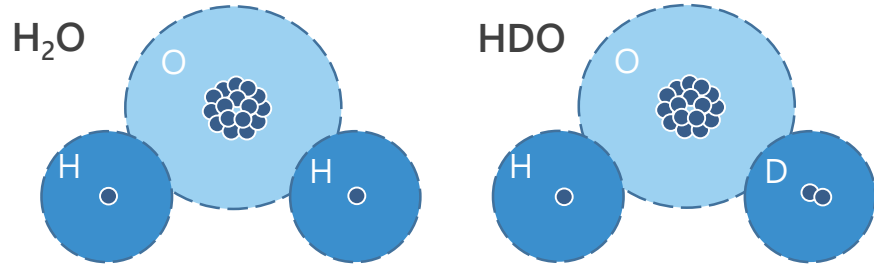


Water vapour isotopologue observations from space and their scientific potential: an update on MUSICA IASI activities

Matthias Schneider, Christopher J. Diekmann, Frank Hase,
Nga Ying Lo, and Kanwal Shahzadi

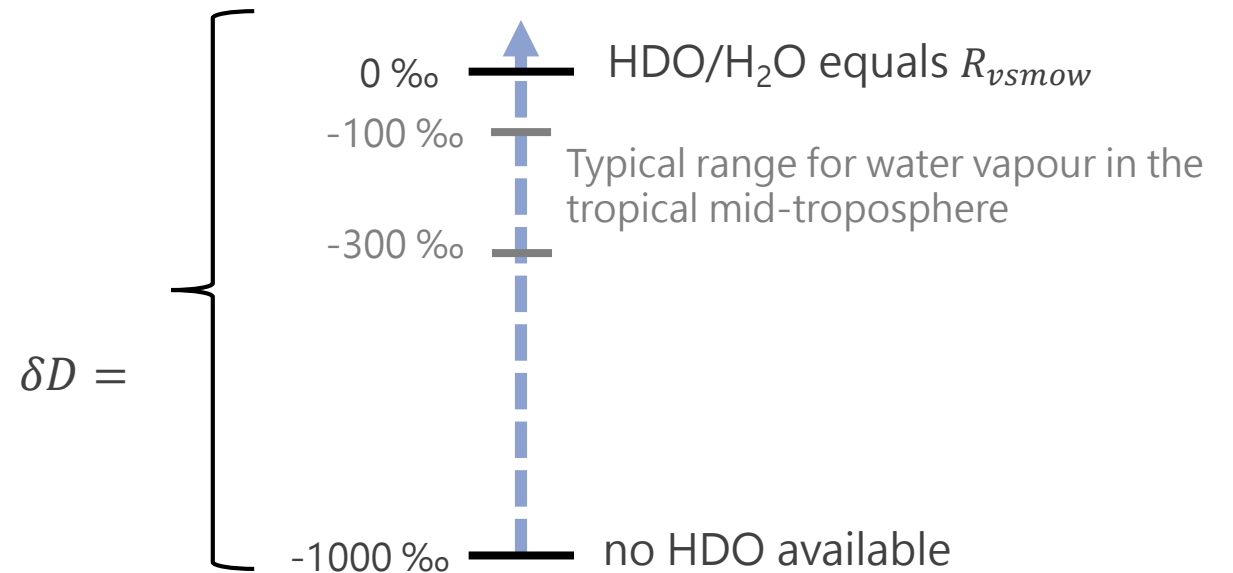
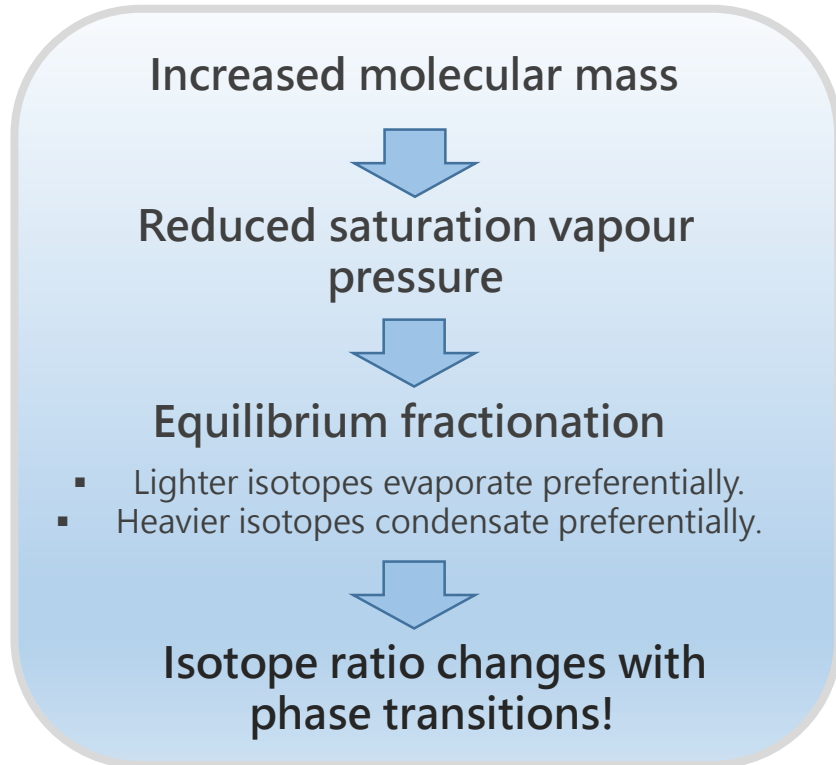
- Introduction to atmospheric water vapour isotopologues
- MUSICA IASI isotopologue retrieval and data set
- Example of moisture transport studies using the MUSICA IASI isotopologue data
- Summary

Isotopic fractionation



$$\delta D = \left(\frac{HDO/H_2O}{R_{vsmow}} - 1 \right) * 1000$$

Water isot.	H ₂ ¹⁸ O	H ₂ ¹⁷ O	HDO	...
R _{vsmow}	0.201 %	0.039 %	0.031 %	...



➔ Unique potential for tracking moisture processes

The MUSICA IASI retrieval

Optimal estimation of trace gas ratio data (isotopologue ratios are the interesting data):

(1) Transfer the problem to the logarithmic scale: $\partial \ln x = \frac{1}{x} \partial x$

(2) Optimal estimation of ratio (δD) proxies: $\ln \left[\frac{\hat{x}_{\text{HDO}}}{\hat{x}_{\text{H}_2\text{O}}} \right] = \ln \hat{x}_{\text{HDO}} - \ln \hat{x}_{\text{H}_2\text{O}}$

(3) Post-processing to generate H₂O and δD products having the same sensitivity: {H₂O, δD } pairs

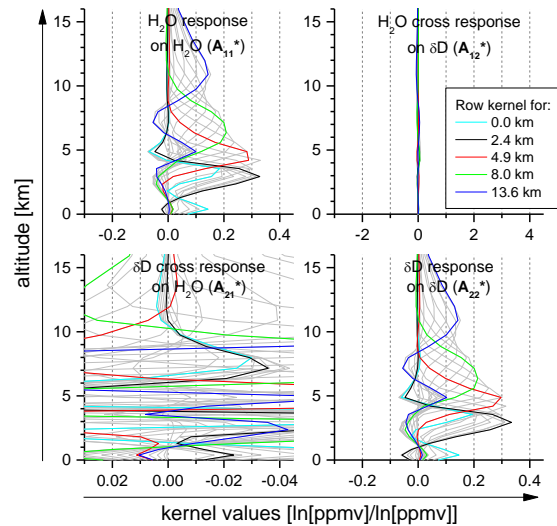
Individual optimal estimation
of H₂O and HDO



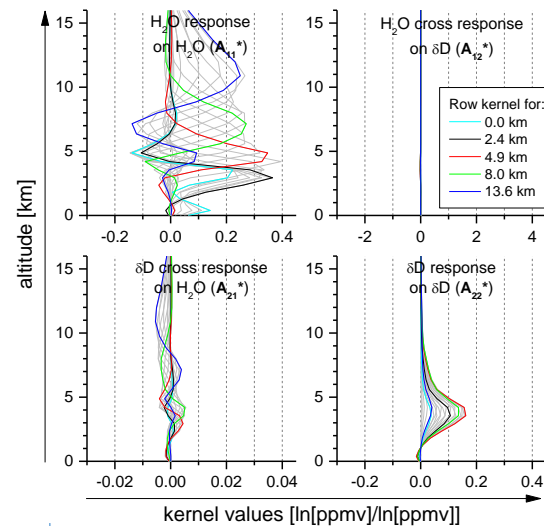
(1+2) Optimal estimation
of H₂O and δD proxies



