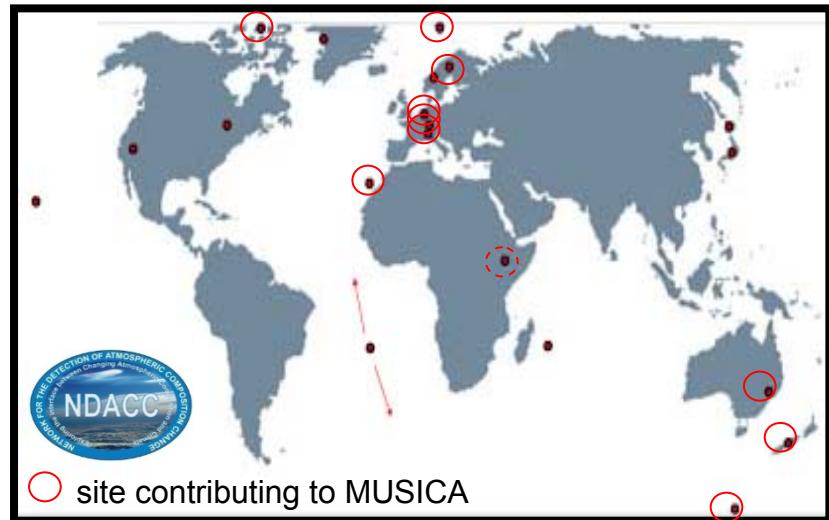
⇒ Aim:

provide common S/W package for calculating uncertainty budget for each data point, to be reported in the data file (random part and systematic part).

Example: The project MUSICA: consistent ground- and space-based water vapour products

MUSICA (MULTi-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water) combines NDACC ground-based FTS observations and IASI / METOP observations (and in-situ observations for validation purposes).

The MUSICA project team (M. Schneider et al.) at the Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, and the Agencia Estatal de Meteorología (AEMET), Santa Cruz de Tenerife, Spain



Schneider and Hase (2011);
Schneider et al. (2012)

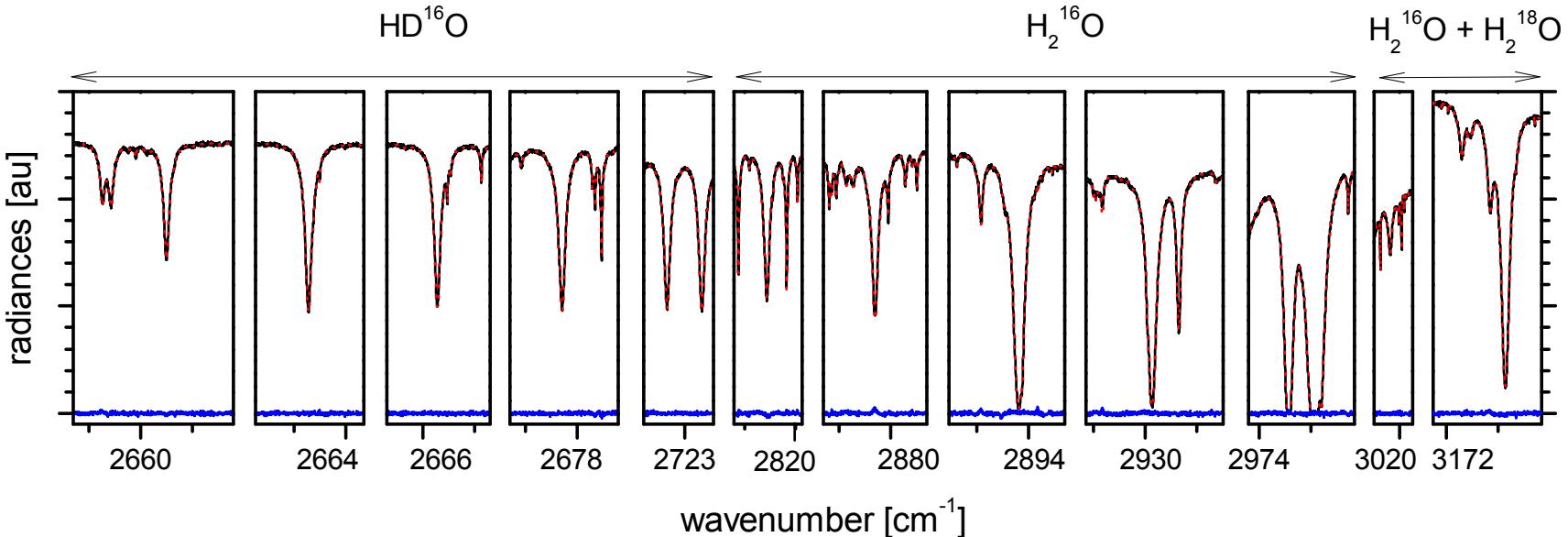
<http://www.imk-asf.kit.edu/english/musica>

Acknowledgement: MUSICA is funded by the European Research Council under the European Community's Seventh Framework Programme (FP7/2007-2013) / ERC Grant agreement n° 256961.

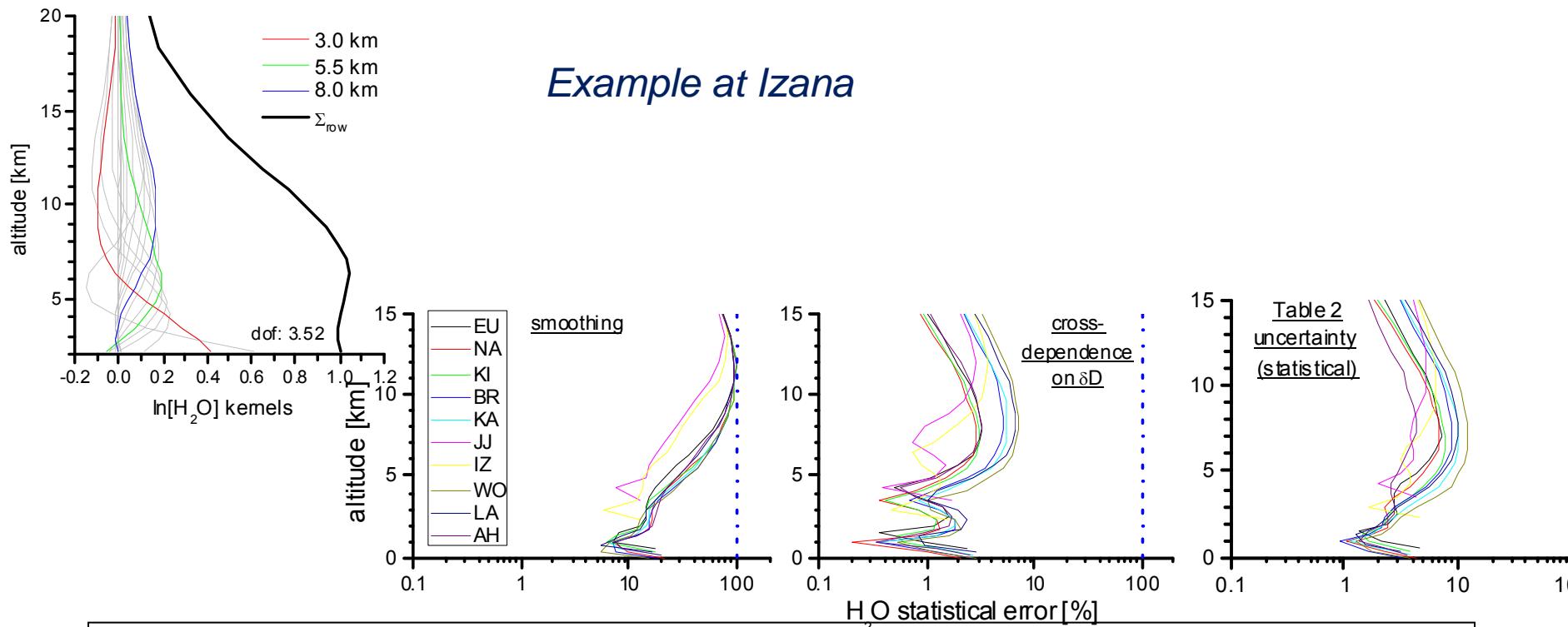
MUSICA's ground-based FTIR spectral windows

