MUSICA H2O and δD (HDO/H2O) data: in-situ, ground-based FTIR, and IASI

I. The MUSICA strategy for generating global long-term data with traceable quality

II. FTIR: experiment, processing chain, uncertainty estimation, empirical quality documentation

III. IASI: processing, uncertainty, consistency with FTIR

IV. Water vapour isotopologue data: MUSICA and beyond

MUSICA:

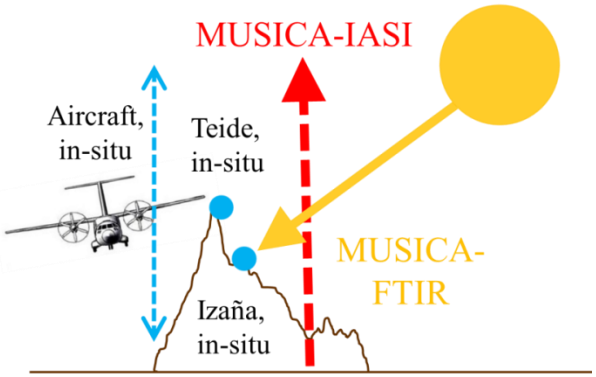
MUlti-platform remote **S**ensing of **I**sotopologues for investigating the **C**ycle of **A**tmospheric water

Scientific objective: Use the isotopic signals in water vapour for constraining the tropospheric moisture pathways and the associated uncertainty in climate models (equilibrium sensitivity, Sherwood et al., Nature 2014).

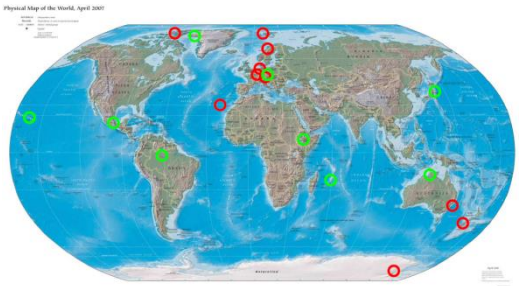
1st step and focus of MUSICA: Generate high quality observational data (H_2O and δD).

Strategy: Combination of different measurement techniques and platforms.

Reference data by calibrated in-situ observations

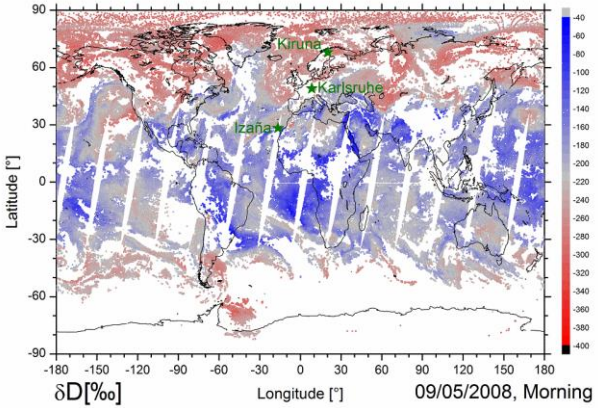


Long-term data from a ground-based remote sensing network:



NDACC/FTIR

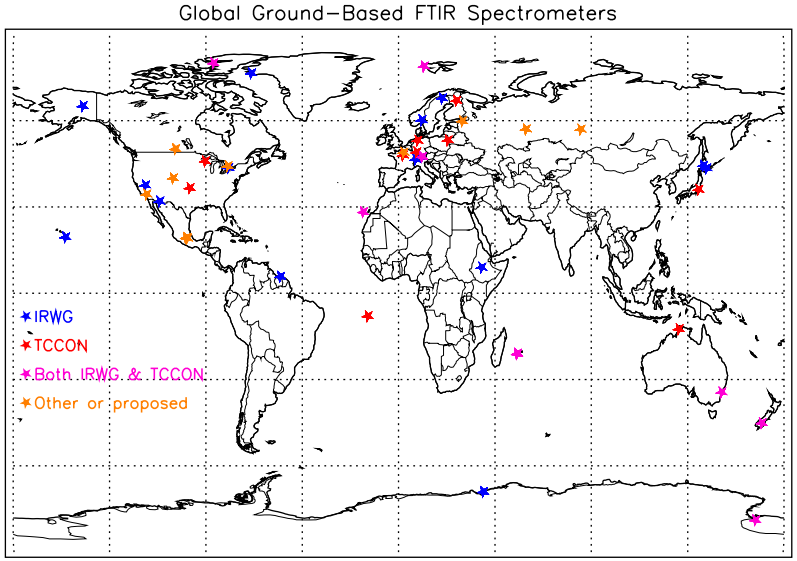
Global coverage with space-based remote sensing:

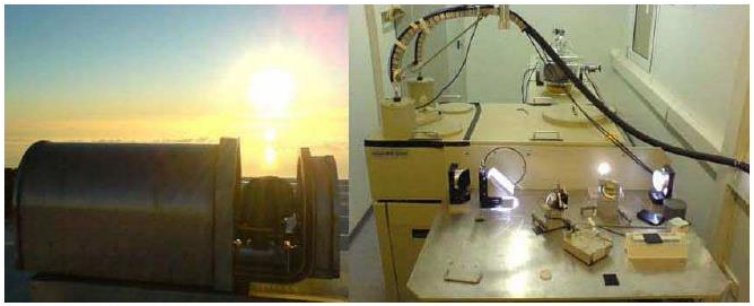


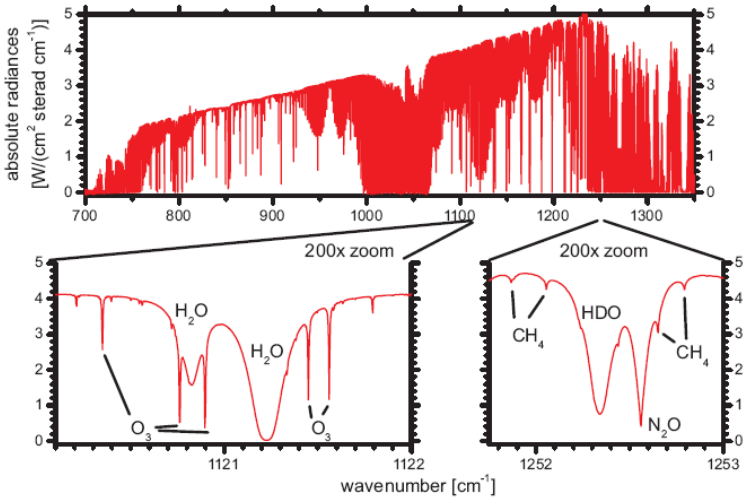
METOP/IASI

Schneider and Hase (2011); Schneider et al. (2012); Wiegele et al. (2014); Barthlott et al. (2014); Schneider et al. (2015); Dyroff et al. (2015)

FTIR experiments







FTIR networks: NDACC + TCCON

MUSICA works with a subset of NDACC stations. Data are centrally processed.

