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

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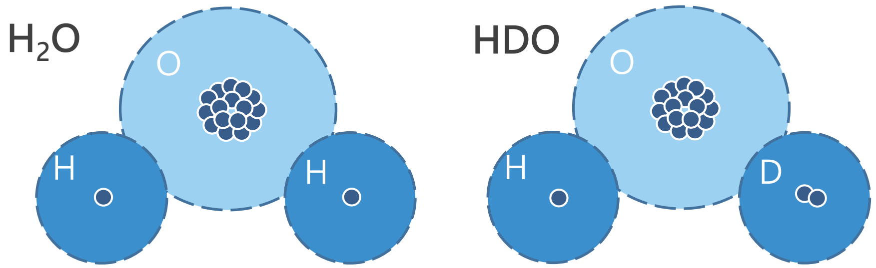
- Introduction to atmospheric water vapour isotopologues
- Our IASI retrieval processor “MUSICA*” and the isotopologue data set
- Example of moisture transport studies using water vapour isotopologue data
- Conclusion

*MUSICA: **MU**lti-platform remote **S**ensing of **I**sotopologues for investigating the **C**ycle of **A**tmospheric water

Water vapour isotopologues



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

Water isot.	$H_2{}^{18}O$	$H_2{}^{17}O$	HDO	...
R_{vsmow}	0.201 %	0.039 %	0.031 %	...

$\delta D =$

0 ‰ — HDO/H_2O equals R_{vsmow}

-100 ‰

Typical range for water vapour in the tropical mid-troposphere

-300 ‰

-1000 ‰ — no HDO available

Increased molecular mass

Reduced saturation vapour pressure

Equilibrium fractionation

- Lighter isotopes evaporate preferentially.
- Heavier isotopes condensate preferentially.

Isotope ratio changes with phase transitions!

Unique potential for tracking moisture processes

The MUSICA IASI retrieval

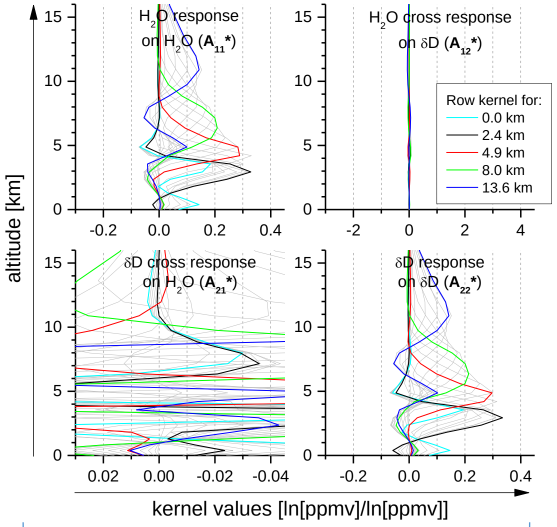
Optimal estimation of trace gas ratio data (isotopologue ratios are the interesting data):

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

(2) Optimal estimation of ratio (δD) proxies: $\ln\left[\frac{\hat{x}_{\mathrm{HDO}}}{\hat{x}_{\mathrm{H2O}}}\right] = \ln \hat{x}_{\mathrm{HDO}} - \ln \hat{x}_{\mathrm{H2O}}$

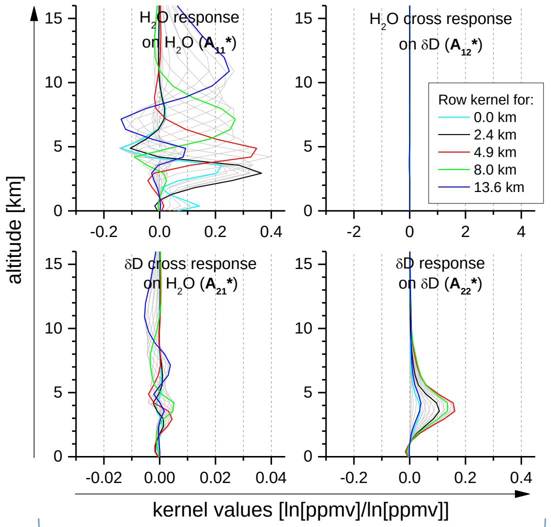
(3) Post-processing to generate H_2O and δD products having the same sensitivity:{H_2O,δD} pairs

Individual optimal estimation of H_2O and HDO



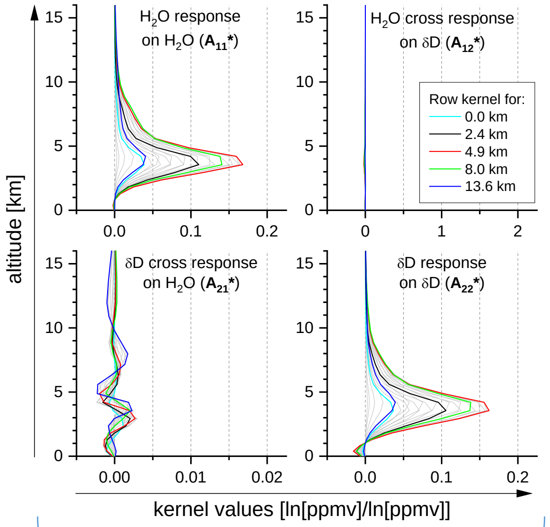
Not useful

(1+2) Optimal estimation of H_2O and δD proxies



MUSICA IASI retrieval output

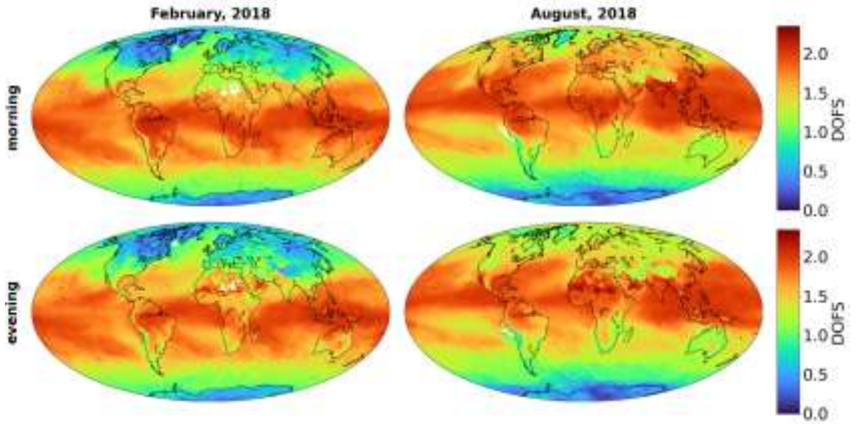
(3) Post processing: generation of {H_2O,δD} pairs