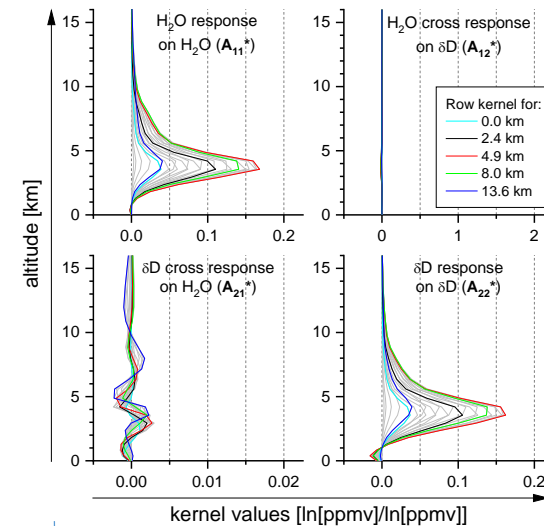
(3) Post processing:
generation of {H₂O, δD } pairs



Not useful

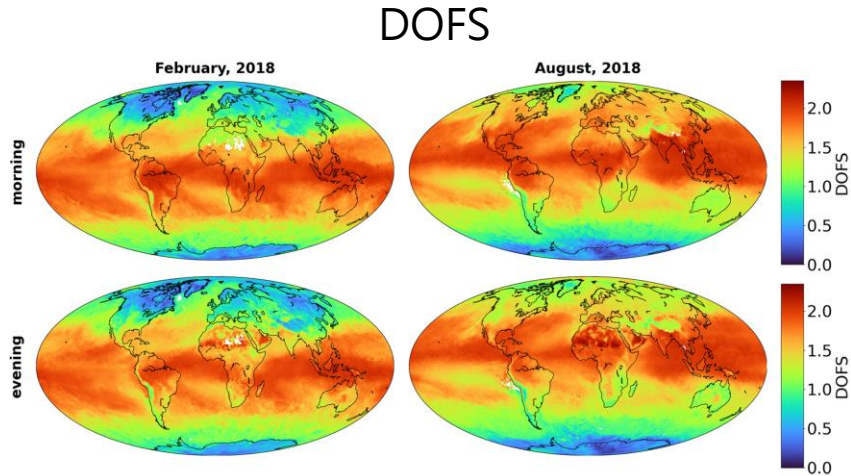


MUSICA IASI retrieval output

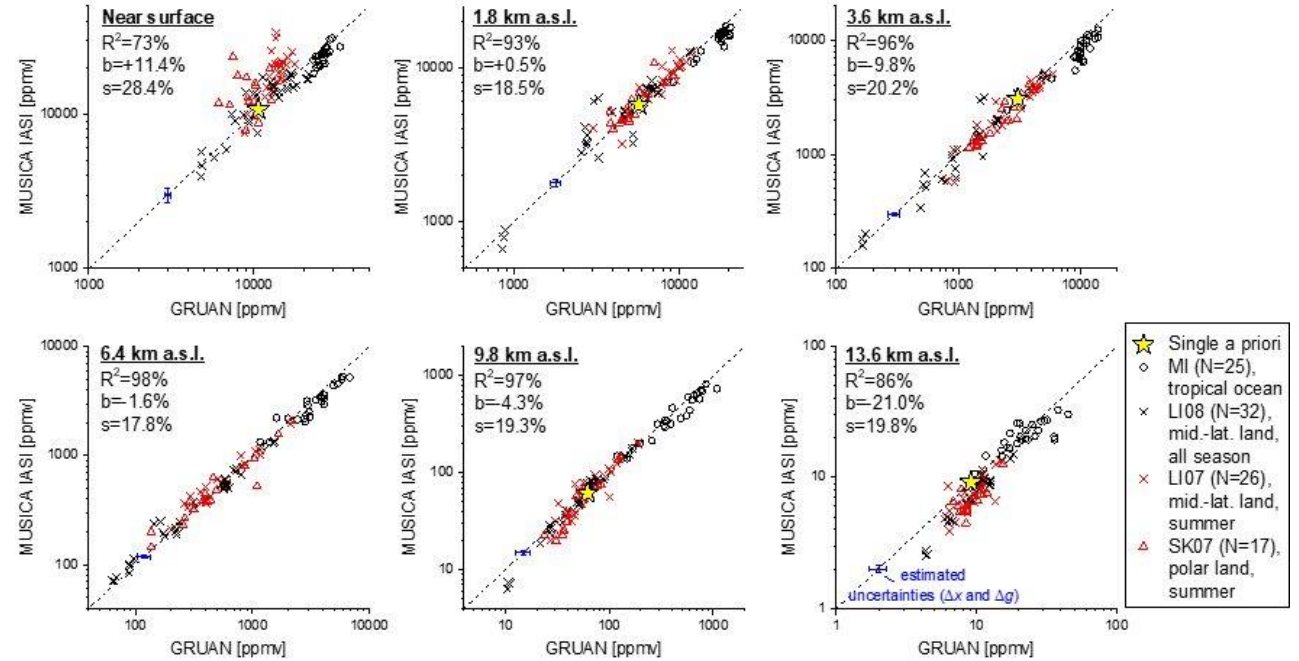


This is the MUSICA IASI
{H₂O, δD } pair product!