Simultaneous observation of absorption signatures of many different trace gases:

H_2O, HDO, O_3, N_2O, CH_4, HNO_3, CCl_2F_2, CCl_3F, $CHClF_2$, COF_2, $ClONO_2$, ClO, NO, NO_2, HCl, C_2H_6, HF, HCN, C_2H_2, CO, CO_2 ,OCS, NH_3, $COCl_2$, N_2

Traceable processing chain: measured spectra → retrieval + uncertainty estimation

MUSICA uses the PROFFIT retrieval code, F. Hase

Ground-based FTIR data processing (very similar for IASI)

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

⇒ Spectral fitting + Regularisation or Optimal Estimation Method

⇒ Minimize cost function: Rodgers (2000)

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

Optimal Estimation in Practice & Error estimation of State vector

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

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

```
y    = measurement
f()  = forward model
x    = state vector
b    = parameters required by fm
ε    = experimental errors
Sa   = covariance of a priori
Sε   = covariance of measurement
Kx   = sensitivity to measurement of fm
Kb   = sensitivity to param. b of fm
x̂    = best estimate for x
```

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

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

Optimal Estimation in Practice & Error estimation of State vector

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

Optimal Estimation in Practice & Error estimation of State vector

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

$$\hat{\vec{x}}-\vec{x}=(\mathbf{A}-\mathbf{I}_n)(x-x_a)$$ – Smoothing

$$+\mathbf{D}_y\mathbf{K}_b(\vec{b}-\hat{\vec{b}})$$ – Model parameters

$$+\mathbf{D}_y\varepsilon$$ – Measurement

Model error is neglected

K_b - Sensitivity of forward model to parameter b

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

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

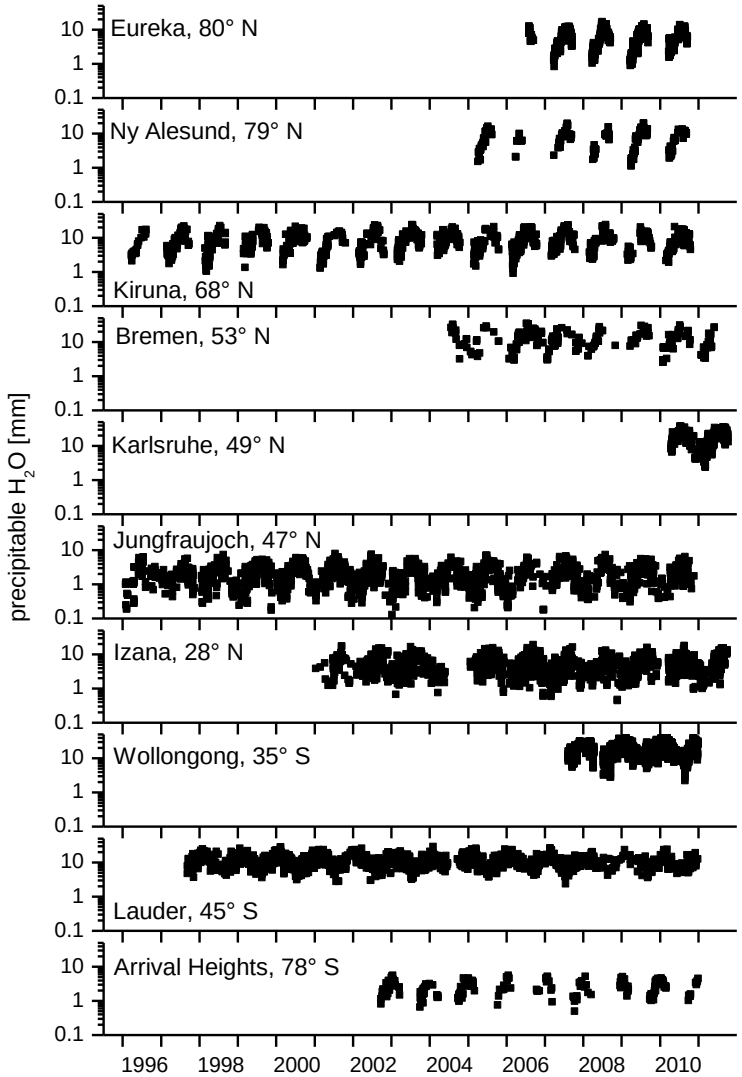
$$\mathbf{S}_b=\mathbf{D}_y\mathbf{K}_b\mathbf{S}_{par}\mathbf{K}_b^T\mathbf{D}_y^T \qquad \mathbf{S}_m=\mathbf{D}_y\mathbf{S}_\varepsilon\mathbf{D}_y^T$$

Finally determine Random and Systematic components separately

$$\mathbf{S}_{rand}=\sum\mathbf{S}_{bi}+\mathbf{S}_m \qquad \mathbf{S}_{syst}=\sum\mathbf{S}_{syst,i}$$

Provide averaging kernel A ⇒ smoothing error

FTIR H2O: data since mid 90s, …



Total number of available water vapour profiles: ≈15000

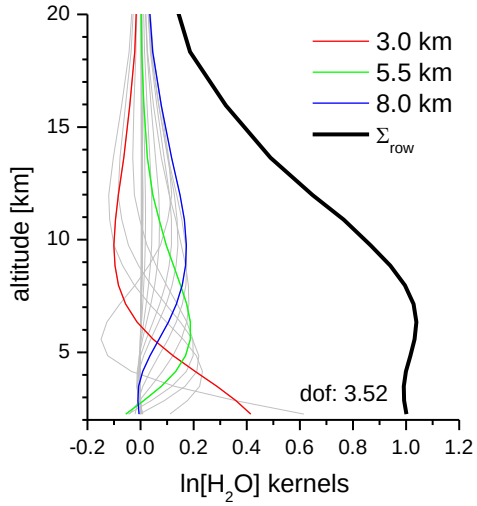
Spectra submitted by instrument PI then centrally processed at KIT

Representative for twelve globally distributed sites:

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

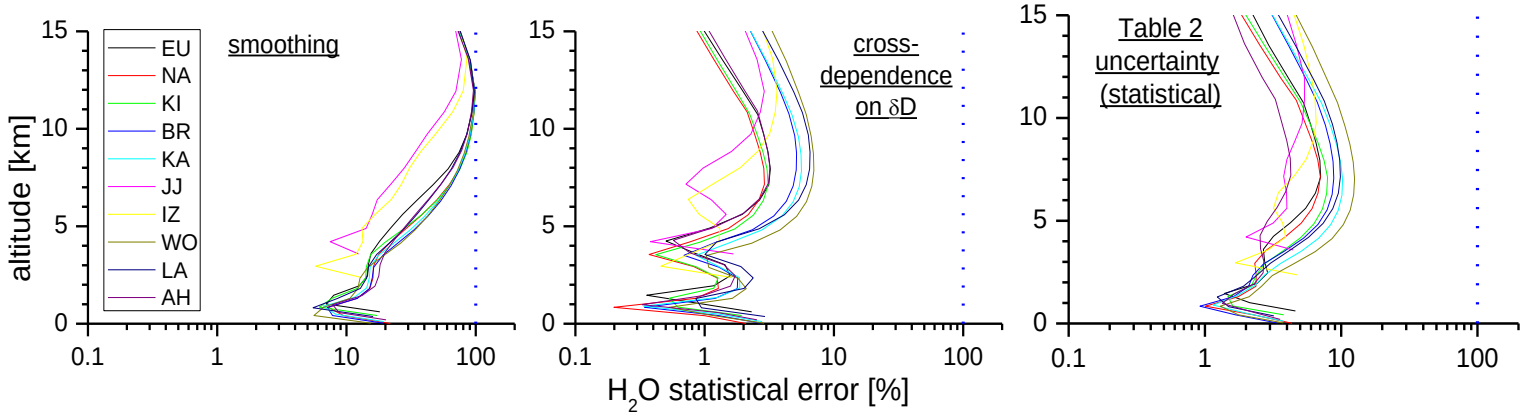
http://www.imk-asf.kit.edu/english/musica

FTIR H2O: Vertical Sensitivity & Error estimation



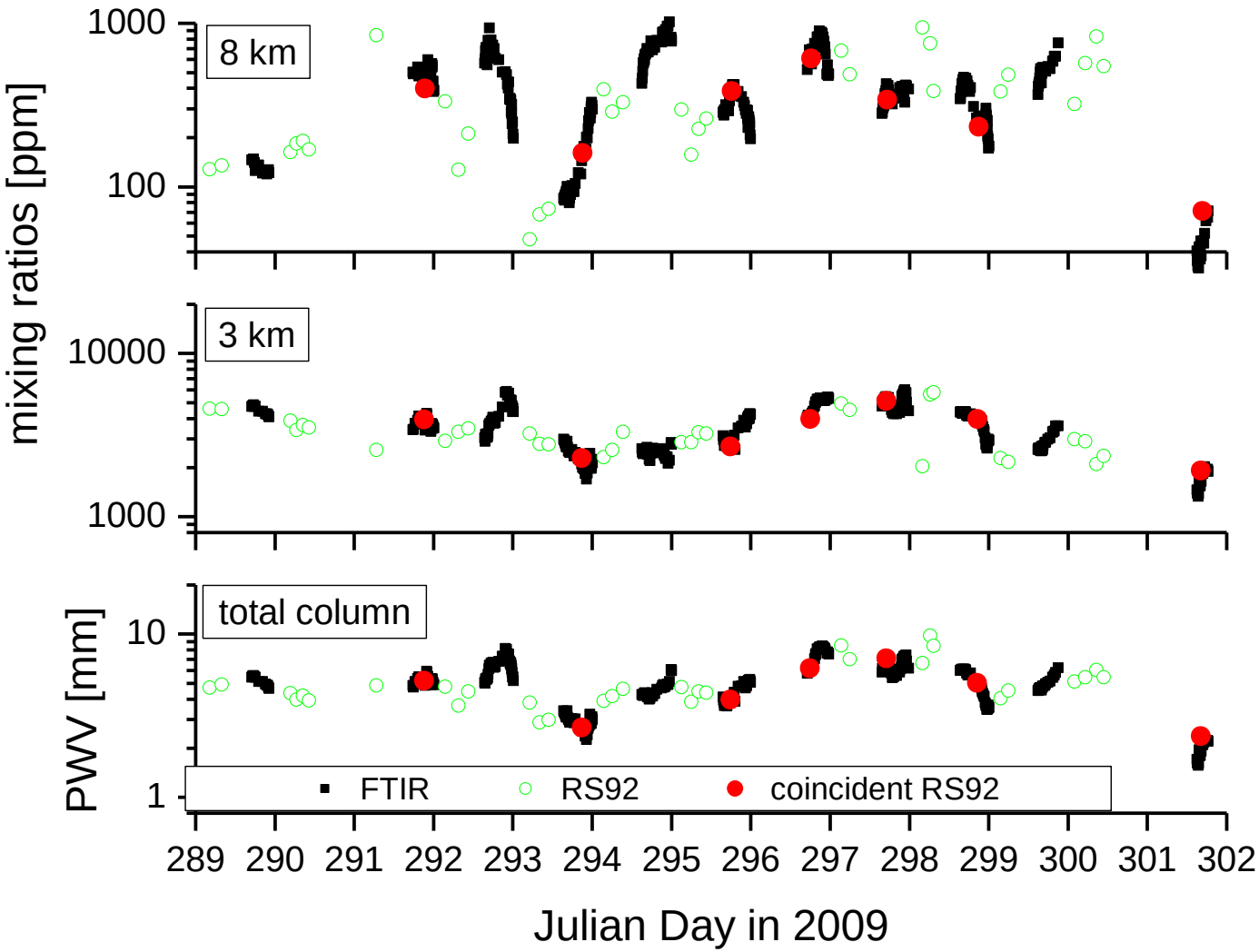
Example for Izana (28°N, 16°W, 2370 m asl)

Within MUSICA the 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"



One example of an empirical quality documentation of FTIR H_2O data

Example for the MOHAVE 2009 campaign:

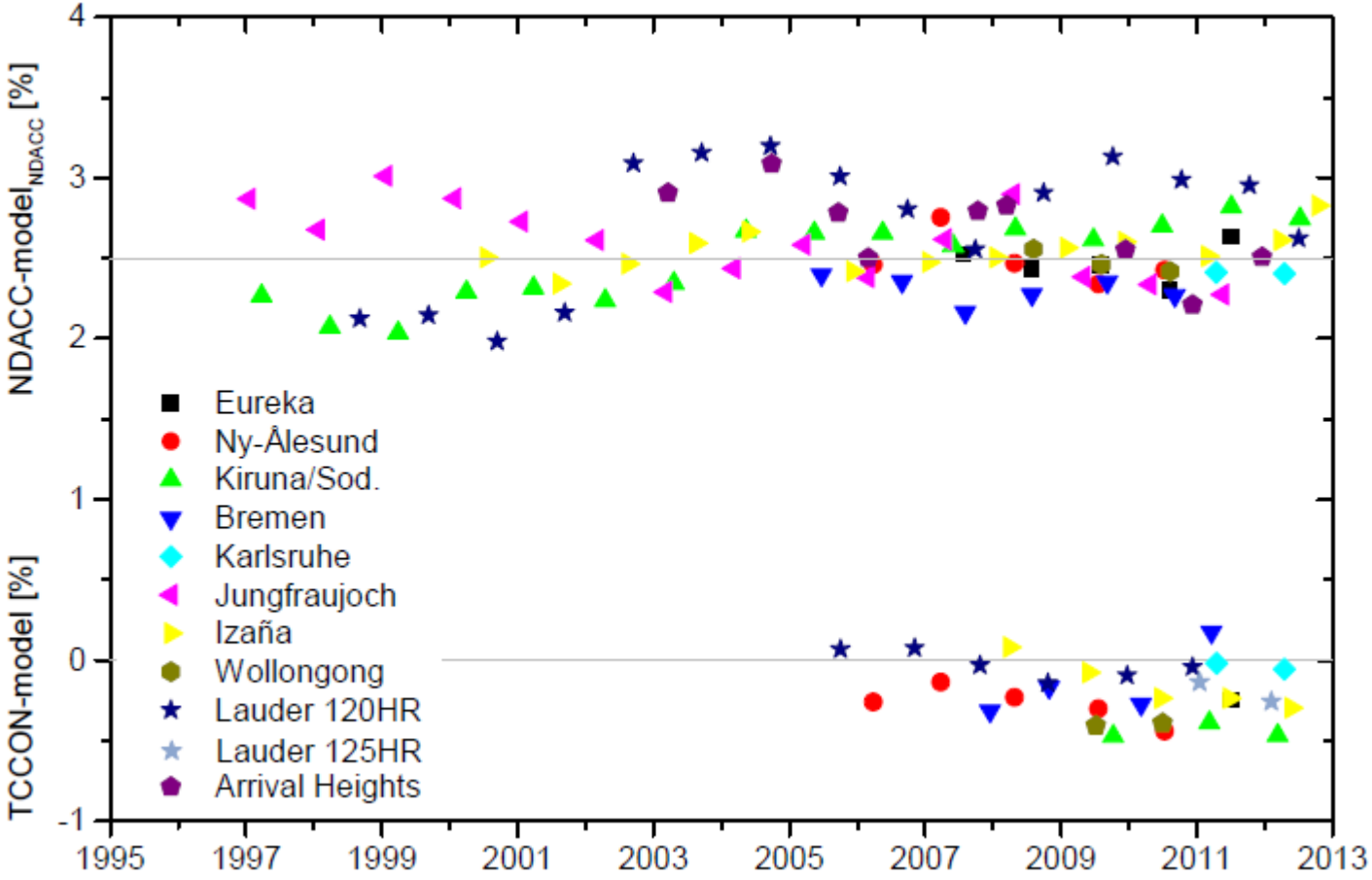


High measurement frequency is important for water vapour, because of the high variability!

<u>Acknowledgement</u>

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

Long-term and network-wide consistency (using CO_2, MIR, or O_2, NIR)

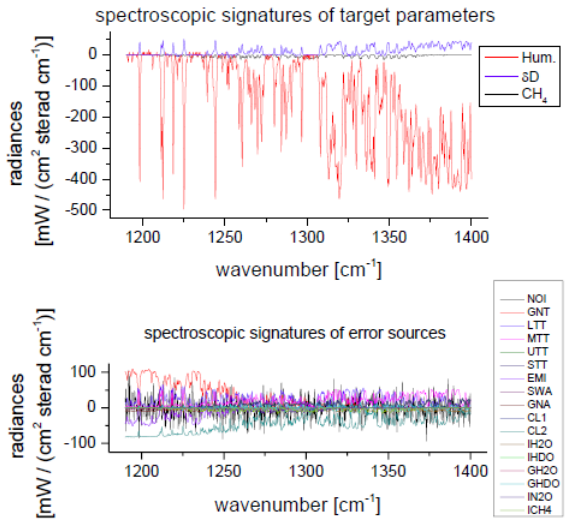


Barthlott et al. (2014)

→ the NDACC / FTIRs produce long-term datasets with a network-wide consistency

IASI: traceable data processing and error estimation

IASI data processing and error estimation



Humidity has a strong variability:
very strong signature

δD and CH4 variability is weak: weak signature!
→ retrieval will be difficult or very difficult!

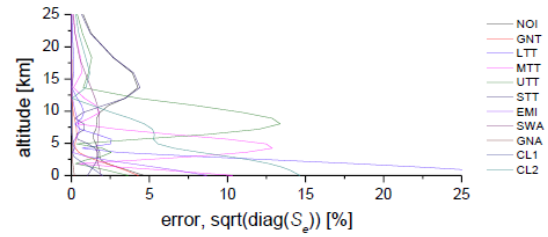
Error signatures (ϵ):

NOI: meas. Noise
GNT: ground temperature
LTT, MTT, UTT, STT: atmos. temp.
EMI: emissivity
SWA: Swath angle
CL1, CL2: low and high cloud
IH2O, IHDO, GH2O, GHDO, IN2O, ICH4: Hitran parameter uncertainty

→

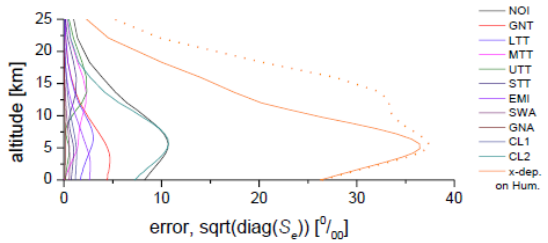
Typical IASI errors for the humidity and δD product

(1): Humidity error covariances: $S_e = G\epsilon\epsilon^T G^T$



Leading error sources:
- Atmospheric temperture uncertainty (LTT - STT)
- High subvisible cloud (CL2)

(2): δD (or HDO/H2O) error covariances (Schneider et al., 2012): $S_e = PG\epsilon\epsilon^T G^T P^T$
Trafo P: { ln[H2O] , ln[HDO] } → { 1/2*ln[H2O]+ln[HDO] , ln[HDO]-ln[H2O] }

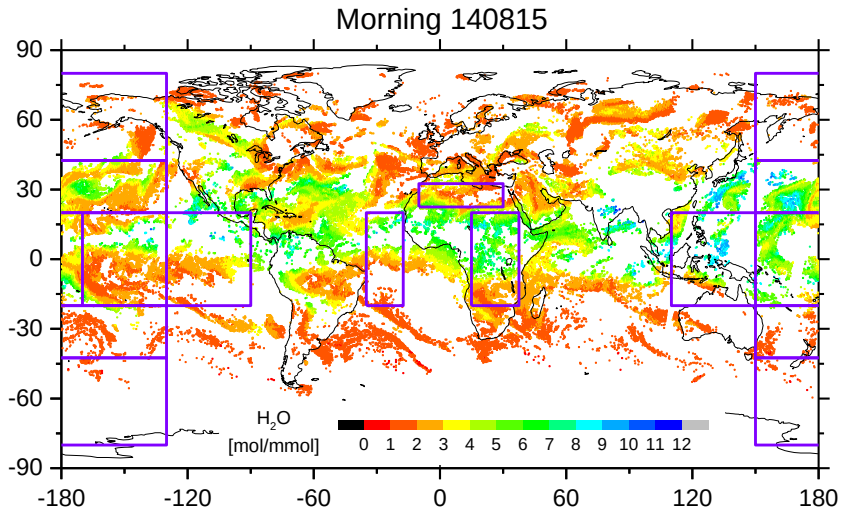


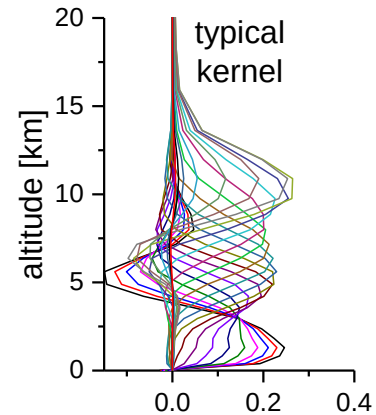
Leading error sources:
- Cross-dependence on humidity
- Measurement noise (NOI)
- High subvisible cloud (CL2)

For the MUSICA FTIR and IASI retrievals the same retrieval code (PROFFIT, F. Hase) is used and the data processing and characterisation is fully traceable and consistent.