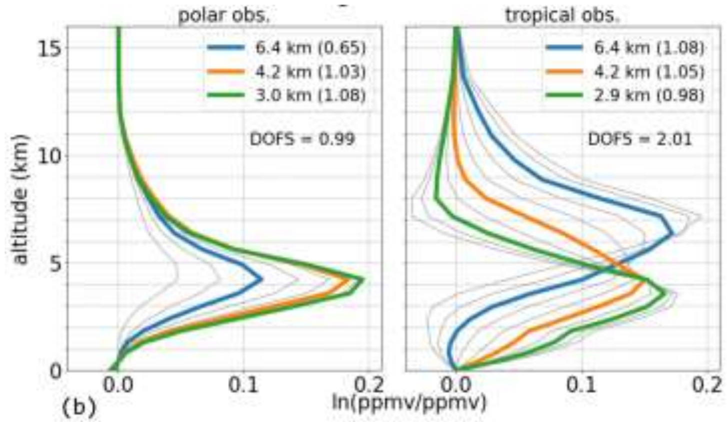
This is the MUSICA IASI {H_2O,δD} pair product!

The MUSICA IASI retrieval

DOFS



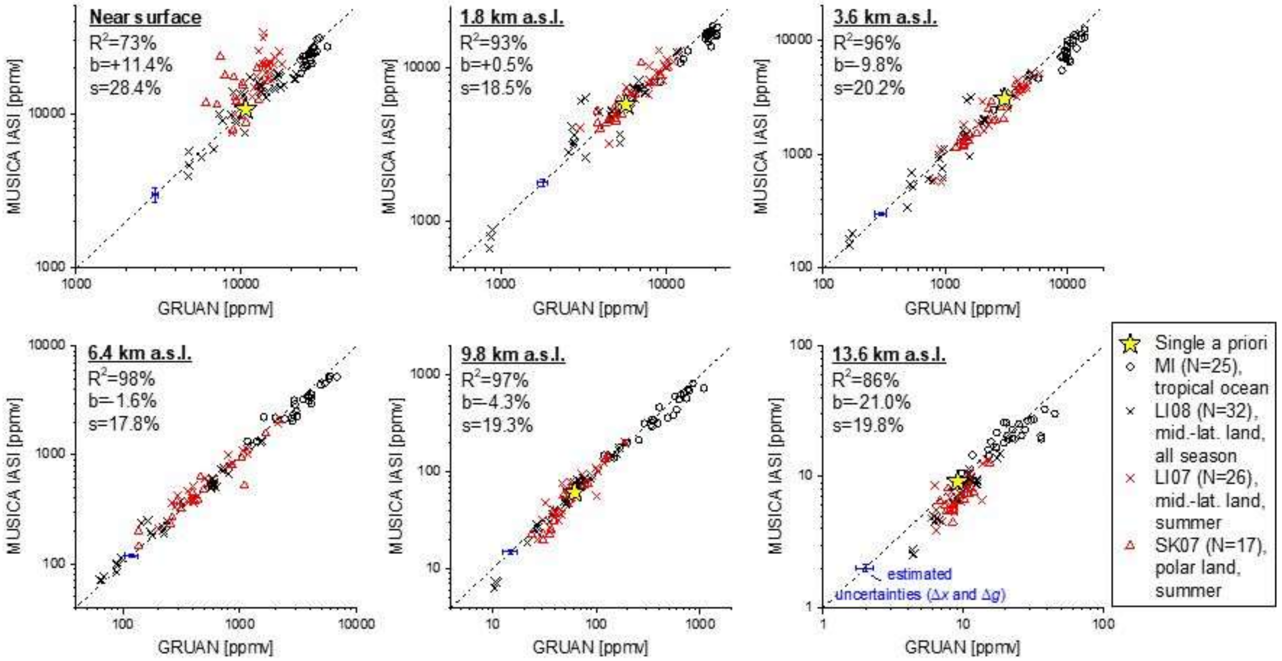
Examples of averaging kernels

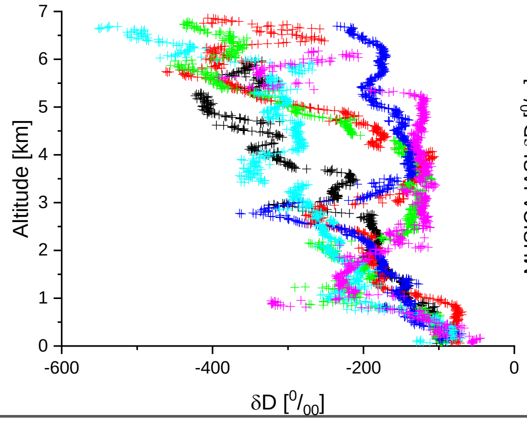


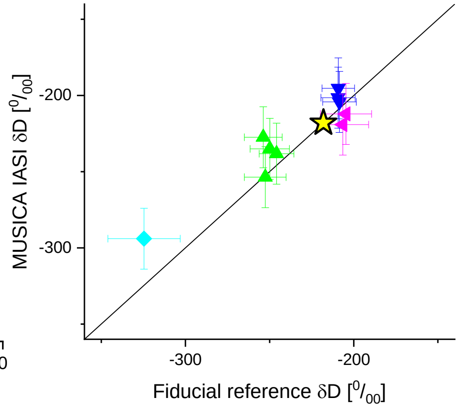
Uncertainties

Typically 10% (H_2O) and 10-20‰ (δD)