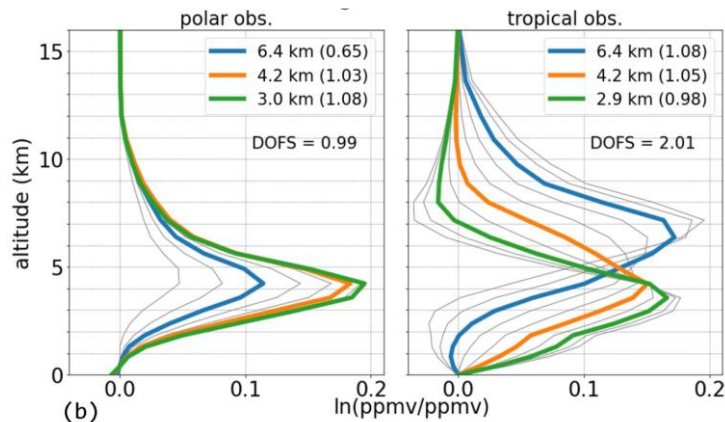
The MUSICA IASI retrieval



Validation with GRUAN and dedicated aircraft campaign

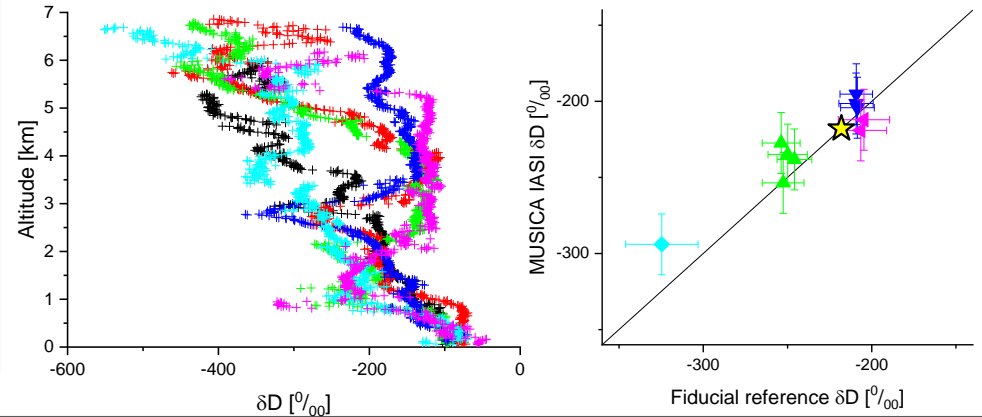


Examples of averaging kernels



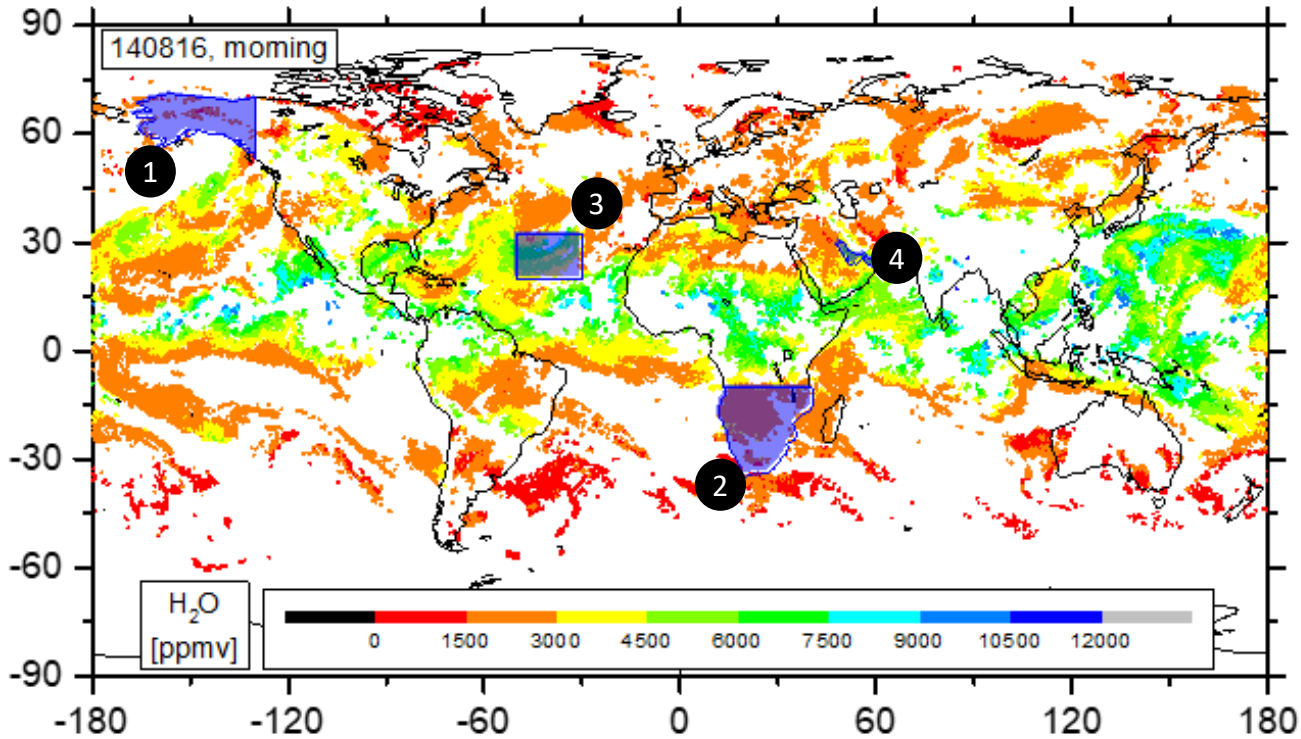
Uncertainties

Typically 10% (H_2O) and 10-20‰ (δD)



Borger et al., 2017; Diekmann et al. 2021; Schneider et al., 2016

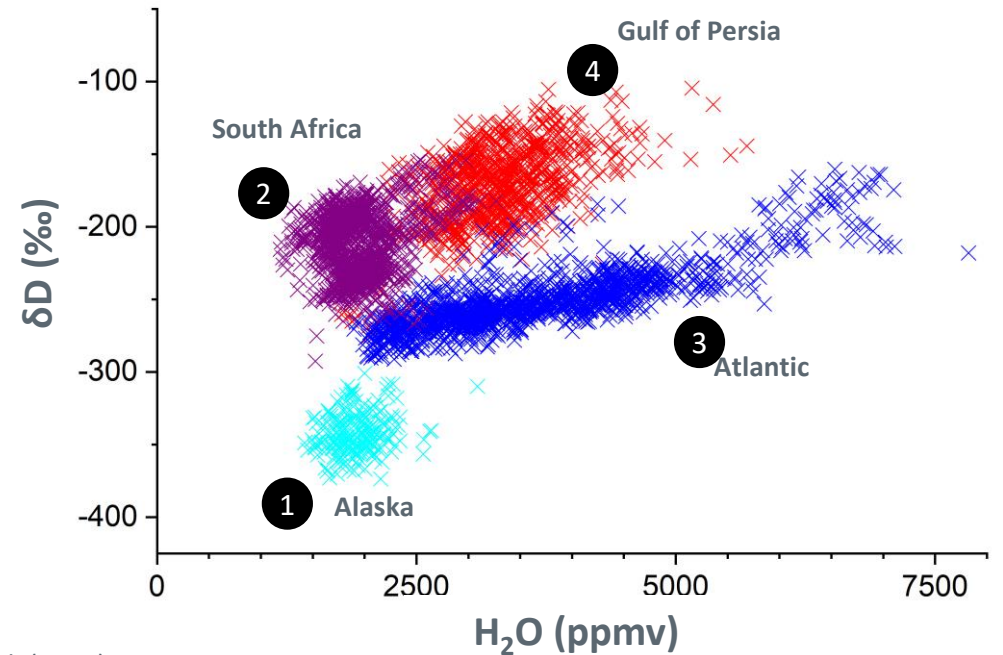
Pairs of H₂O and δD



Global H₂O-distribution in mid-tropospheric water vapour

Schneider et al. (2016)

Pairwise analysis of H₂O and δD in water vapour

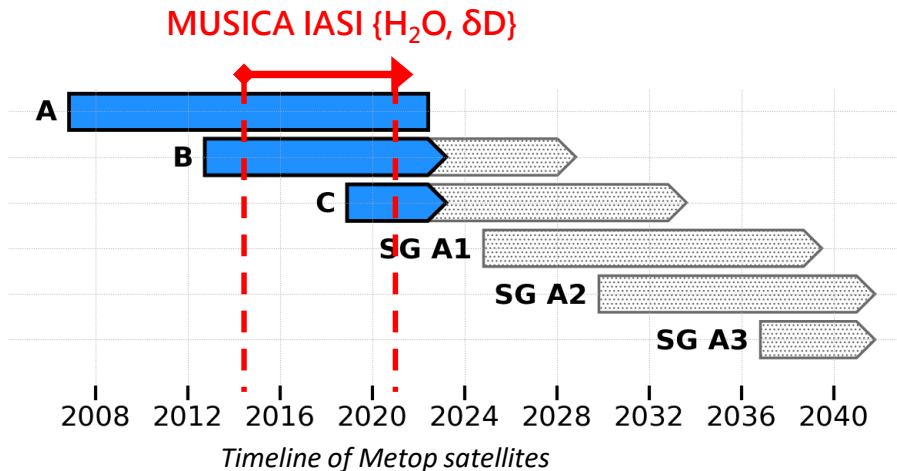
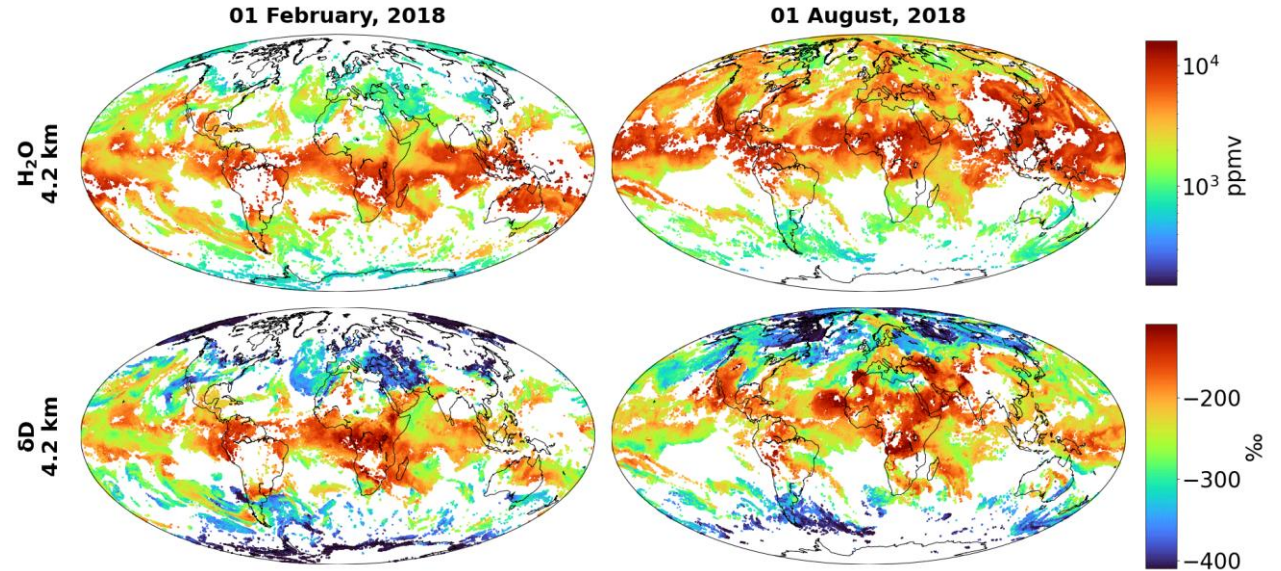