We measure high resolution broadband spectra. For the analysis we select spectral regions where the target species has well isolated absorption signatures:

Example of the spectral windows used for H_2^{16}O and HD^{16}O retrievals:

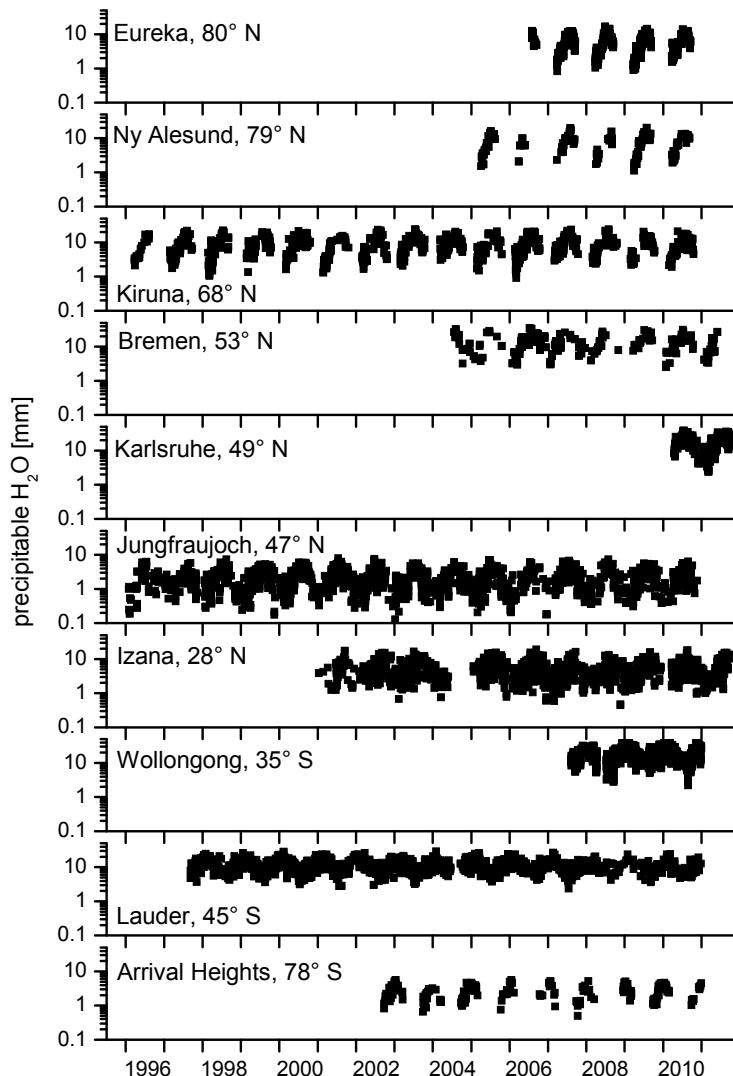


Vertical Sensitivity & Error assessment for MUSICA's g-b FTIR water vapour product



Data quality is well assessed for each individual observation at all stations.
For more details see Schneider et al. (2012), Sect. 4.1: „Characterisation of product type 1: Optimally estimated H₂O profiles”

Current state of MUSICA gb FTS water vapour dataset: 10 stations, data since mid 90s, ...



Total number of available water vapour profiles: ≈ 15000

Spectra submitted by PI then centrally processed at KIT

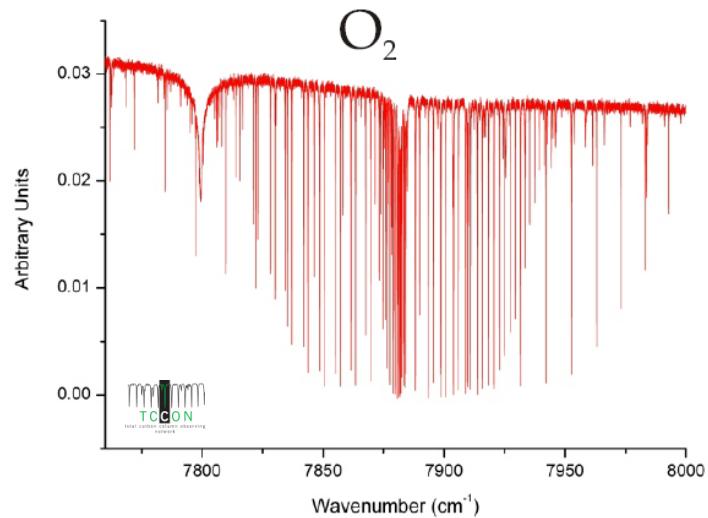
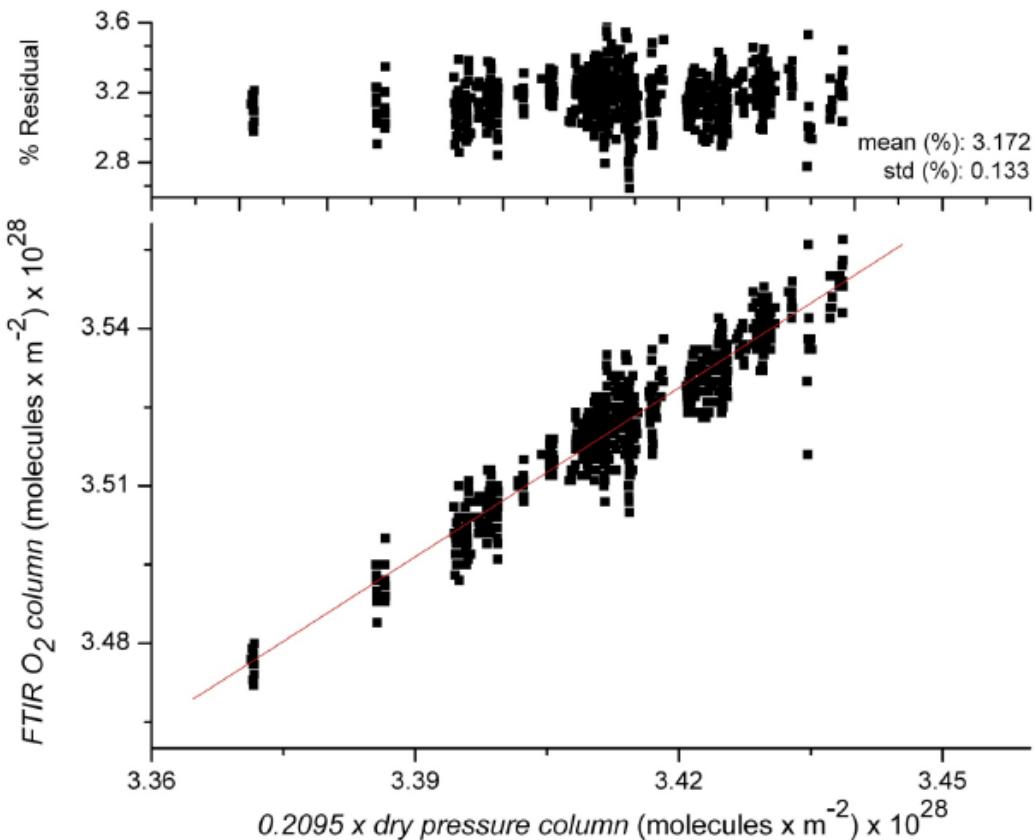
Representative for ten globally distributed sites, :