Validation with GRUAN and dedicated aircraft campaign

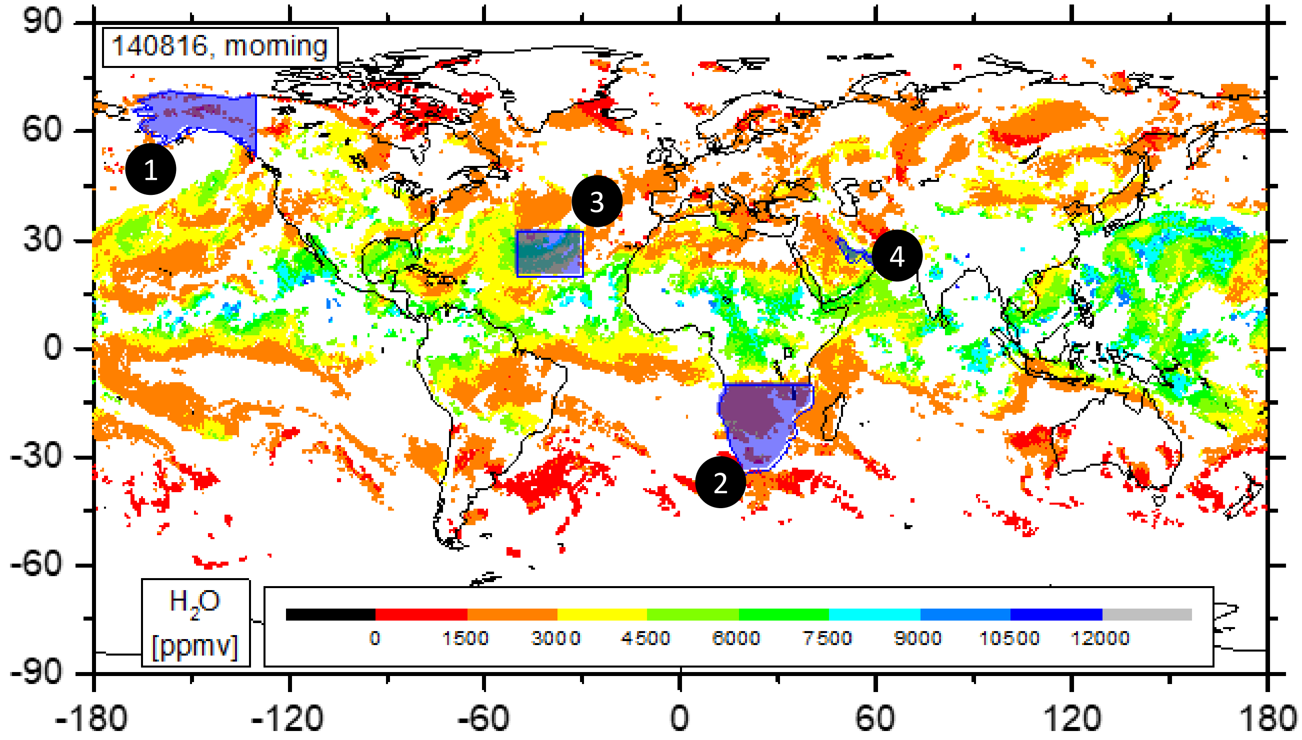






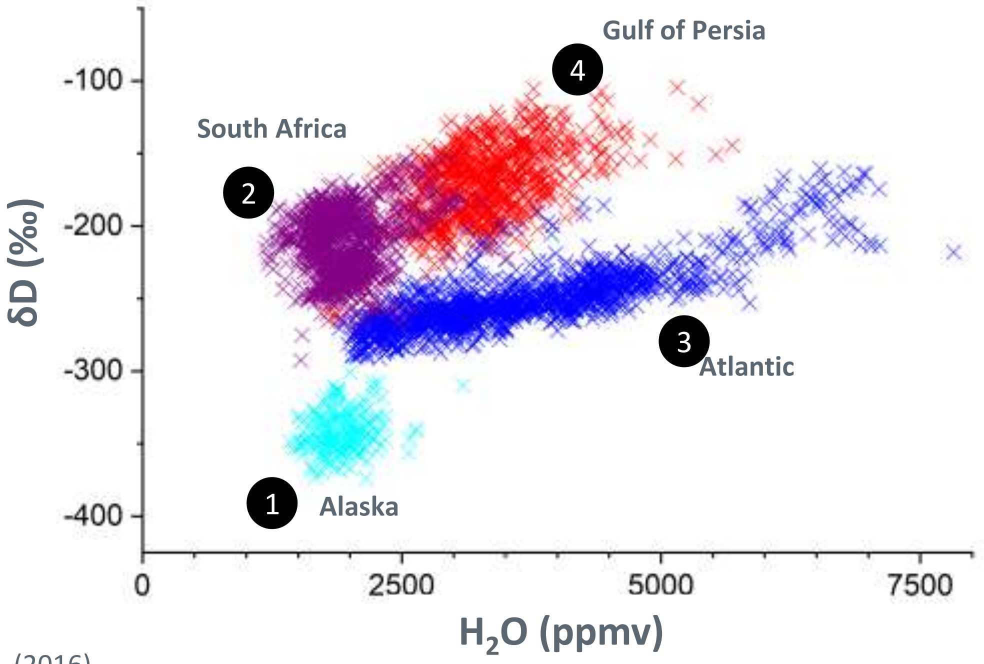
Borger et al., 2017; Diekmann et. al. 2021; Schneider et al., 2016

Pairs of H_2O and δD (2014 – 2021, >2 billion data pairs)



Global H_2O-distribution in mid-tropospheric water vapour

Pairwise analysis of H_2O and δD in water vapour

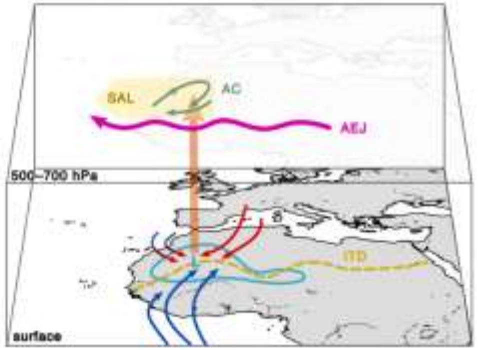


Schneider et al. (2016)

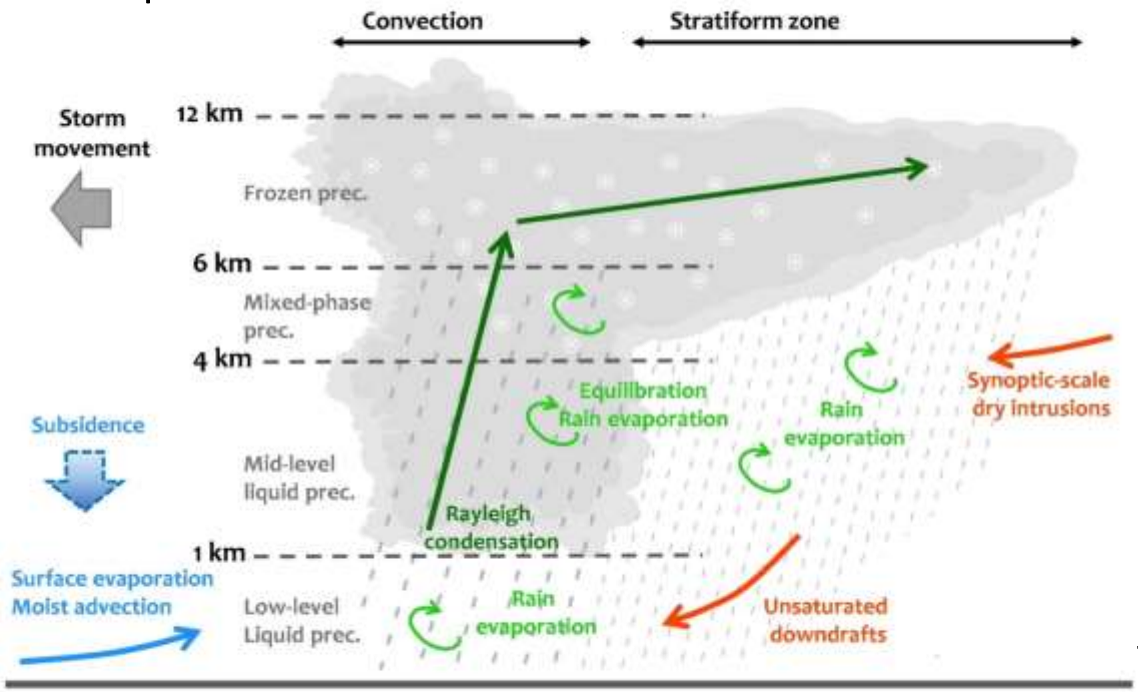
Effects of different moisture processes become visible when analysing the {H_2O, δD}-pair distribution