Effects of different moisture processes become visible when analysing the {H₂O, δD}-pair distribution

MUSICA IASI datasets of $\{H_2O, \delta D\}$ pairs

Unique potential of IASI

- Up to 3 satellites in orbit, allowing up to 500.000 cloud-free quality-filtered and vertically resolved HDO/H₂O observations per day
- Continuity of data availability over several decades
- Current status of data availability (MUSICA IASI processor): full long-term dataset (> 6 years, > 2 billion data points),
 - IASI Retrieval: Schneider et al (2022)
 - $\{H_2O, \delta D\}$ post-processing: Diekmann et al (2021)

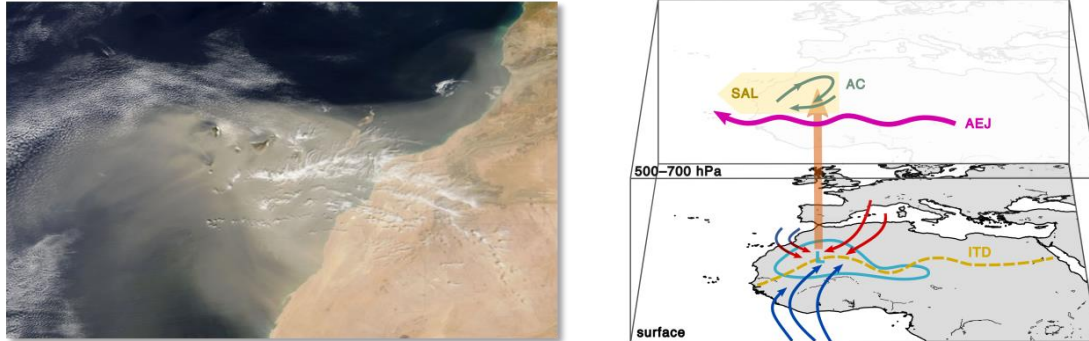


Daily maps of IASI $\{H_2O, \delta D\}$ data

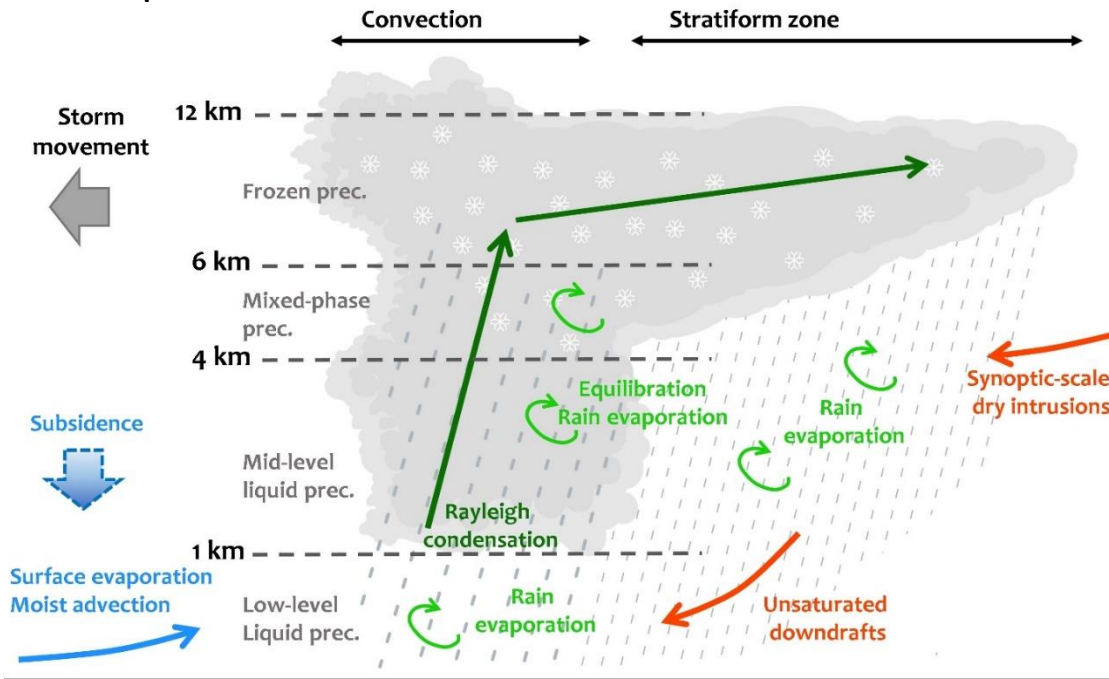
- Morning and evening overpasses
- Two global maps per day
- Cloud-free pixels
- Focus on free troposphere (~ 4.2 km)
- Usage of flags for quality filtering

Moisture transport

Airmass mixing (no phase transitions, e.g., Saharan Air Layer):

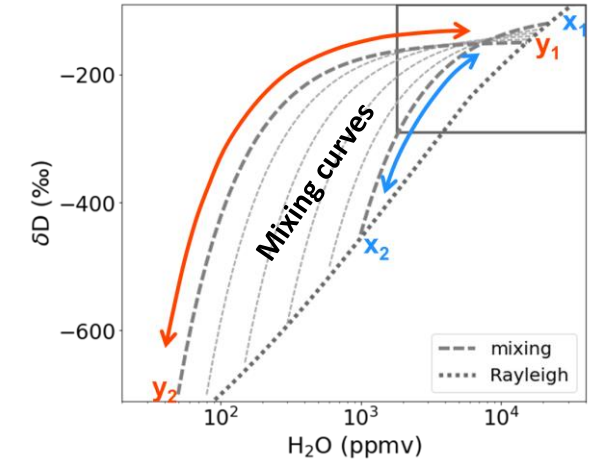


Cloud processes:



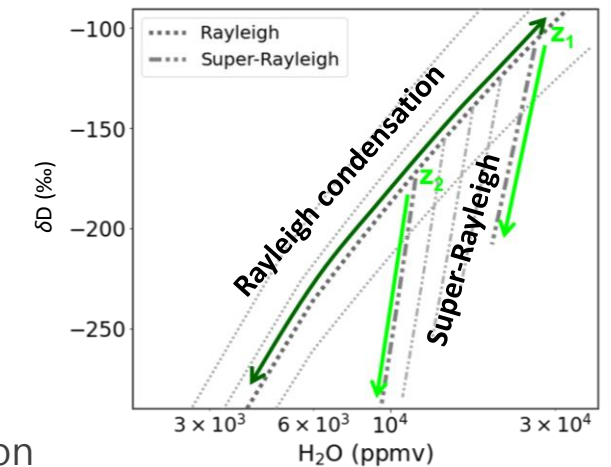
Theoretical process lines in the {H₂O, δD} phase space