NH, SH, polar, mid-latitudes, (sub)-tropics, land surface, ocean surface, lowland, high mountains, etc.



<http://www.imk-asf.kit.edu/english/musica>

Asset (1): very high quality as documented by retrieved O₂ and pressure correlations



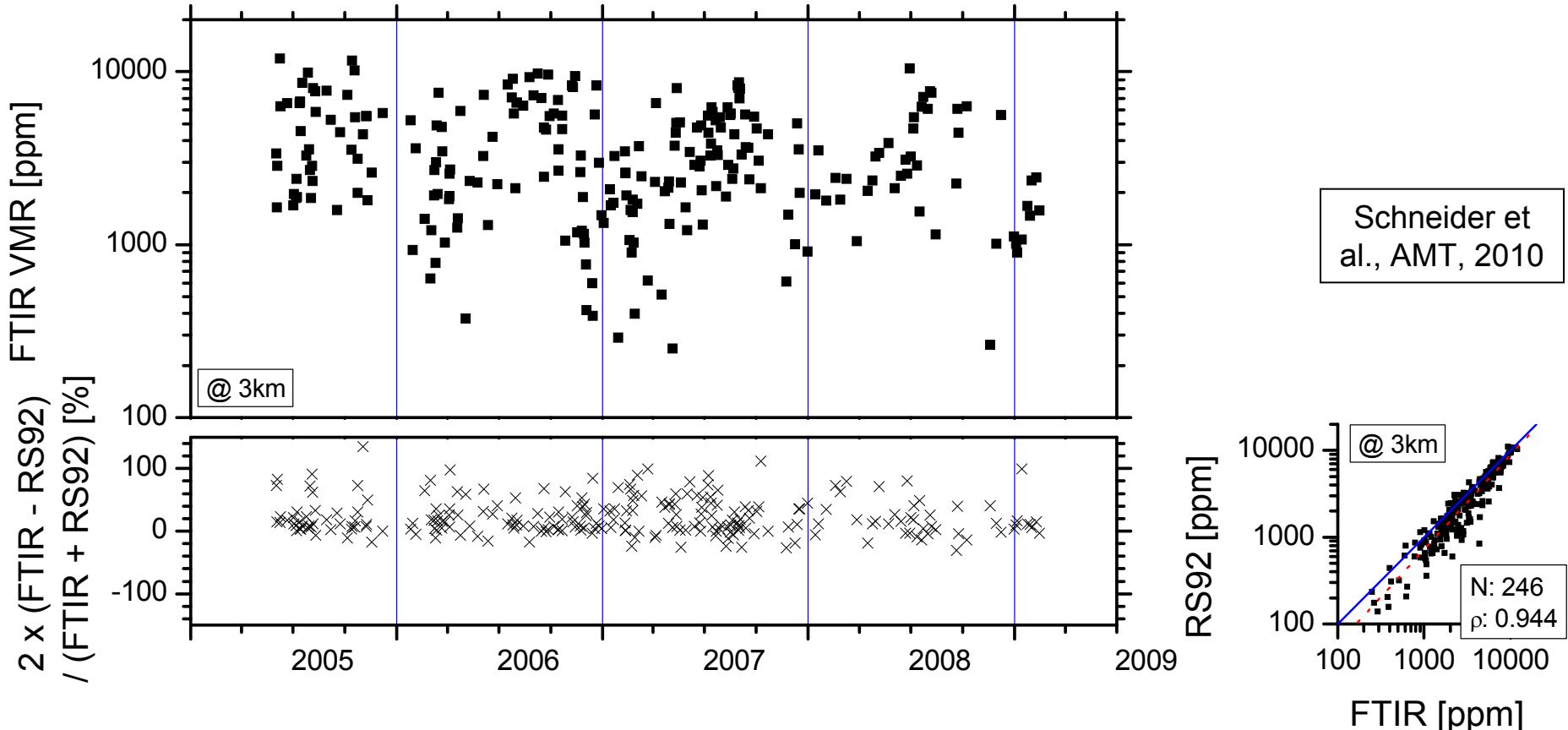
differential absorption principle
→ „self calibrating“