Moisture transport with {H_2O,δD} (Rayleigh and beyond)

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

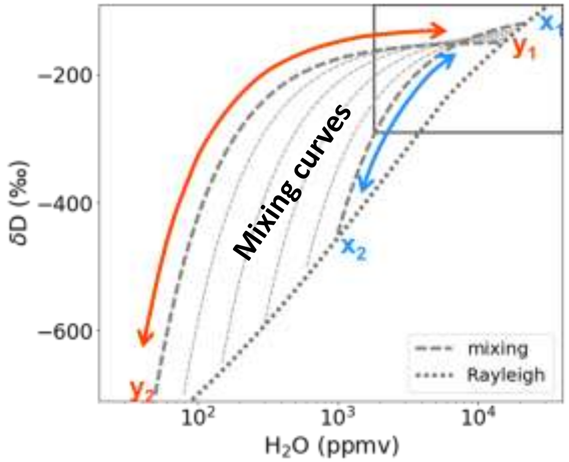


Cloud processes:



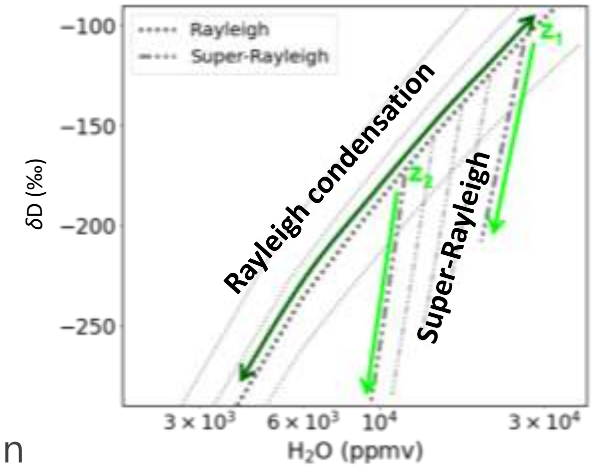
Theoretical process lines in the {H2O, δD} phase space

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



Rayleigh Condensation
Rain condensation during moist adiabatic ascent

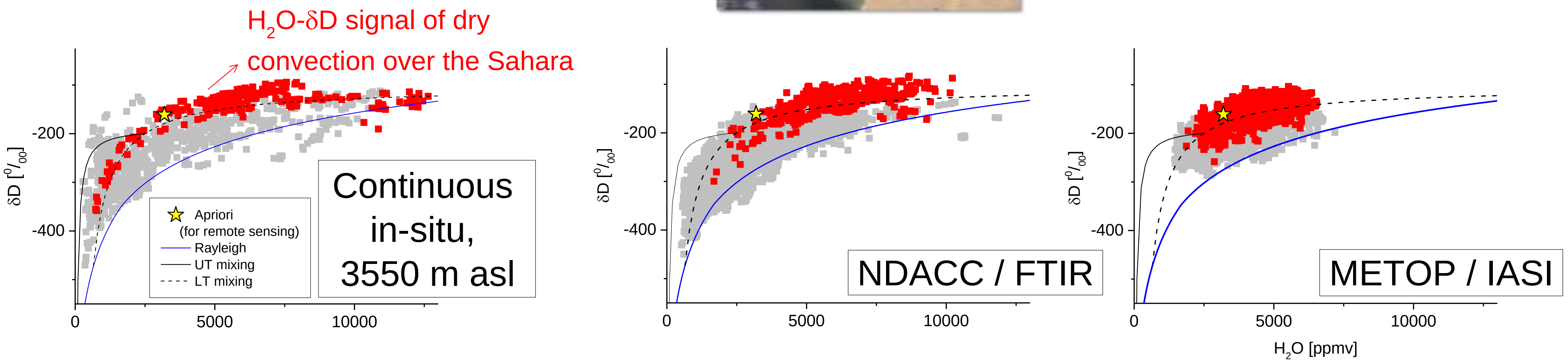
Super-Rayleigh Signals
Special case of Rayleigh condensation, which is overlaid by partial rain evaporation and equilibration



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

Moisture transport

Well-studied airmass mixing (Saharan Air Layer):

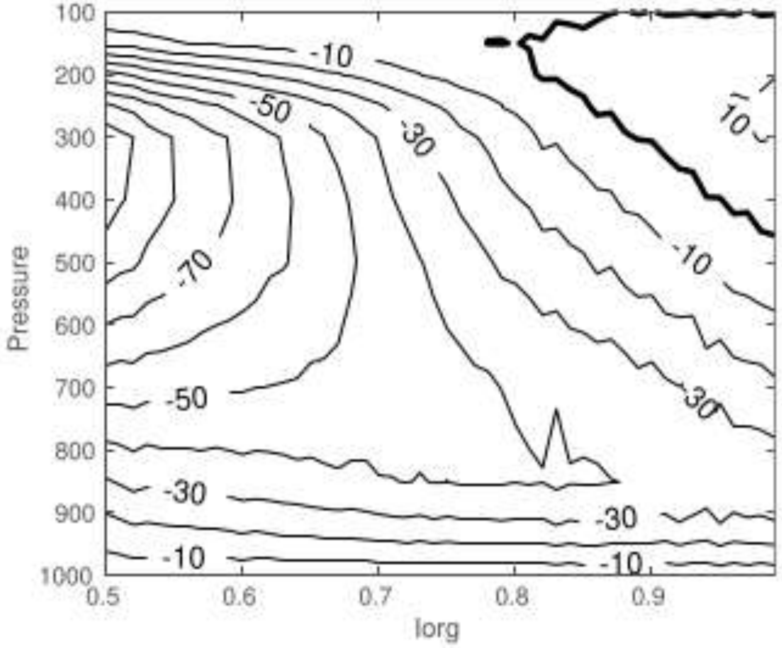


Serves also as process-based validation of the MUSICA IASI {H2O,δD}-pair distribution (Schneider et al., 2016)