Mixing of air masses
Mixing curves for air mass mixing without fractionation



Rayleigh Condensation
Rain condensation during moist adiabatic ascent

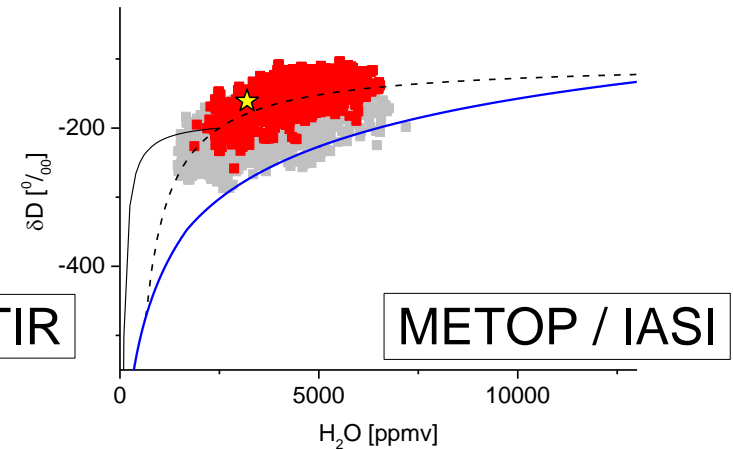
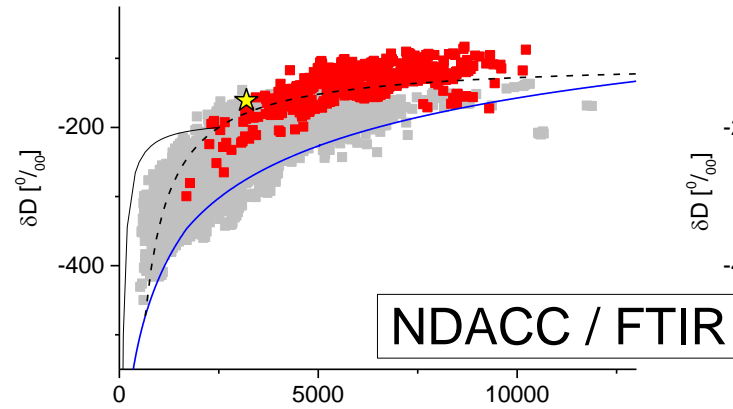
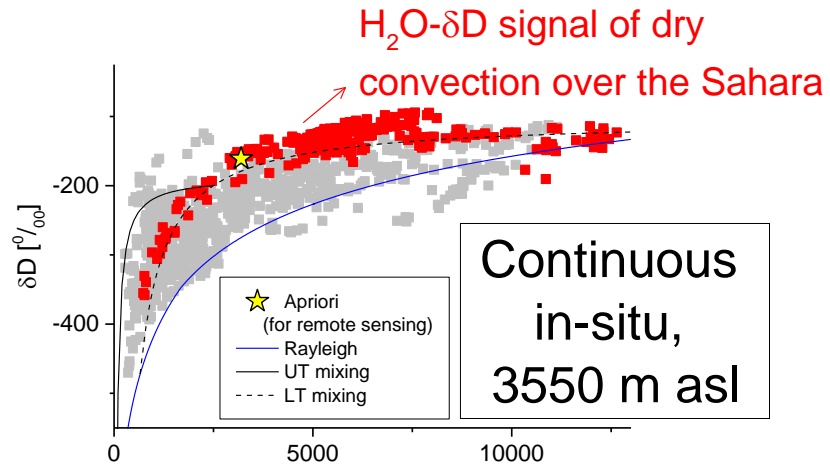
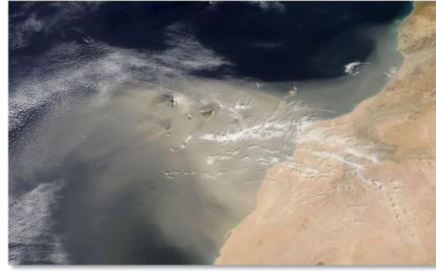
Super-Rayleigh Signals
Special case of Rayleigh condensation, which is overlaid by partial rain evaporation and equilibration



Noone et al, 2012; Diekmann et al, 2021b

Moisture transport

Well-studied airmass mixing (Saharan Air Layer):

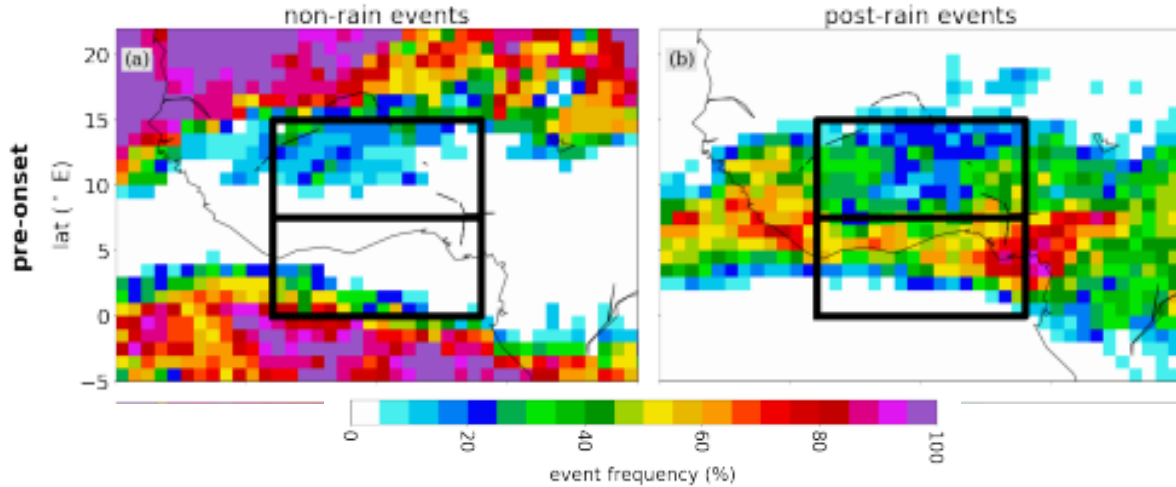


Serves also as process-based validation of the MUSICA IASI {H₂O, δ D}-pair distribution (Schneider et al., 2016)

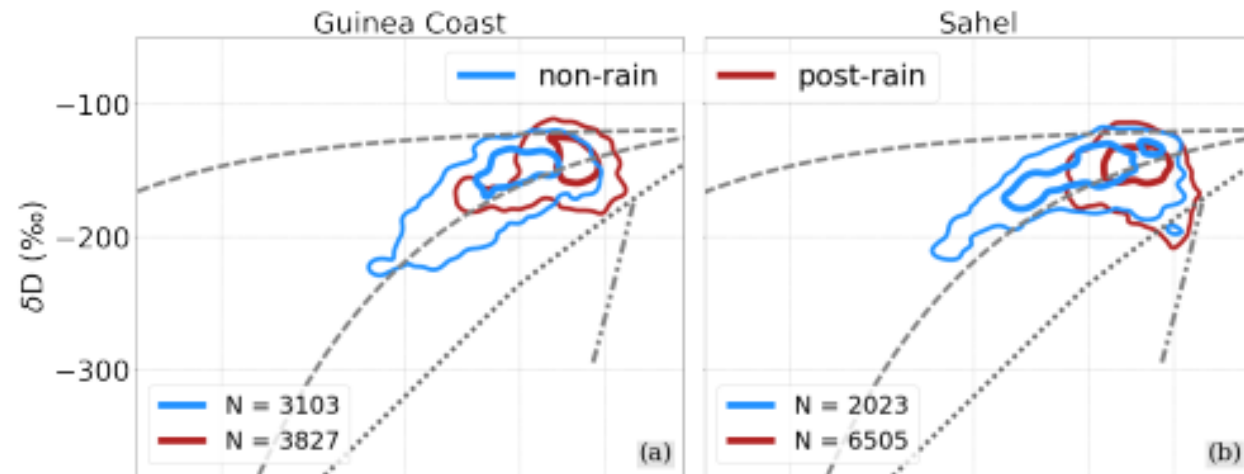
Moisture transport

Example West African Monsoon, Diekmann et al., 2024

Classification: rain versus non-rain (IMERG)

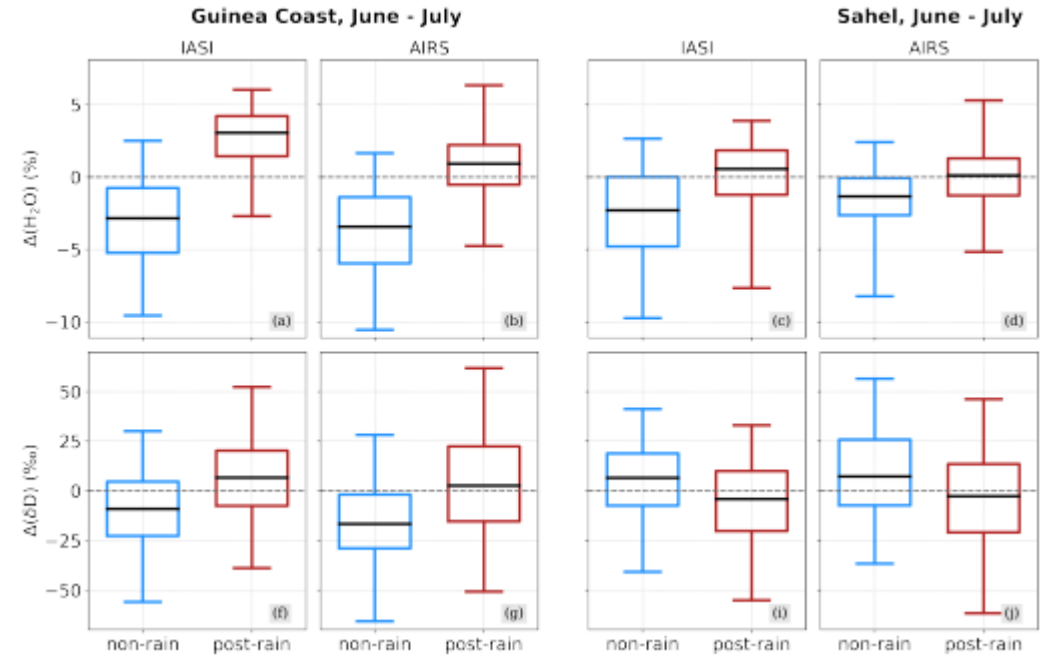


{H₂O, δD} distribution: rain versus non-rain



Figures adopted from Diekmann et al. (2024)