The plots are courtesy by E. Sepúlveda

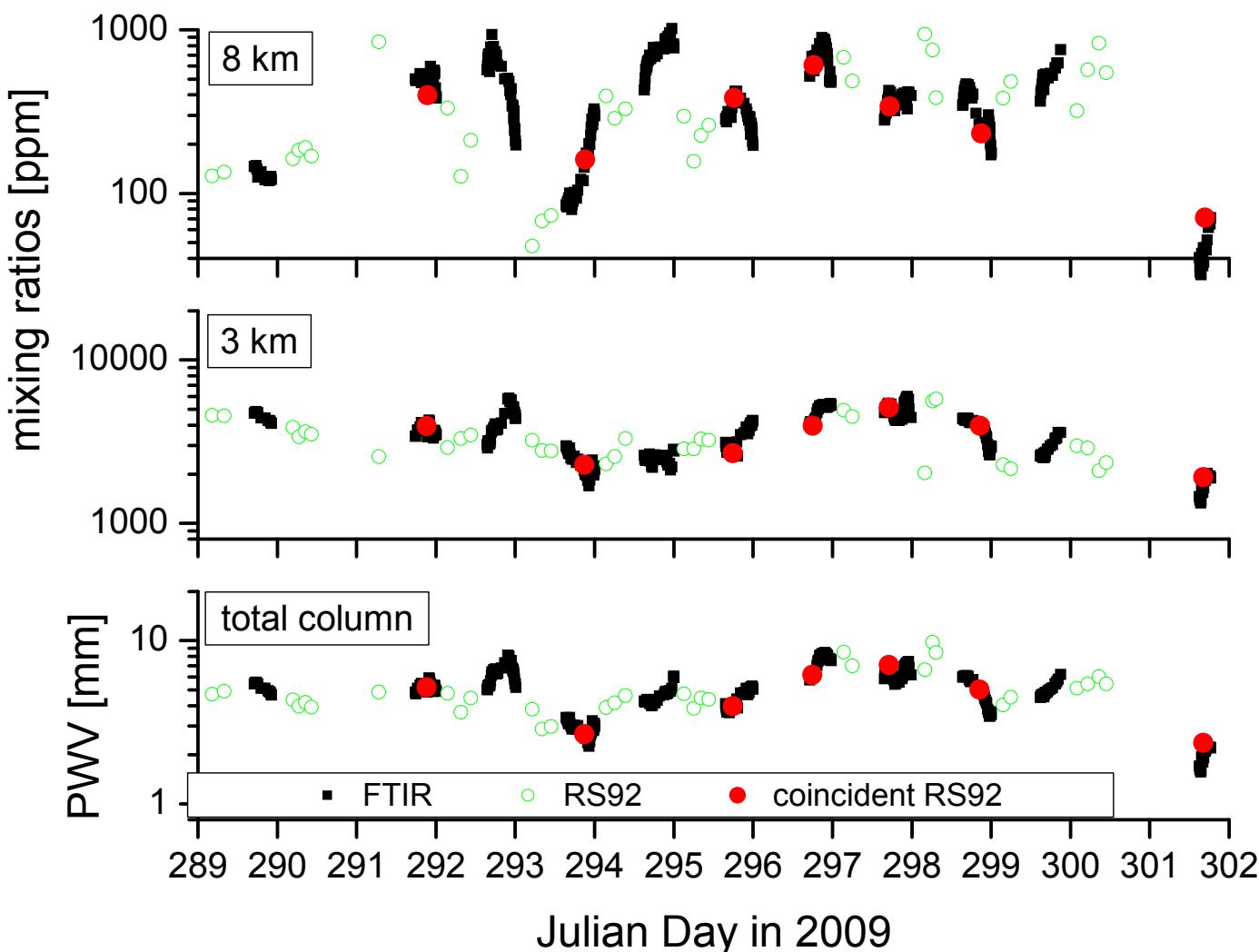
→ the gb FTS technique can produce very precise long-term data sets

Asset (2): „profiles“ of high quality, example study 2005-2009, FTS vs. Vaisala RS92

lower troposphere (3 km):



Asset (3): high measurement frequency, example MOHAVE-2009 campaign



High measurement frequency is important for water vapour, because of the high variability!

Acknowledgement
FTIR spectra and RS92 data were provided by G. Toon, J.F. Blavier, and T. Leblanc, JPL, California, USA



■ Progress in **NORS** (EU FP7 project, Nov. 2011- mid 2014):

Objective: tailor NDACC FTIR, LIDAR, MICROWAVE, and UVVIS DOAS products to the needs of supporting the quality assessment of the GMES (Copernicus) Atmospheric Service.

In progress

- Rapid data delivery within 1 month
- Full characterisation of products (uncertainties, sensitivities, horizontal and vertical averaging kernels, uncertainties, ...)
- Data user guide
- Data uncertainties guide
- Data consistency checks (whenever redundancy, and versus satellite data)

Summary

- The ground-based FTIR remote sensing technique offers high precision and long-term stability (cf. cell measurements)
- Existing networks are in place and adaptable for evolving requirements
- Working towards more homogeneous data products, furthered by
 - Instrumentation standards,
 - Certification protocol
 - Consistent retrieval parameters,
 - Consistent error analysis.
- Water vapour (and HDO/H₂O) profiles of a carefully documented quality are produced within the project MUSICA and available for ten globally distributed sites (for some stations dating back to the mid 90s)
- Valuable reference dataset due to combination of high quality, long-term availability, profiling capability, and high measurement frequency
- NDACC data are delivered in GEOMS compliant HDF files including metadata, and uncertainties; all data are referenced to SI units
- Ancillary data (surface temperature, pressure water vapor profile & column are included)
- Data already widely used for satellite and model validation

Issues raised in GRUAN:

- Central storage of raw (L1) data,
 - Not implemented (but all PI's save their raw data)
 - 'Level' of raw tbd (eg. spectrum or interferogram?)
 - Depending on level & measurement frequency, data rate could be to a Gb/day
- Quantified uncertainties with every data point
 - Desired by all - in progress
- Traceability
 - As in HITRAN, NCEP – OK
 - TCCON includes calibration to in-situ aircraft data
 - Further calibration may be required by GRUAN
 - HDF file does not include full traceability information
- Central processing,
 - in place for MUSICA, not wider NDACC, but possible
 - is an implemented part of TCCON but not standard
- Homogeneity of the measurements across the network:
 - Active, in everyone's interest – how to prove they are not?
- Redundant observations:
 - Partly dealt with in NORS for ozone, CO and CH4, in MUSICA for H₂O

EXTRA SLIDES

For details please refer to the recent publications on the MUSICA dataset

Schneider, M., S. Barthlott, F. Hase, Y. González, K. Yoshimura, O.E. García, E. Sepúlveda, A. Gomez-Pelaez, M. Gisi, R. Kohlhepp, S. Dohe, T. Blumenstock, A. Wiegele, E. Christner, K. Strong, D. Weaver, M. Palm, N.M. Deutscher, T. Warneke, J. Notholt, B. Lejeune, P. Demoulin, N. Jones, D.W.T. Griffith, D. Smale, and J. Robinson:

Ground-based remote sensing of tropospheric water vapour isotopologues within the project MUSICA,
Atmos. Meas. Tech., 5, 3007-3027, 2012.

Schneider, M. and F. Hase:

Optimal estimation of tropospheric H₂O and δD with IASI / METOP,
Atmos. Chem. Phys., 11, 11207-11220, 2011.

Ground-based FTS retrieval principle

We invert the spectra by an optimal estimation method.

Minimise the cost function:

$$\underbrace{[\vec{y} - \vec{f}(\vec{x}, \vec{b}, \vec{p})]^T S_{\epsilon}^{-1} [\vec{y} - \vec{f}(\vec{x}, \vec{b}, \vec{p})]}_{\text{measurement information}} + \underbrace{[\vec{x} - \vec{x}_a]^T S_a^{-1} [\vec{x} - \vec{x}_a]}_{\text{a priori information}}$$