Moisture transport

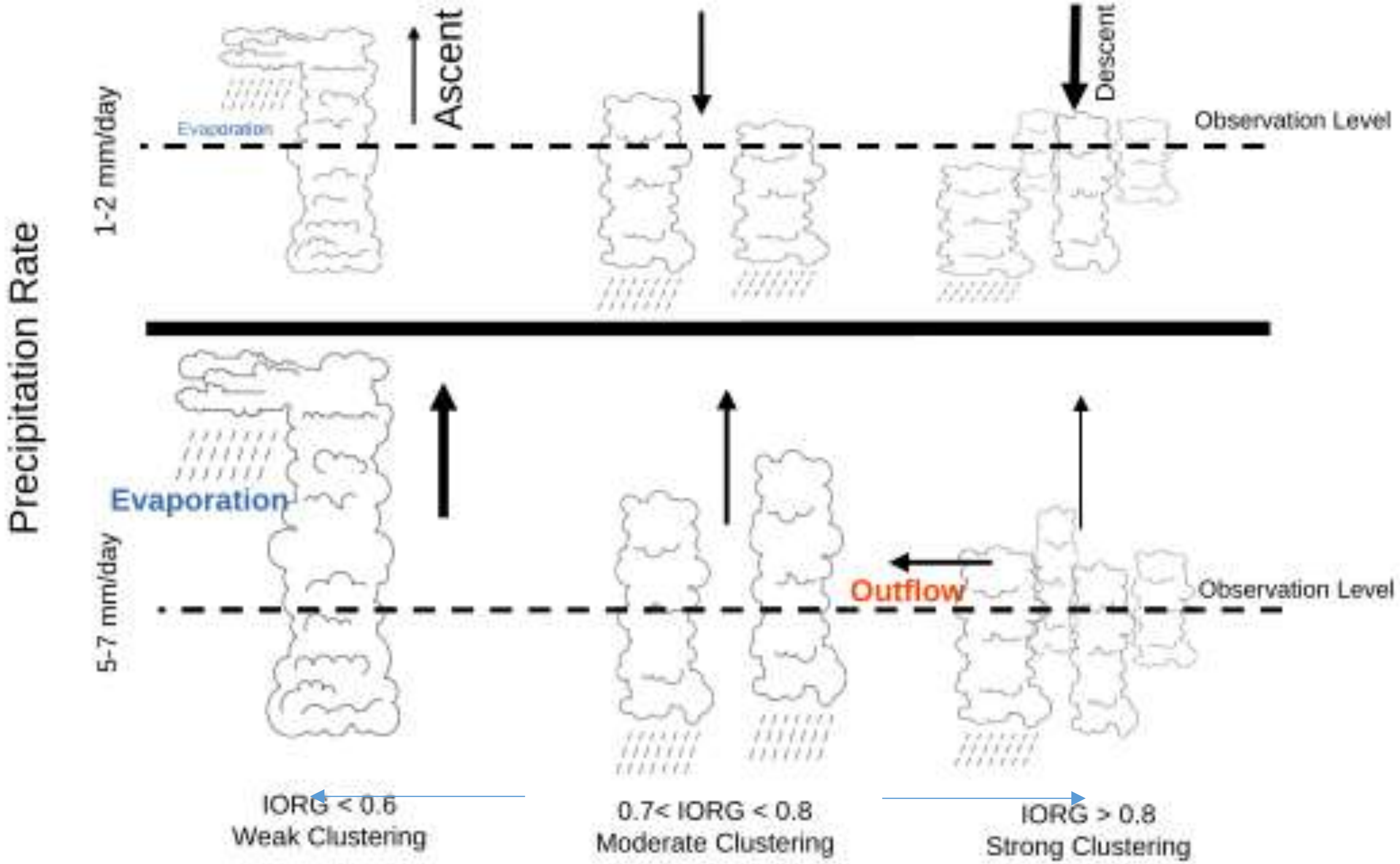
Galewsky et al. (2023): Convective intensity, convective organization, and mid-tropospheric water vapour isotopologues
Identification of convection has been made with OLR minima.