Anti-correlation between H₂O and δD



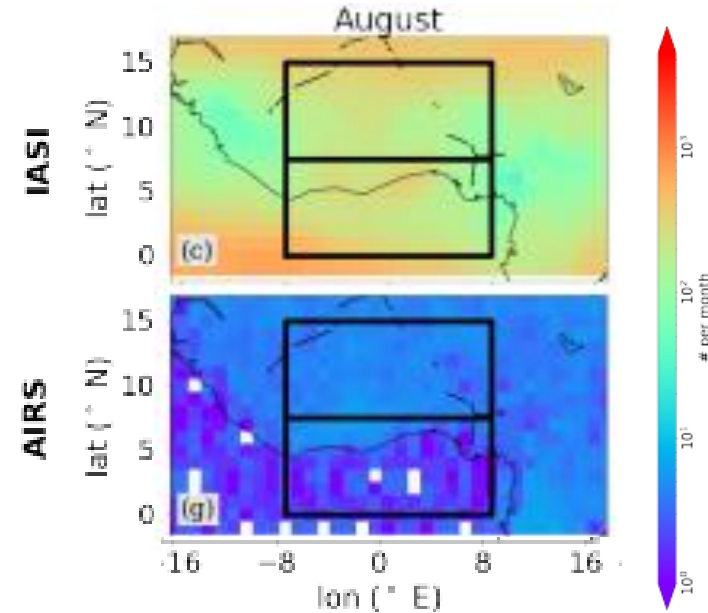
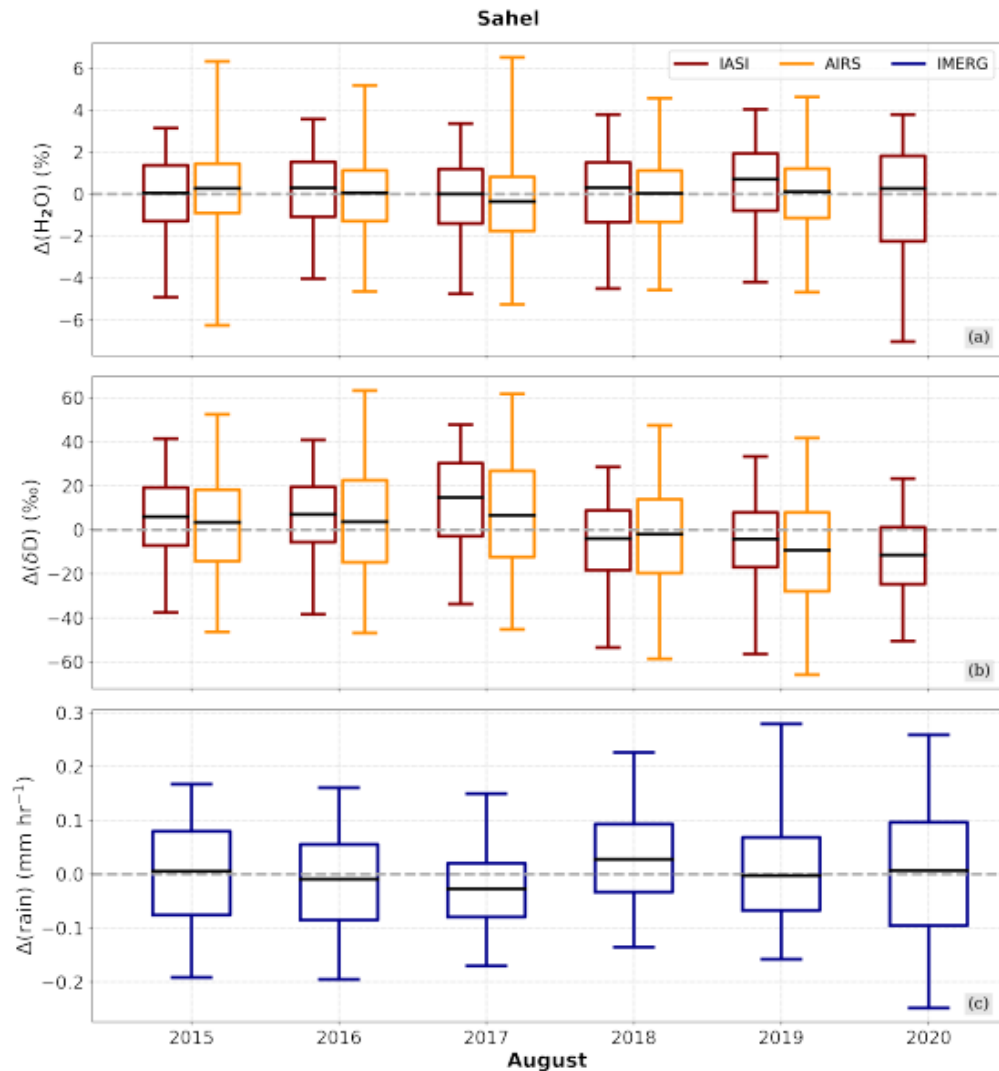
Guinea Coast: generally positive correlation between H₂O and δD

Sahel: super-Rayleigh {H₂O, δD} distribution significantly more frequent after rain events.

-> Anti-correlation between H₂O and δD.

Moisture transport

Covariation of West African Monsoon precipitation intensity and middle tropospheric water vapour isotopologues, Diekmann et al., 2024



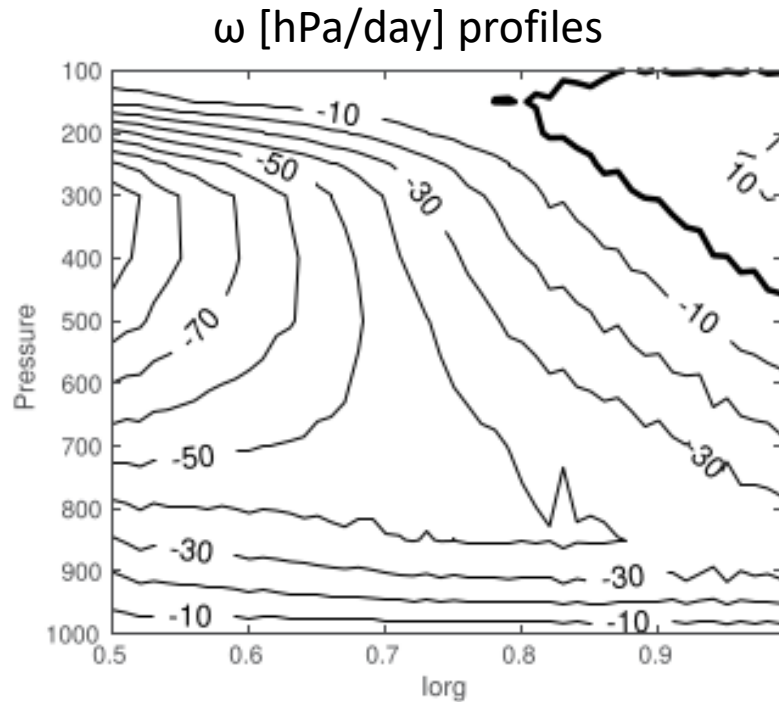
Study using middle tropospheric $\{\text{H}_2\text{O}, \delta\text{D}\}$ data from IASI and ARIS

2017: weakest HDO depletion (weakest super-Rayleigh signal) for lowest mean rainfall
2015-2017 versus 2018-2020: increasing peak rain intensity is correlated with stronger super-Rayleigh signal.