Unique coverage of IASI data

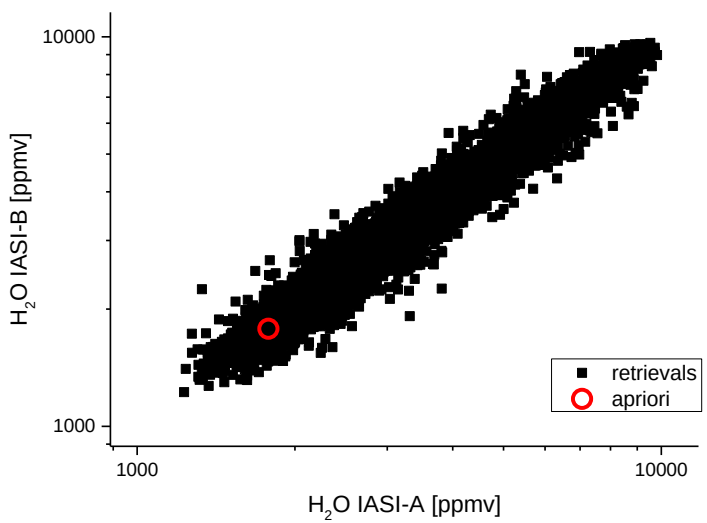
Example for a morning overpass on a single day:





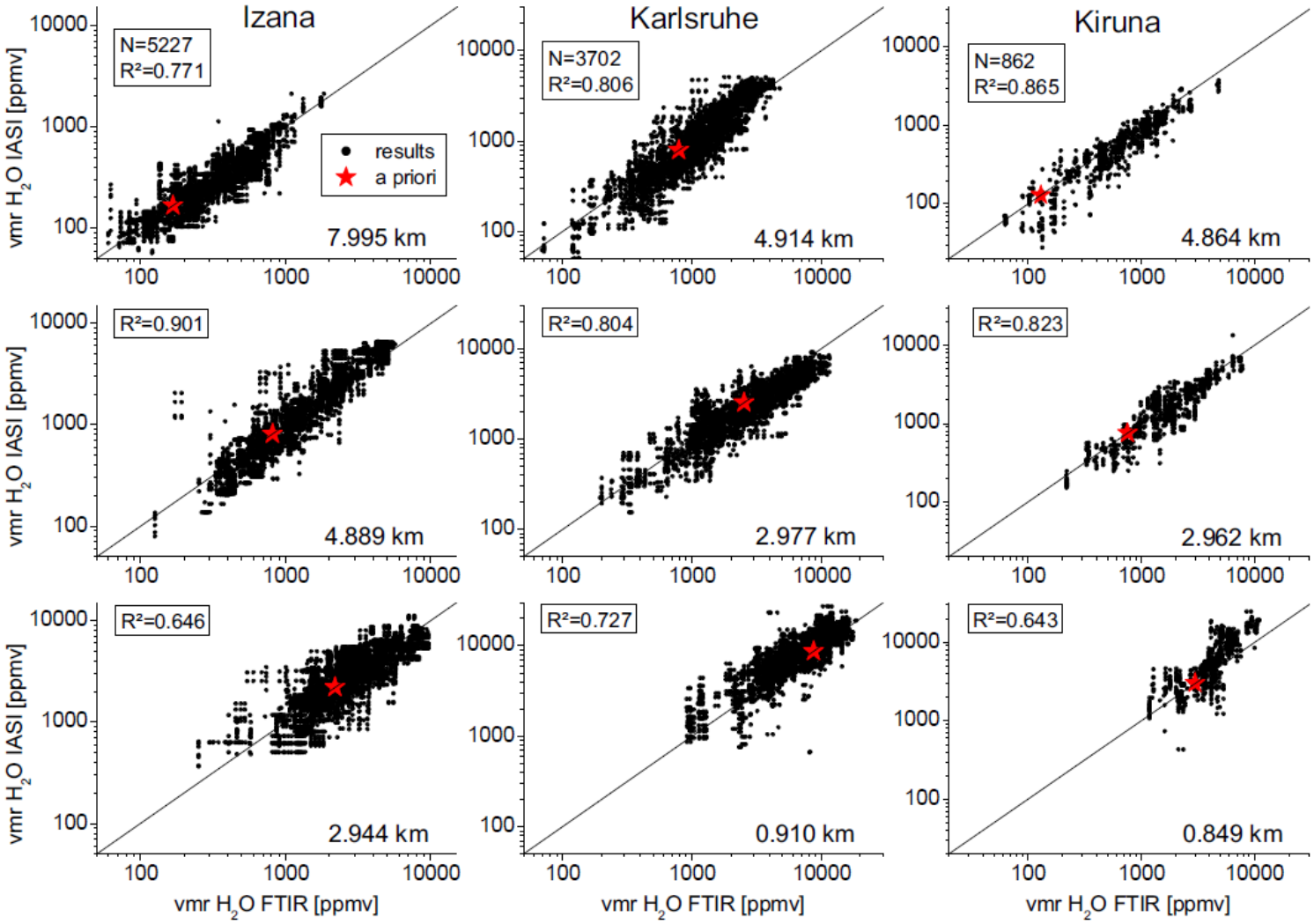
Filtered for reasonable sensitivity with respect to H2O and isotopologues.

IASI-A versus –B (coincidence criterion: within 1 hour and within 0.25° x 0.25°)



Very good agreement between IASI-A and -B!

IASI versus ground-based FTIR (H_2O): overview



Wiegele et al., 2014

Upper air water vapour isotopologue data

Tropospheric moisture transport affects atmospheric circulation (transport of latent heat and radiative forcing of clouds and water vapour) and the evolution of clouds, which in their turn are major uncertainties in climate models.
Water vapour isotopologues offer unique possibilities for tracking moisture pathways and thus for diagnosing the performance of climate models.