ω [hPa/day] profiles



deep = unaggregated

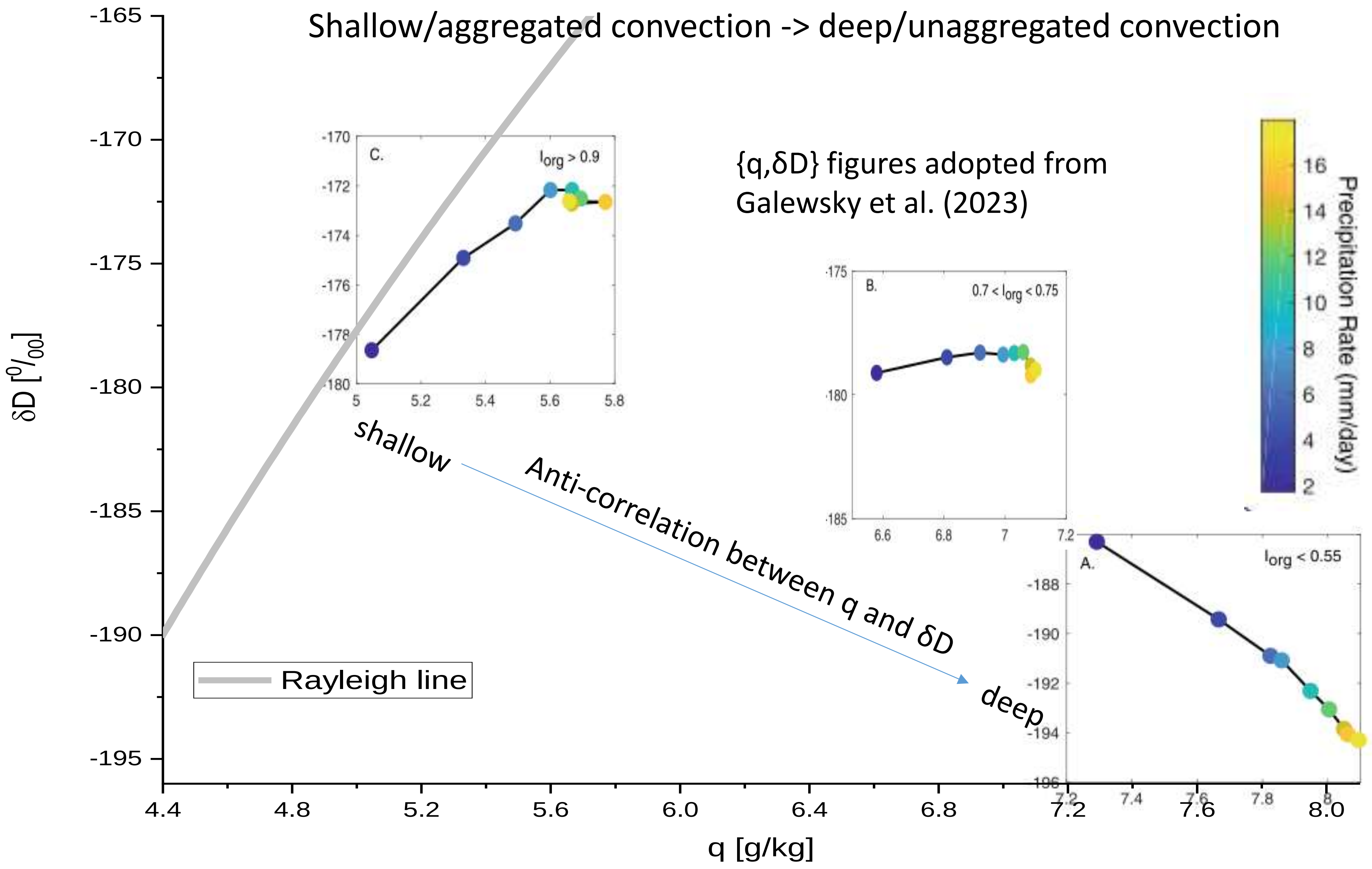
shallow = aggregated



deep = unaggregated

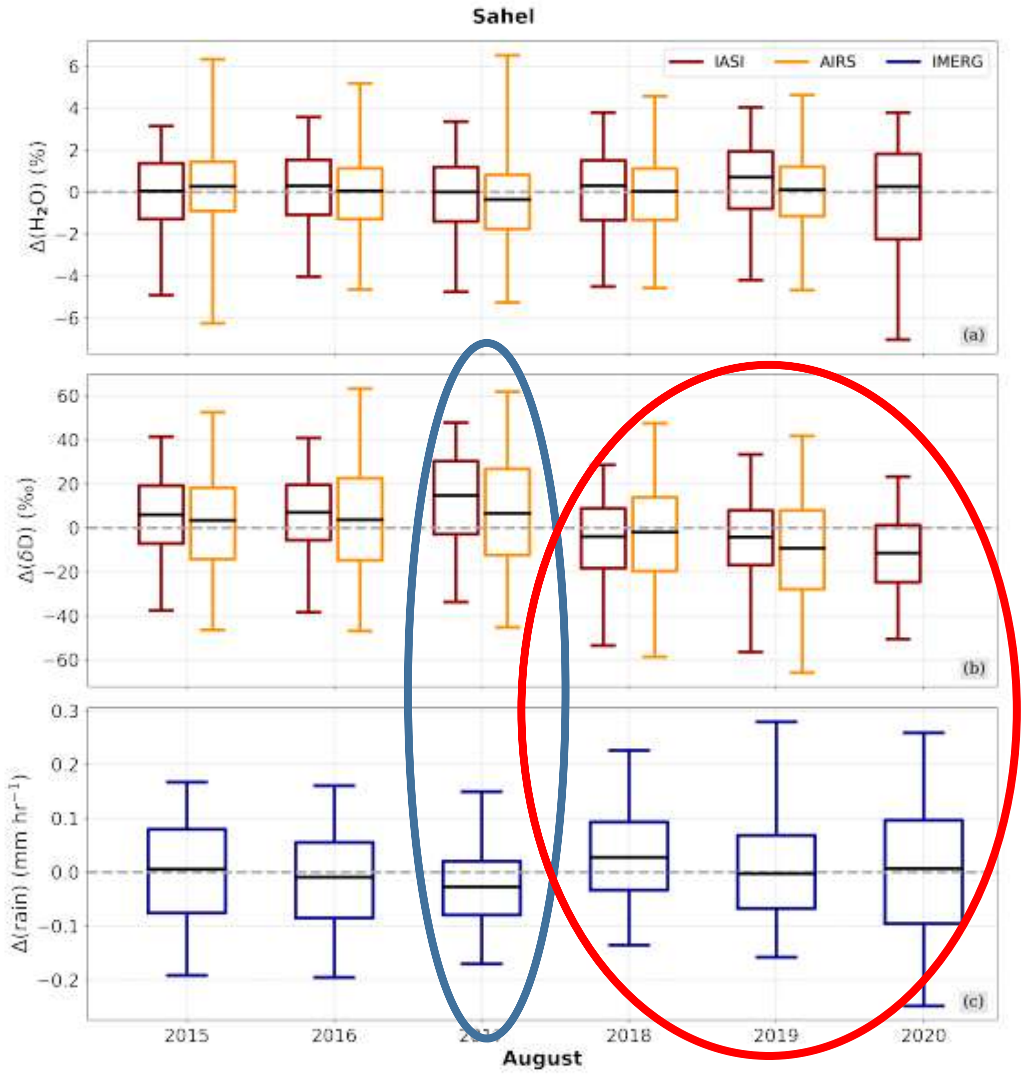
shallow = aggregated

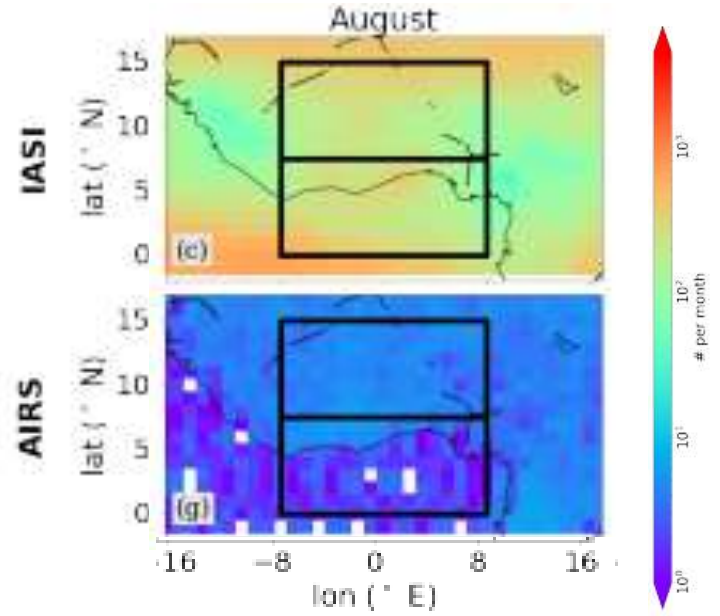
Moisture transport



Moisture transport

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





Study using middle tropospheric $\{H_2O,\delta D\}$ data from IASI and ARIS

2017: weakest HDO depletion (weakest super-Rayleigh signal), less intense convection, lowest mean rainfall