Moisture transport

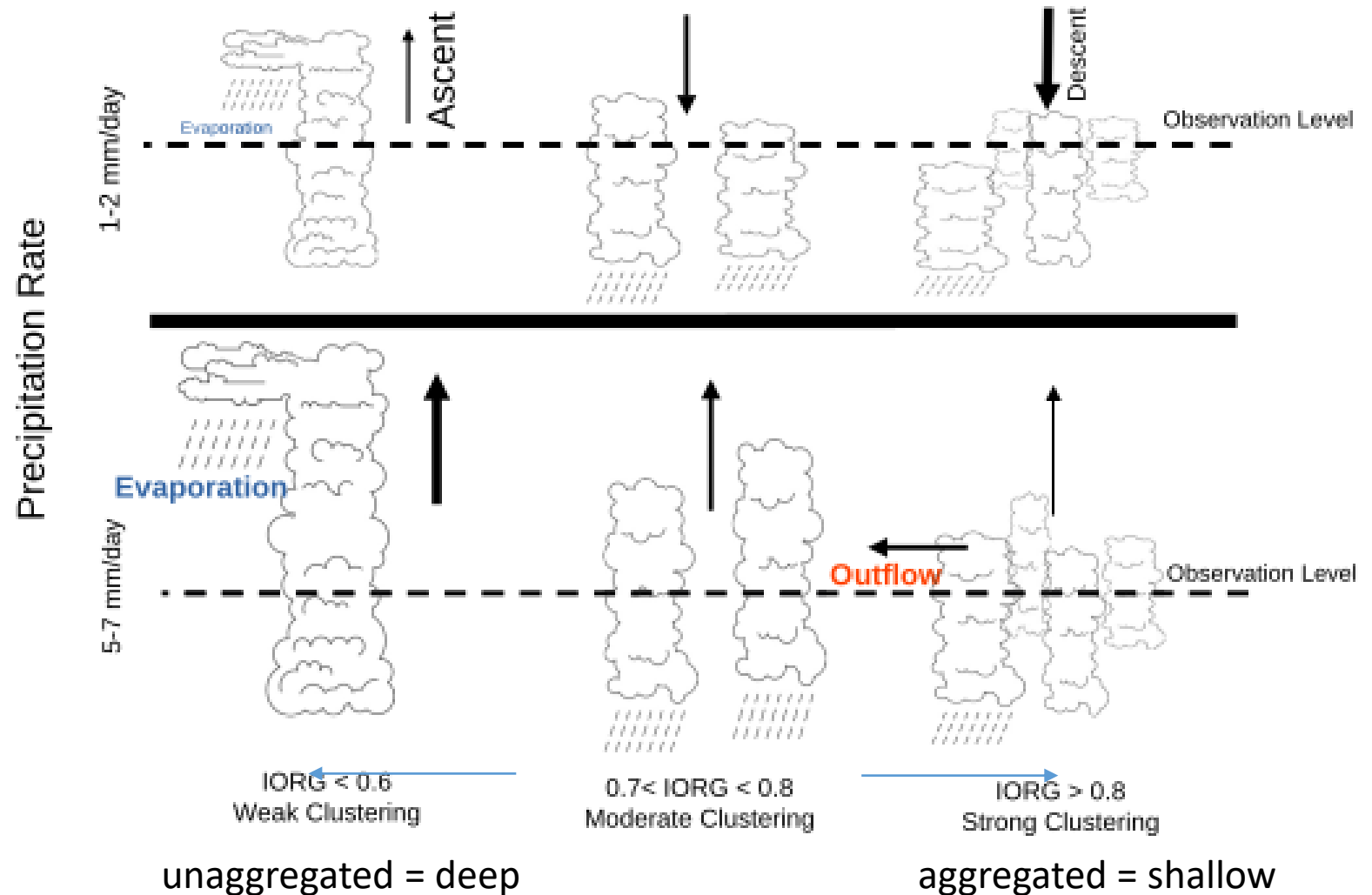
Galewsky et al. (2023): Convective organization and mid-tropospheric water vapour isotopologues

Convection intensity and degree of organization



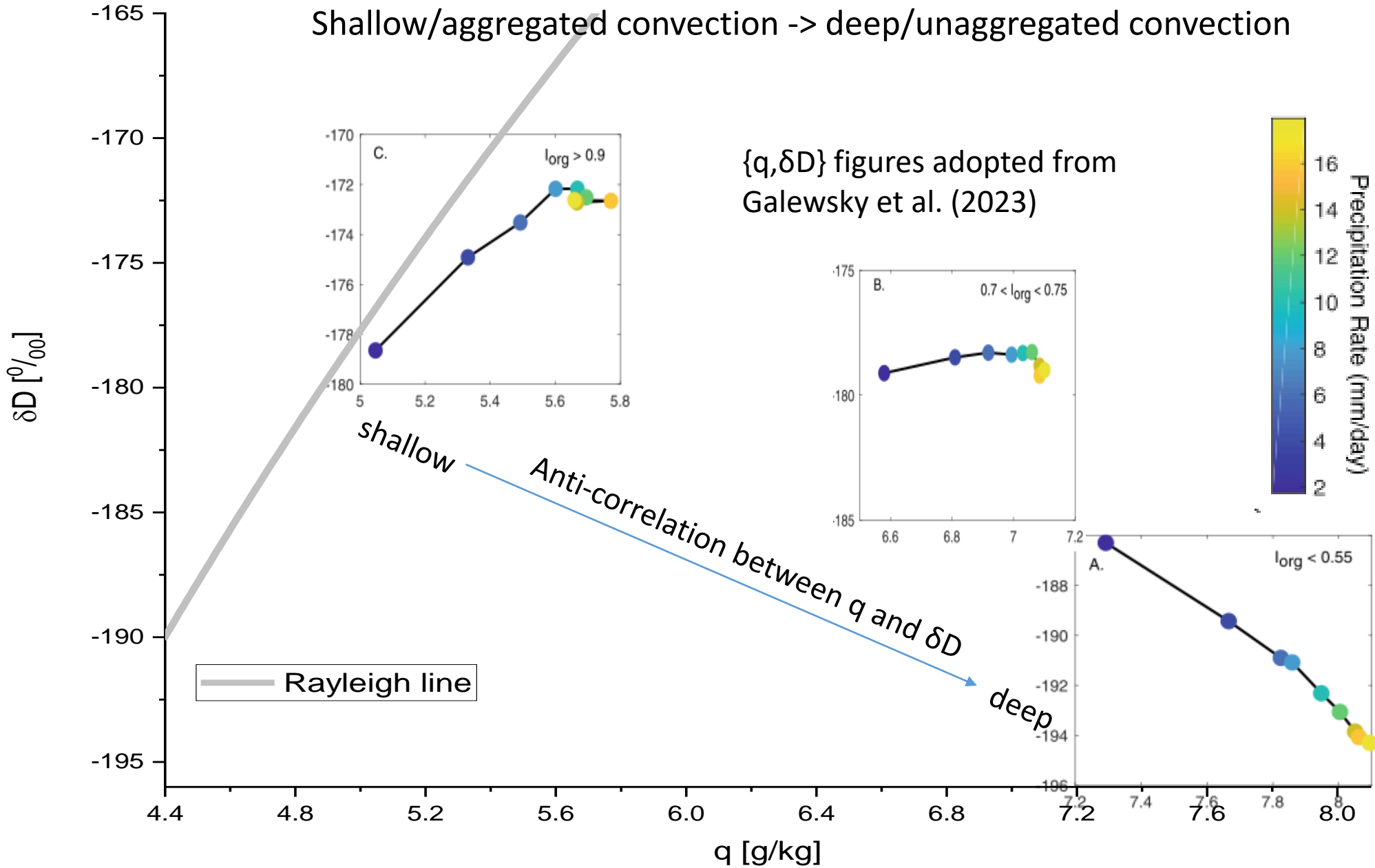
← unaggregated
= deep

→ aggregated
= shallow



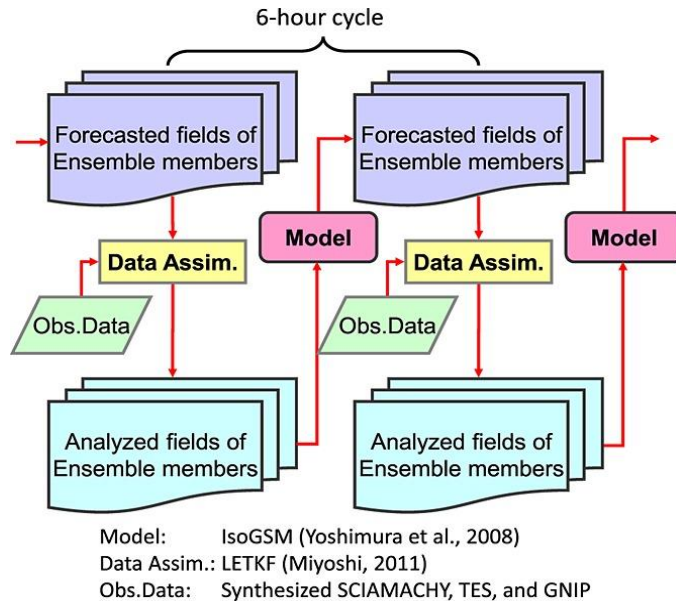
Moisture transport

Shallow/aggregated convection -> deep/unaggregated convection



Data assimilation of water isotopologues

The LETKF assimilation system



Data assimilation, basic equations

$$x^a(t_i) = x^b(t_i) + \mathbf{G}_{t_i} [y(t_i) - \mathbf{H}_{t_i} x^b(t_i)]$$

$$\mathbf{G}_{t_i} = \mathbf{S}_{t_i}^b \mathbf{H}_{t_i}^T [\mathbf{H}_{t_i} \mathbf{S}_{t_i}^b \mathbf{H}_{t_i}^T + \mathbf{S}_{\varepsilon}]^{-1}$$