Sherwood et al. (Nature, 2014): free tropospheric moisture transport pathways determine model climate sensitivity

ARTICLE

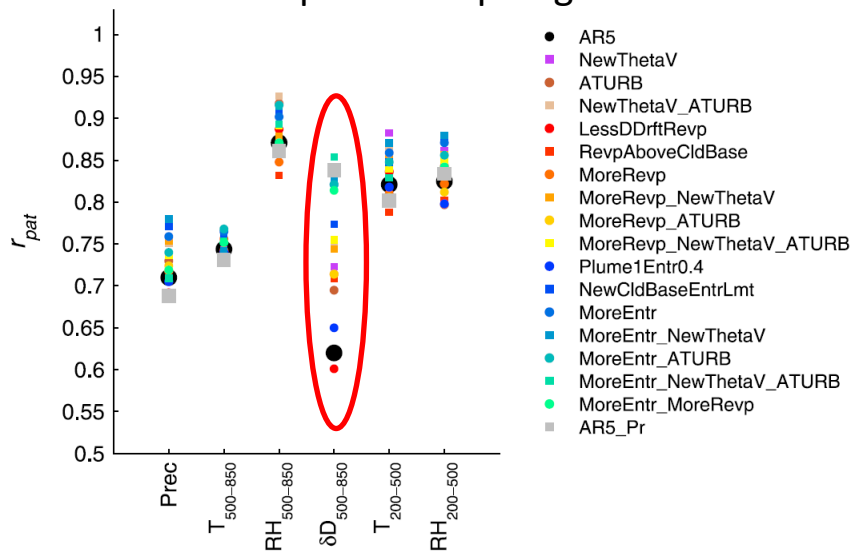
doi:10.1038/nature12829

Spread in model climate sensitivity traced to atmospheric convective mixing

Steven C. Sherwood[1], Sandrine Bony[2] & Jean-Louis Dufresne[2]

Equilibrium climate sensitivity refers to the ultimate change in global mean temperature in response to a change in external forcing. Despite decades of research attempting to narrow uncertainties, equilibrium climate sensitivity estimates from climate models still span roughly 1.5 to 5 degrees Celsius for a doubling of atmospheric carbon dioxide concentration, precluding accurate projections of future climate. The spread arises largely from differences in the feedback from low clouds, for reasons not yet understood. Here we show that differences in the simulated strength of convective mixing between the lower and middle tropical troposphere explain about half of the variance in climate sensitivity estimated by 43 climate models. The apparent mechanism is that such mixing dehydrates the low-cloud layer at a rate that increases as the climate warms, and this rate of increase depends on the initial mixing strength, linking the mixing to cloud feedback. The mixing inferred from observations appears to be sufficiently strong to imply a climate sensitivity of more than 3 degrees for a doubling of carbon dioxide. This is significantly higher than the currently accepted lower bound of 1.5 degrees, thereby constraining model projections towards relatively severe future warming.

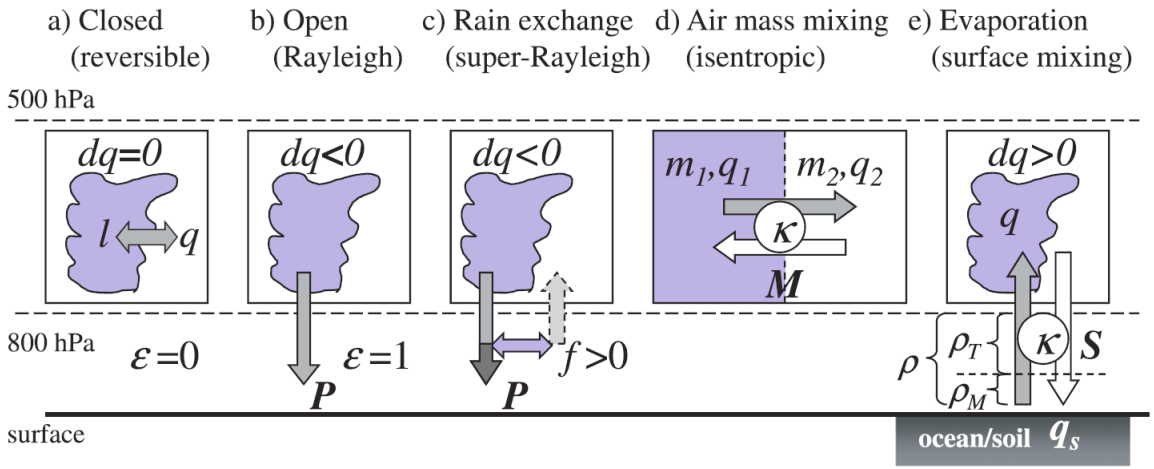
Field et al. (GRL, 2014): diagnosis opportunities of water vapour isotopologues

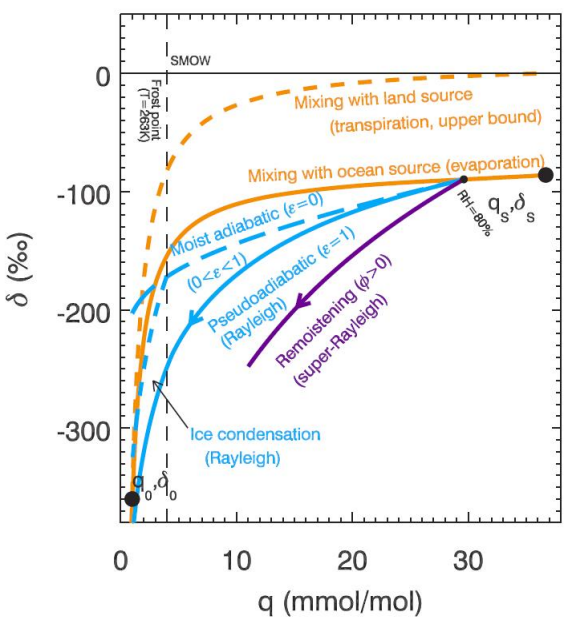


In addition, the water vapour isotopologues offer a link to the paleo-climate community: Icecore water isotoplogue analyses are a main fundament of paleo-climate research.