2015-2017 versus 2018-2020: super-Rayleigh signal, more intense convection. increasing peak rain intensity

Data assimilation of water isotopologues

The LETKF assimilation system

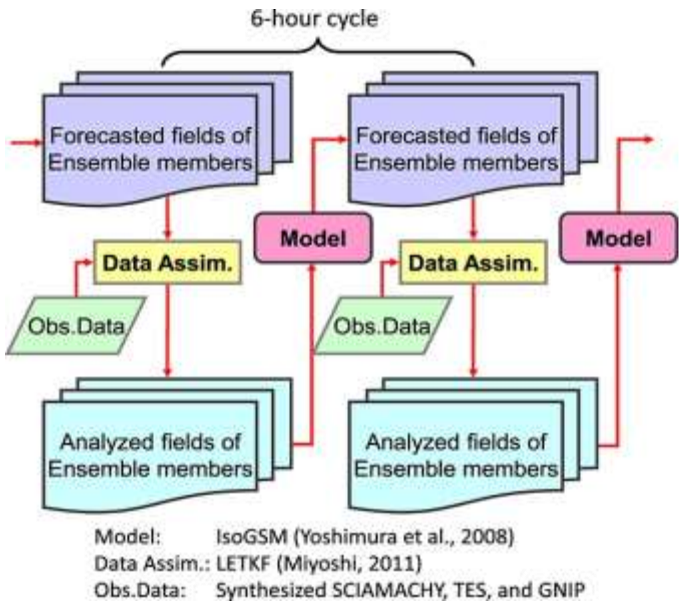


Figure taken from Yoshimura et al. (2014)

Data assimilation, basic equations

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

$$\mathbf{G}_{t_i} = \mathbf{S}^b_{t_i}\mathbf{H}^T_{t_i}\left[\mathbf{H}_{t_i}\mathbf{S}^b_{t_i}\mathbf{H}^T_{t_i} + \mathbf{S}_\varepsilon\right]^{-1}$$

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
$\mathbf{S}^b_{t_i}$: background state error covariances matrix
$\mathbf{S}_\varepsilon$: measurement state error covariances matrix

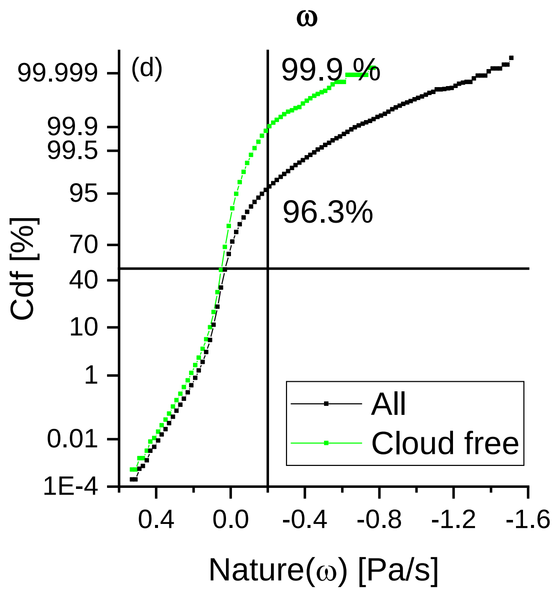
If $\mathbf{S}^{b,I\to A}_{t_i} = \mathbf{S}^{b,A\to I}_{t_i} \neq 0$, the isotopologue observations (y^I) will have an impact on the analysed atmospheric fields $(x^{a,A})$.

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

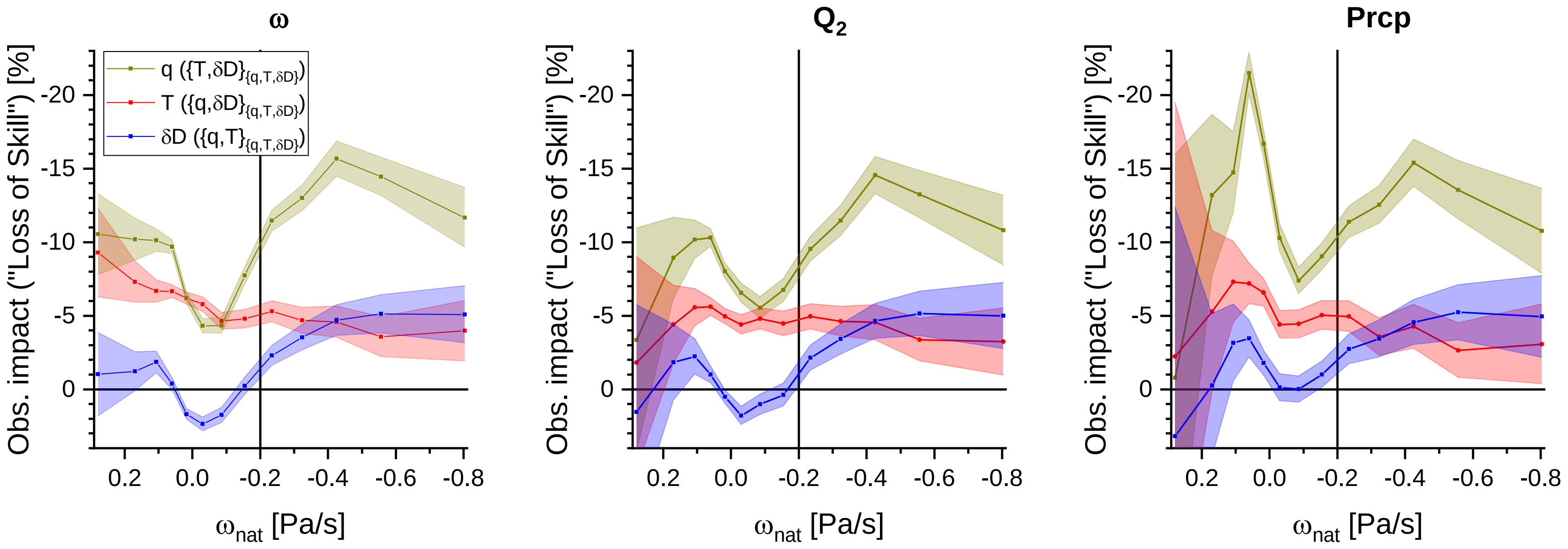
Data assimilation of water isotopologues