Variables and operators:

t_i : time step

$x^a(t_i)$: analysed state vector

$x^b(t_i)$: background (or forecast) state vector

$y(t_i)$: measurement state vector (the observation)

\mathbf{G}_{t_i} : Kalman gain matrix

\mathbf{H}_{t_i} : measurement forward operator matrix

$\mathbf{S}_{t_i}^b$: background state error covariances matrix

\mathbf{S}_{ε} : measurement state error covariances matrix

Figure taken from Yoshimura et al. (2014)

If $\mathbf{S}_{t_i}^{b,I \rightarrow A} = \mathbf{S}_{t_i}^{b,A \rightarrow I} \neq 0$, the isotopologue observations (y^I) will have an impact on the analysed atmospheric fields ($x^{a,A}$).

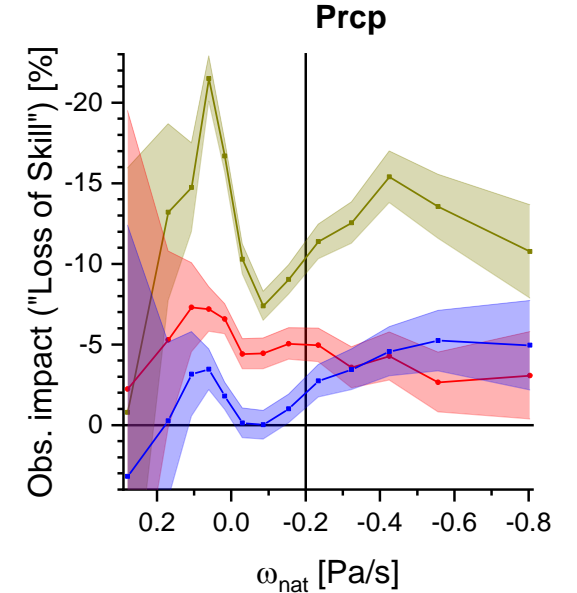
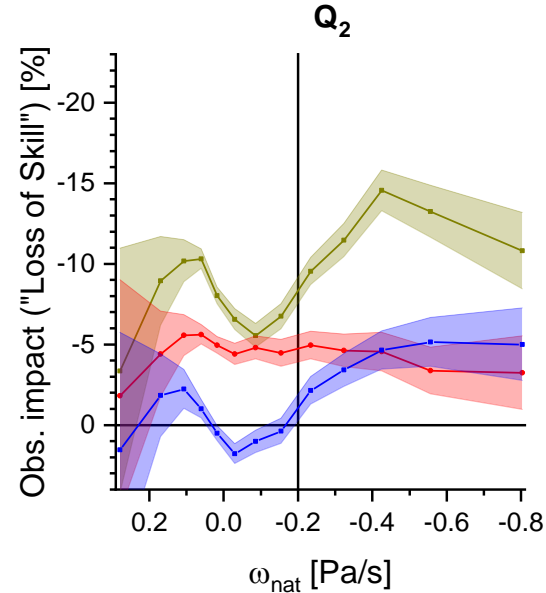
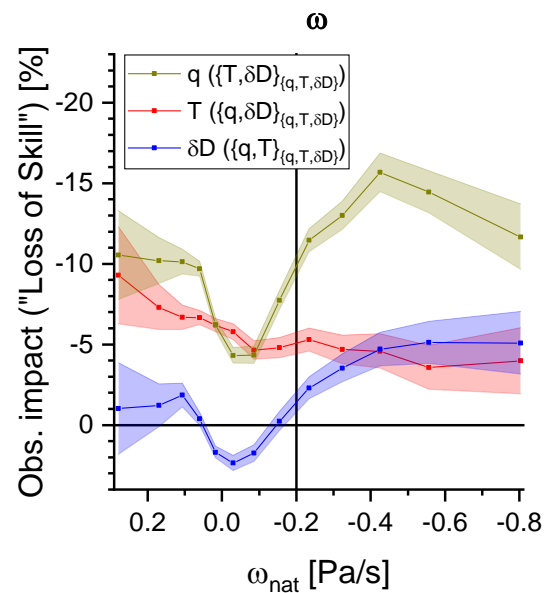
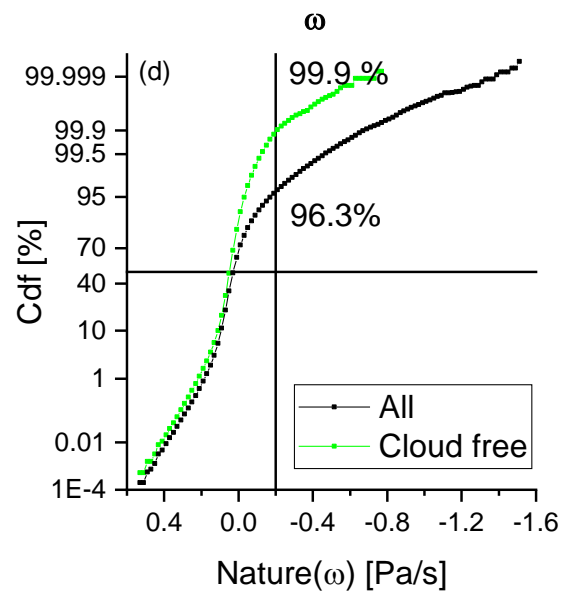
$$\left\{ \begin{array}{l} \mathbf{S}_{t_i}^b = \begin{pmatrix} \mathbf{S}_{t_i}^{b,A \rightarrow A} & \mathbf{S}_{t_i}^{b,I \rightarrow A} = \mathbf{S}_{t_i}^{b,A \rightarrow I} \\ \mathbf{S}_{t_i}^{b,A \rightarrow I} = \mathbf{S}_{t_i}^{b,I \rightarrow A} & \mathbf{S}_{t_i}^{b,I \rightarrow I} \end{pmatrix} \\ \mathbf{G}_{t_i} = \begin{pmatrix} 0 & \mathbf{S}_{t_i}^{b,I \rightarrow A} \mathbf{H}_{t_i}^{I \rightarrow I^T} (\mathbf{H}_{t_i}^{I \rightarrow I} \mathbf{S}_{t_i}^{b,I \rightarrow I} \mathbf{H}_{t_i}^{I \rightarrow I^T} + \mathbf{S}_{\varepsilon}^I)^{-1} \\ 0 & \mathbf{S}_{t_i}^{b,I \rightarrow I} \mathbf{H}_{t_i}^{I \rightarrow I^T} (\mathbf{H}_{t_i}^{I \rightarrow I} \mathbf{S}_{t_i}^{b,I \rightarrow I} \mathbf{H}_{t_i}^{I \rightarrow I^T} + \mathbf{S}_{\varepsilon}^I)^{-1} \end{pmatrix} \end{array} \right.$$

Data assimilation of water isotopologues

Schneider et al., 2024. Potential of satellite water isotopologue observations for improving the analyses of convective events

(Almost) no observations assimilated for $\omega < -0.2$ Pa/s

BUT: strongest impact of δD observations for $\omega < -0.2$ Pa/s



Summary

- MUSICA IASI {H₂O,δD}-pair data: about 2 billion data points, 2014 – 2021:
<https://www.imk-asf.kit.edu/english/musica-data.php>
- Mid-tropospheric {H₂O,δD}-pair distributions give insight into convective processes (monitoring of convective processes?)
- Assimilation of isotopologues can improve the analysis of a convective atmosphere: benefit for climate monitoring and/or weather forecasts?

Thanks for your attention!