Water vapour isotopologue data: the δD-H2O pairs

Figures 1 and 2 from Noone (Journal of Climate, 2011):

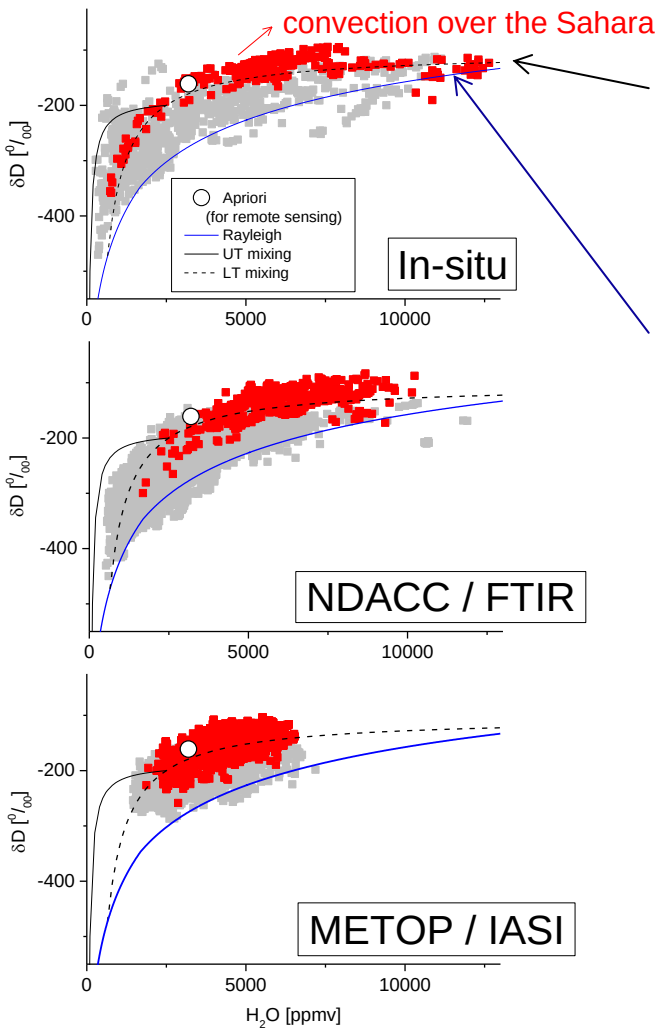




Simultaneous δD-H2O measurements reveal atmospheric moisture transport pathways.

Validation of isotopologue data: validate H2O-δD pairs!

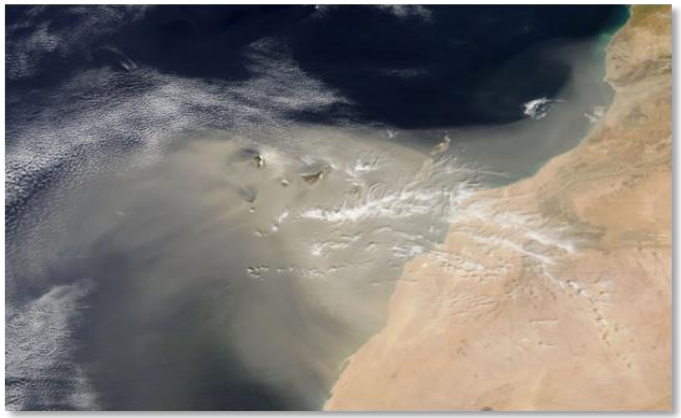
In situ and remote sensing observations west of the Sahara (at 650 hPa), a validation exercise:



Mixing lines: drying by mixing between humid and dry airmass (no condensation, δD is mainly determined by the humid airmass).

Rayleigh line: drying by condensation (vapour becomes increasingly depleted in HDO)

We use the dry convection mixing events over the Sahara for validating the added value of the isotopologues. Example of such event as seen in free tropospheric dust concentrations:

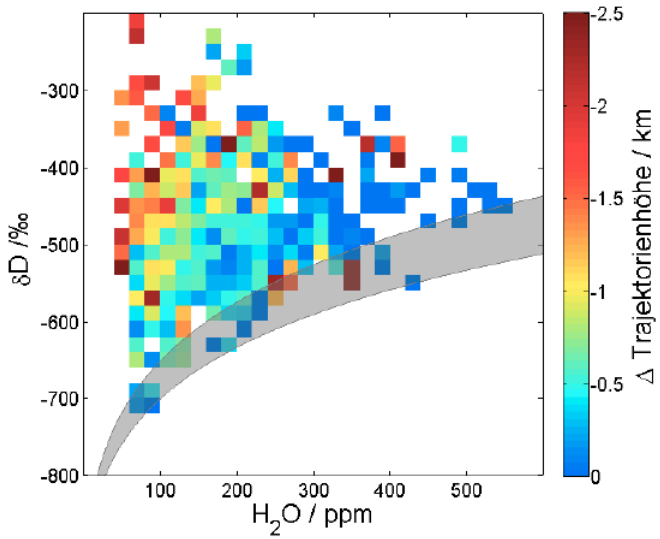


→ The MUSICA remote sensing data can well capture different moisture transport pathways.
→ The remote sensing signals are traced back to in-situ standards (MUSICA aircraft campaign!!!).

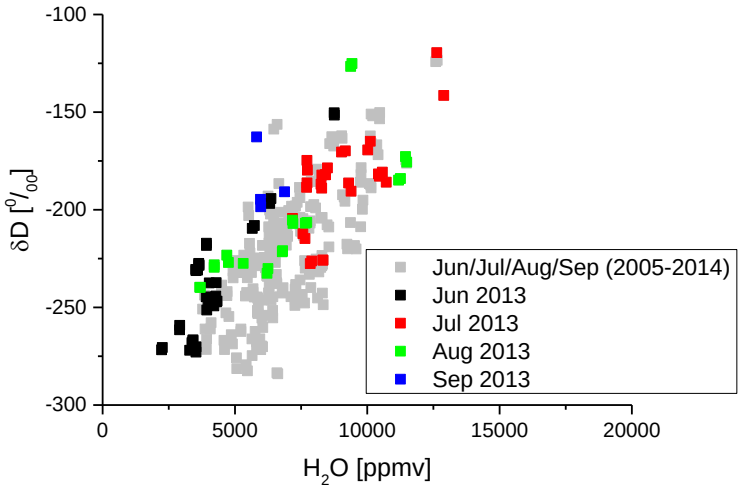
Schneider et al. (2015); Dyroff et al. (2015); González et al. (2015)

Water vapour isotopologue data: some examples

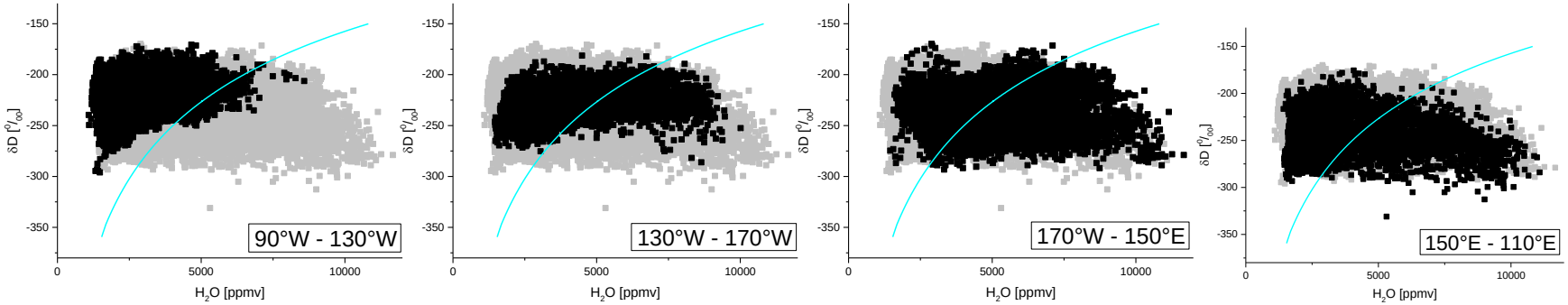
CARIBIC, 15°S-15°N, 10-12km, ice lofting during deep convection, Christner et al., in preparation