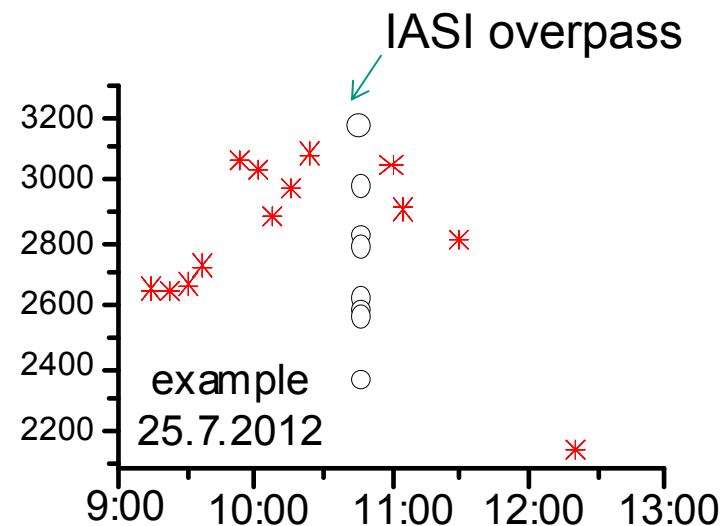
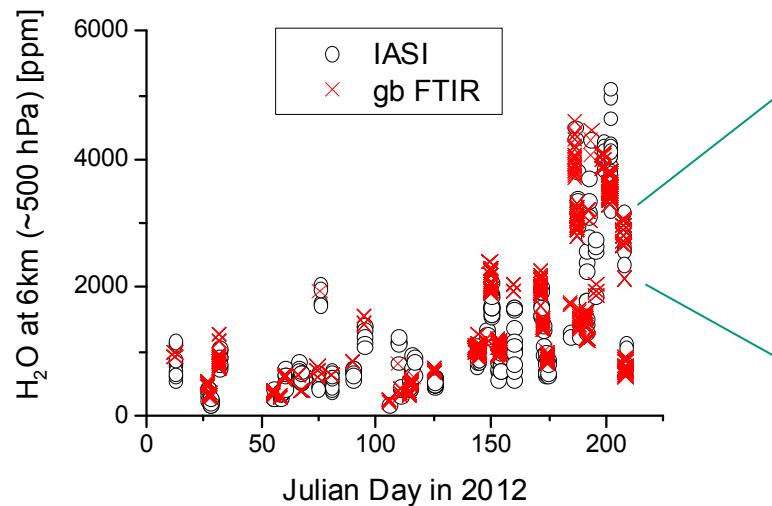
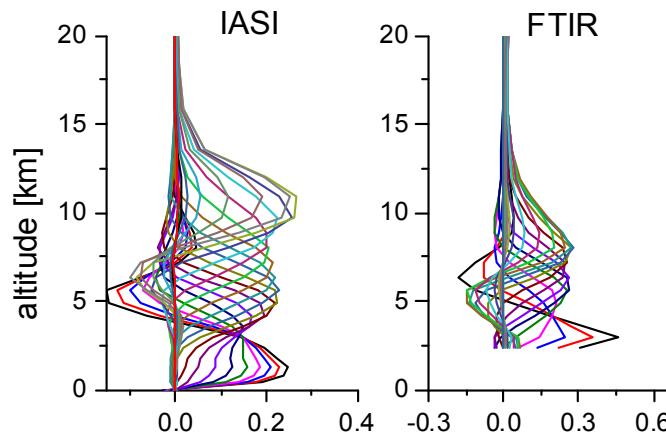
Rodgers (2000)

Ground-based FTIR: an important reference for validating satellite sensors

(1): High quality data

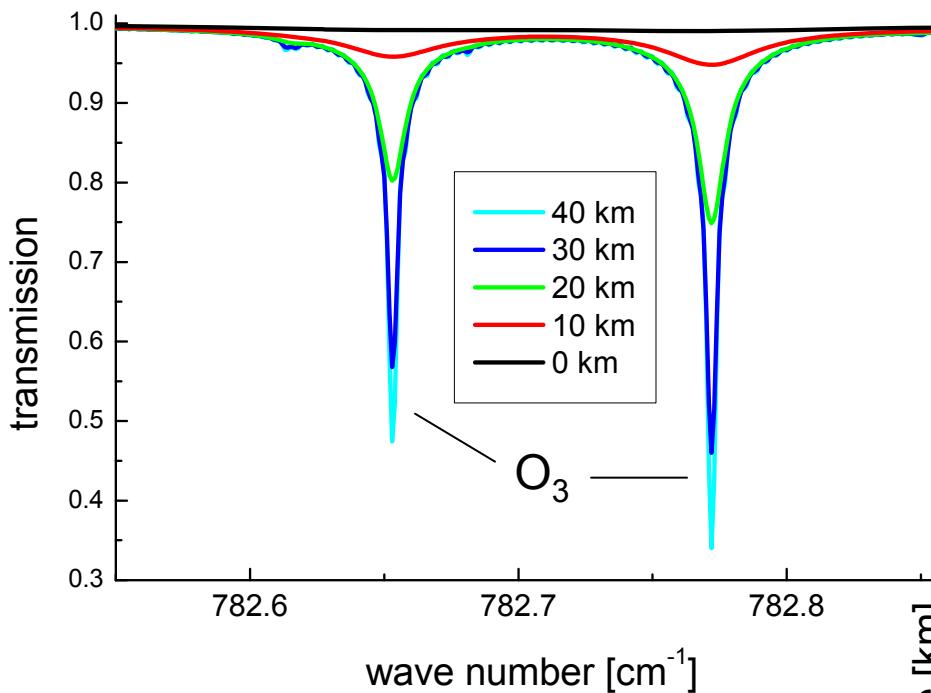
(2): Gb FTIR and satellite sensor kernels overlap, example FTIR and IASI:

(3): Gb FTIR can measure quasi continuously (during daytime), essential for proper validation:



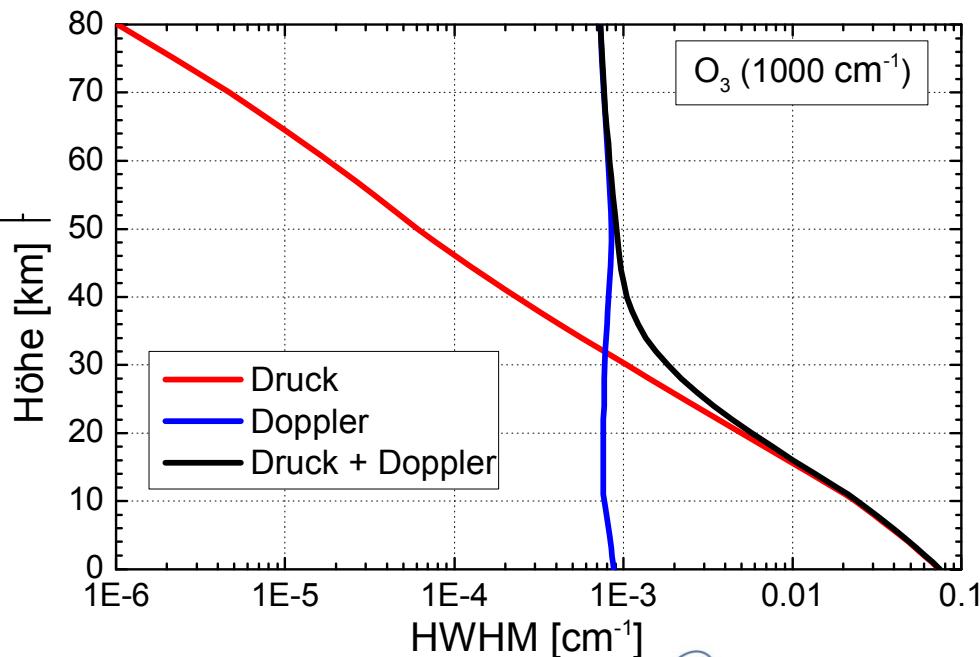
Spectra analysis: information on the absorbers' vertical distribution

Example for O₃:



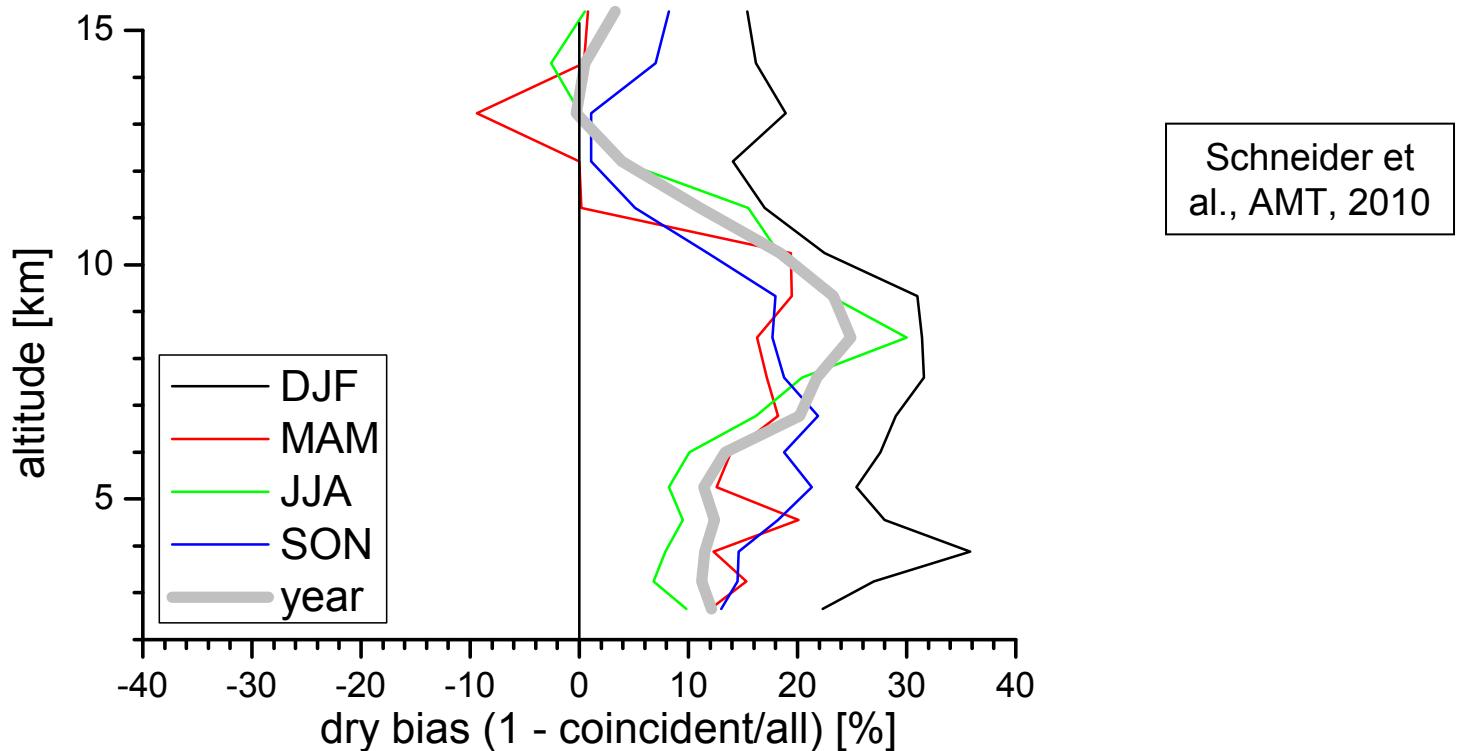
In the middle infrared the pressure broadening determines the line shape between the Earth's surface and about 40 km altitude.

Due to the pressure broadening effect very high resolution spectra contain information about the absorbers vertical distribution

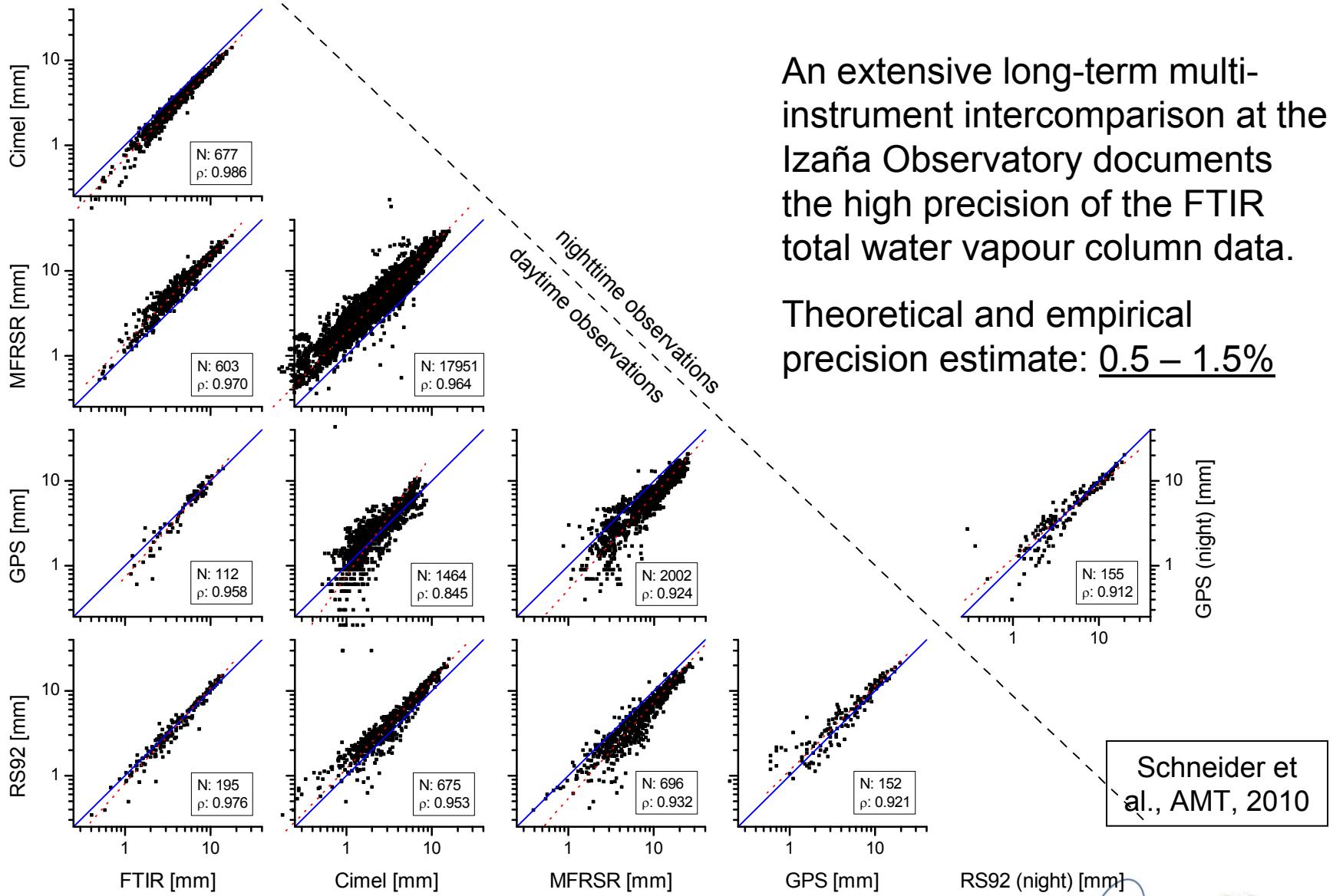


Limitation of the FTS technique: observation only exists for clear sky conditions

Estimated clear sky dry bias at the subtropical Izaña Observatory:



Quality of H_2O total column amounts



Global ground-based FTIR networks

There are two global networks measuring high resolution solar absorption spectra in the infrared applying very high quality instrumentation

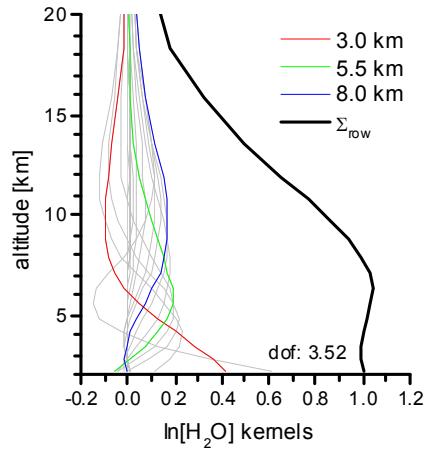
NDACC: Network for the Detection of Atmospheric Composition Change



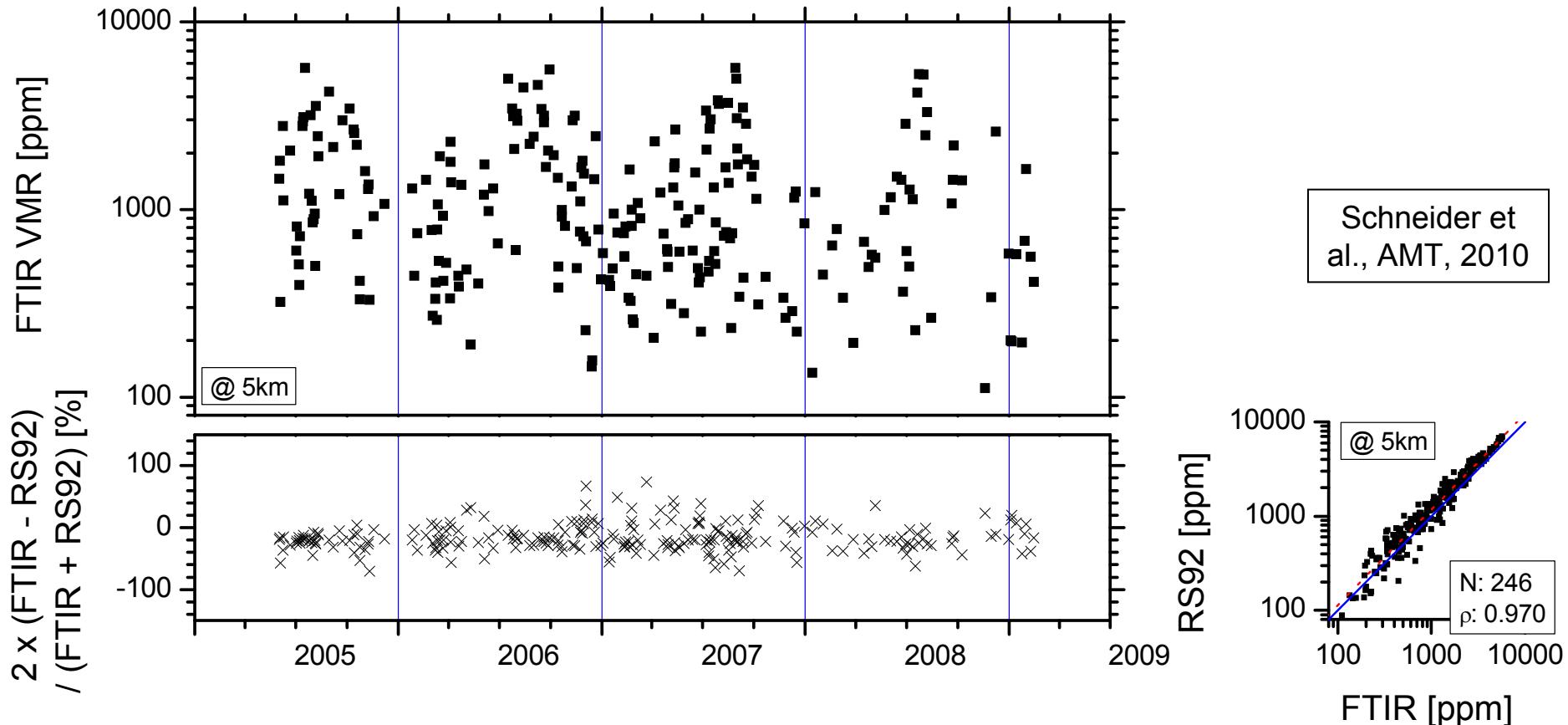
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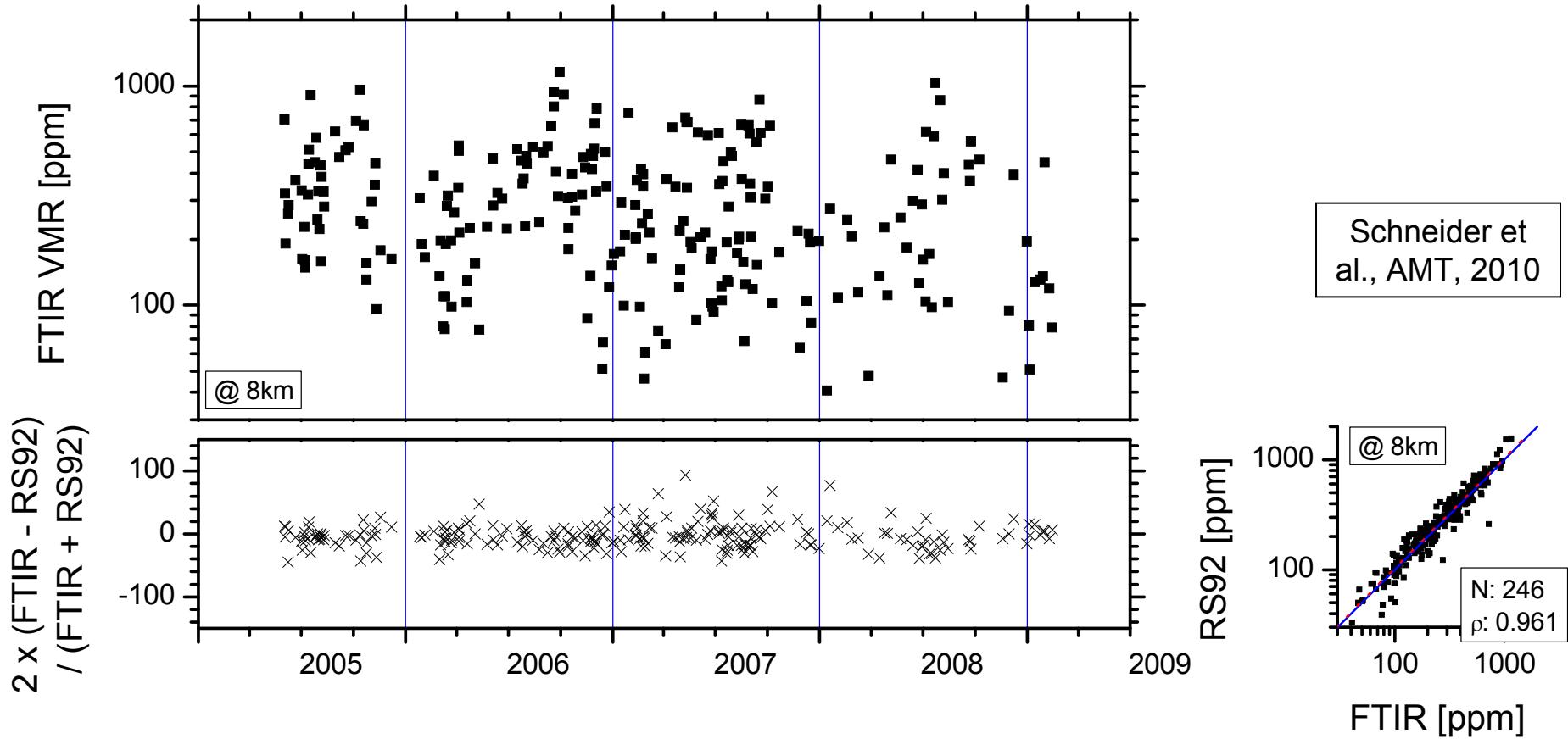
Typical averaging kernels for MUSICA's gb FTIR water vapour product, example Izana