FTIR Ny Alesund (80°N), record sea ice melt in 2013, paper in preparation



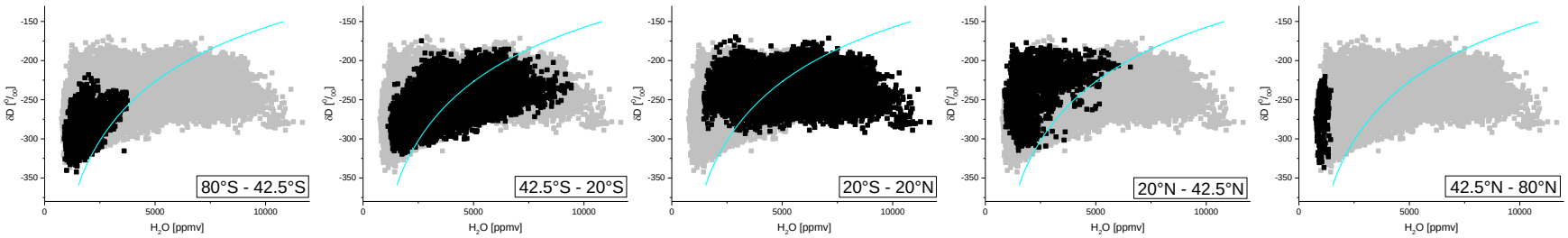
IASI, February 2014, Tropical Pacific, East –> West moistening largely via rain recycling, paper in preparation



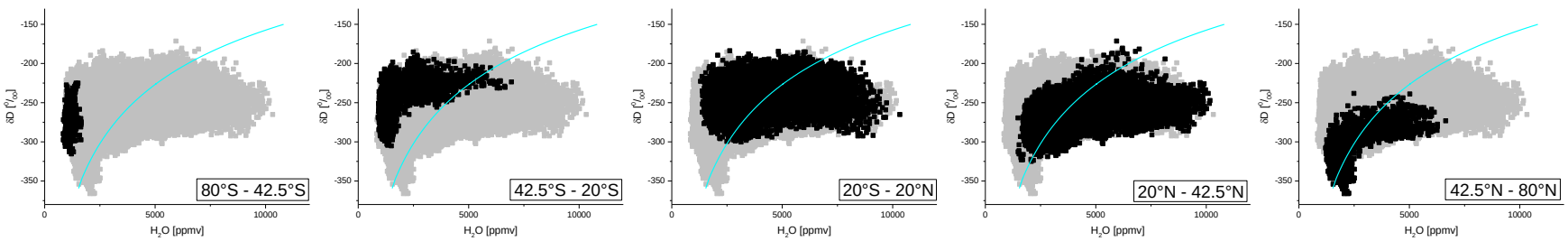
Water vapour isotopologue data: some examples

IASI, Central Pacific (130°W – 150°E) : South – North Cross Section, seasonal variation of the Tropical-Subtropical circulation (Hadley cell), paper in preparation.

February 2014

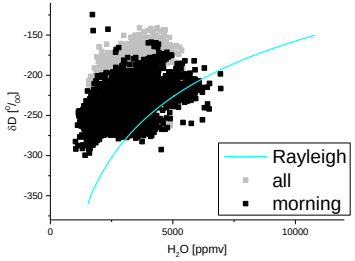


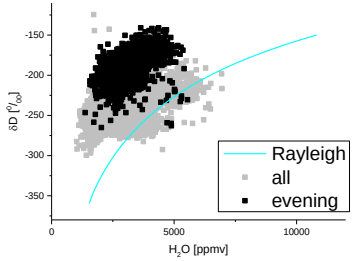
August 2014



Water vapour isotopologue data: morning vs. evening on 140616

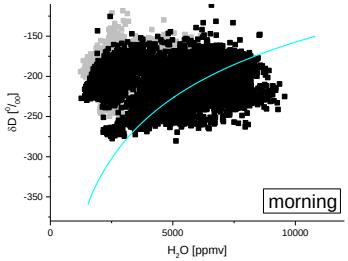
IASI, Northern Africa (Sahara desert, 22.5 – 32.5°N):

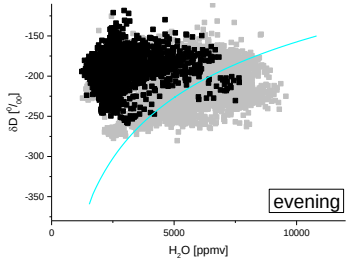




Pronounced diurnal cycle:
Dry Convection !

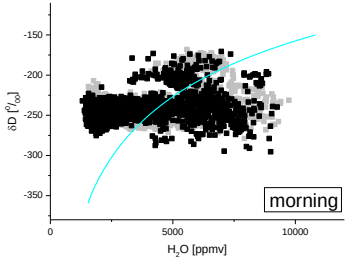
IASI, Tropical Africa (20°S – 20°N):

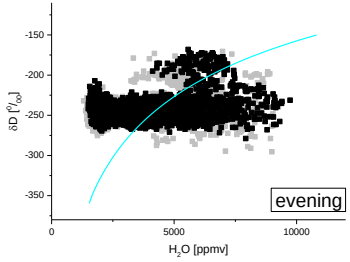




Pronounced diurnal cycle:
In the evening the rain evaporation signal is hidden by clouds

IASI, Tropical Atlantic (20°S – 20°N):





Over the ocean there is no significant diurnal cycle in the δD-H2O distribution.

Water vapour isotopologue data as essential climate variable (ECV)?

<u>Essential climate variables (ECVs) are identified based on the following criteria (Bojinski et al., BAMS 2014):</u>

$\delta D\text{-}H_2O$

"(1) RELEVANCE: The variable is critical for characterising the climate system and its changes."

"(2) FEASIBILITY: Observing or deriving the variable on a global scale is technically feasible using proven, scientifically understood methods."

"(3) COST EFFECTIVENESS: Generating and archiving data on the variable is affordable, mainly relying on coordinated observing systems using proven technology, taking advantage where possible of historical datasets."

Summary

- Two international networks with high resolution ground-based FTIRs: NDACC + TCCON
- MUSICA / FTIR: works with NDACC spectra, central processing, traceable retrieval and error estimation, many different empirical validation exercises
- MUSICA / IASI: optimal consistency to FTIR retrieval (traceability and error estimation), different validation exercises using in-situ or FTIR data, cross-validation between IASI-A and -B
- FTIR and IASI can observe free tropospheric δD-H2O pairs: promising opportunities for studying tropospheric moisture transport pathways and their evolution in a changing climate