middle troposphere:



upper troposphere:

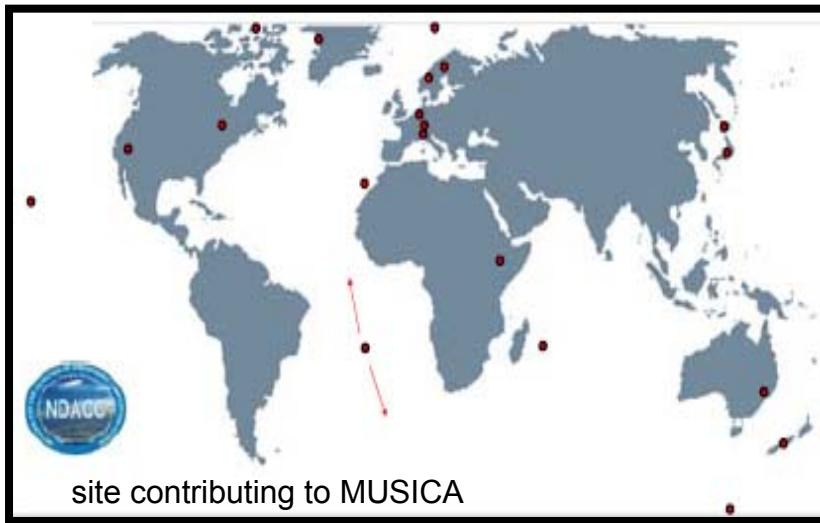


- central storage of raw data,
- quantified uncertainties with every data point,
- traceability,
- central processing,
- homogeneity of the measurements across the network,
- redundant observations.

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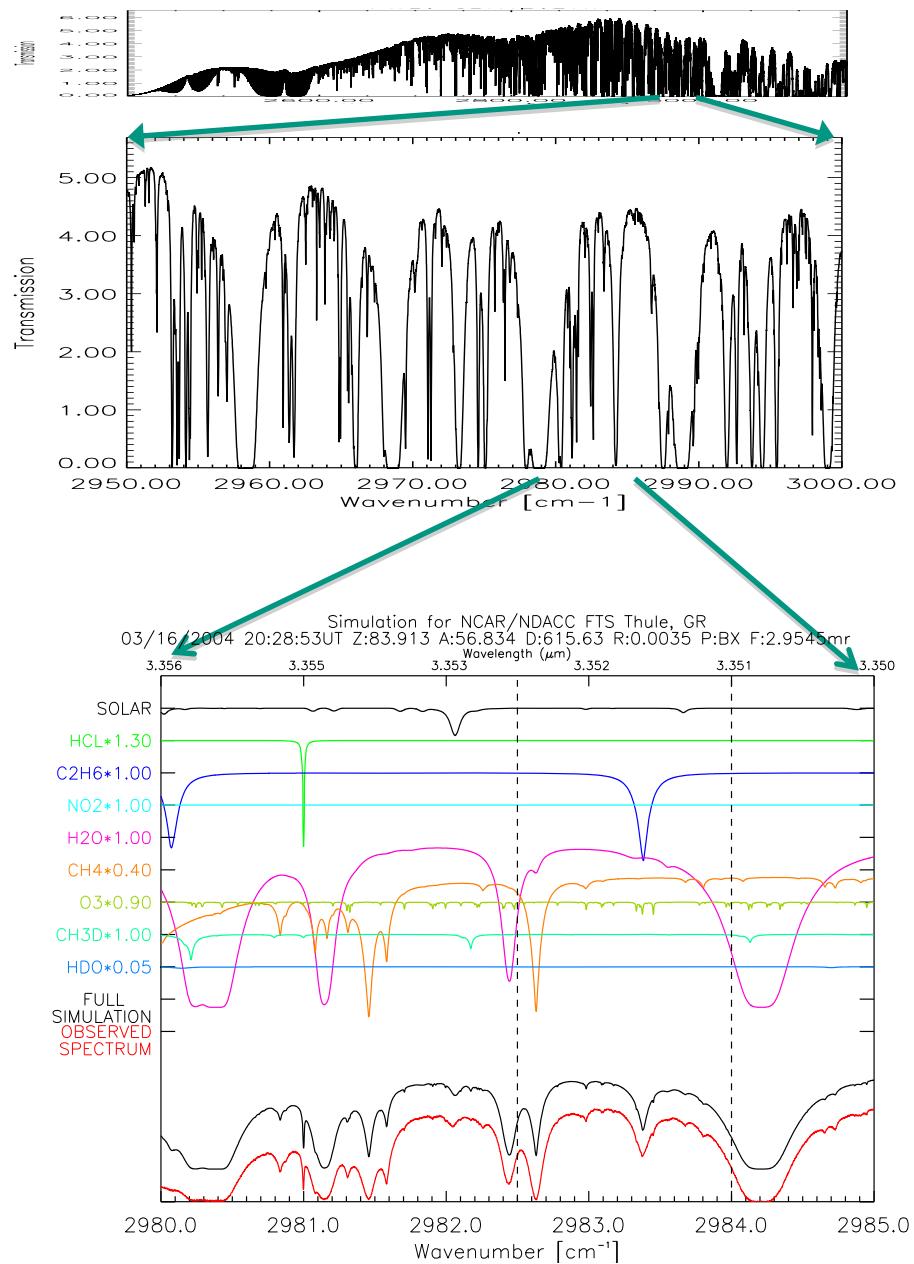
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C₂H₆ Simulation