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

(Almost) no observations assimilated for ω < -0.2 Pa/s



BUT: strongest impact of δD observations for ω < -0.2 Pa/s



Conclusion

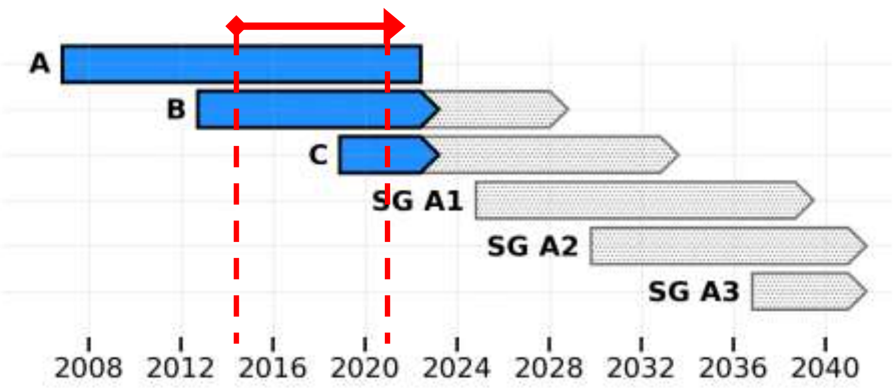
- MUSICA IASI {H_2O,δD}-pair data: about 2 billion data points, 2014 – 2021:
  https://www.imk-asf.kit.edu/english/musica-data.php
- Mid-tropospheric {H_2O,δD}-pair distributions give (detailed) insights into convective processes:
  Monitoring of the occurrence of different convection types?
- Assimilation of isotopologues can improve the (re-)analysis of a convective atmosphere:
  Benefit for detecting trends in the atmospheric water cycle (e.g., changes of convective intensity/occurrence)?

Thanks for your attention!

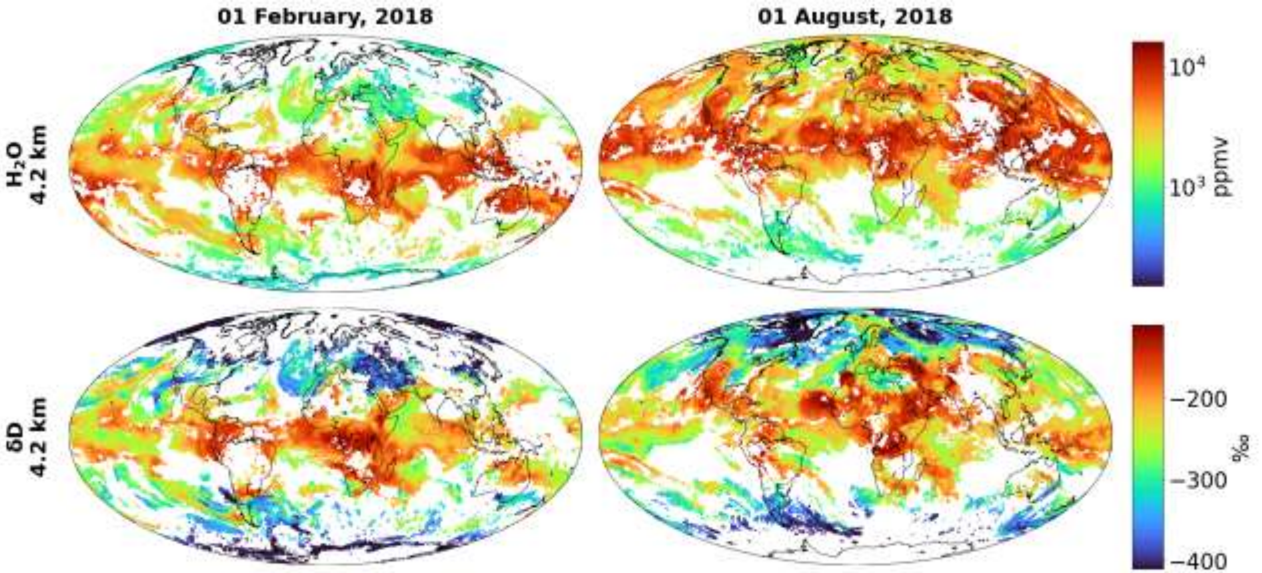
MUSICA IASI datasets of {H_2O, δD} pairs

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, δD} post-processing**: Diekmann et al (2021)



Timeline of Metop satellites



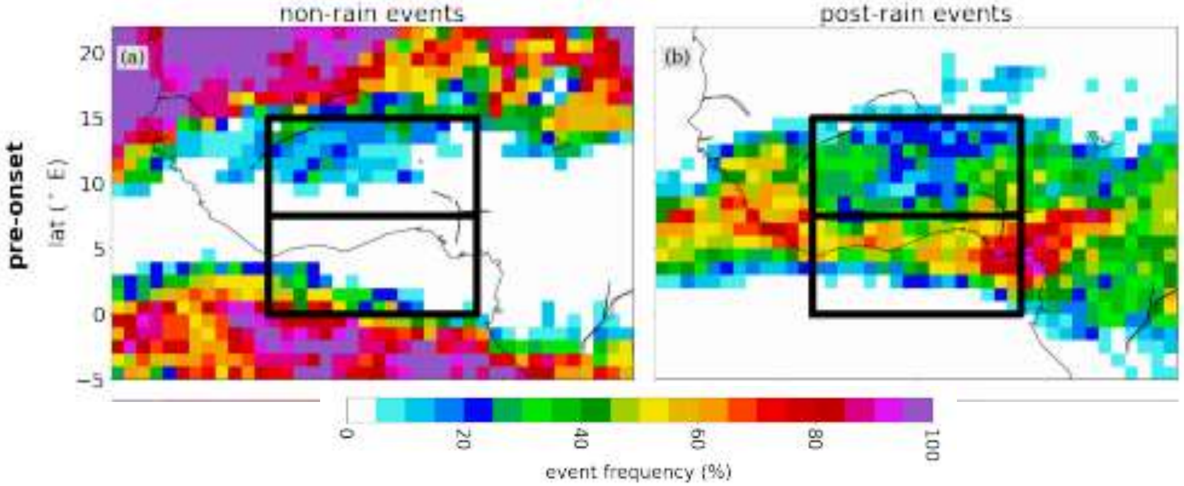
Daily maps of IASI {H_2O, δD} data

- 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

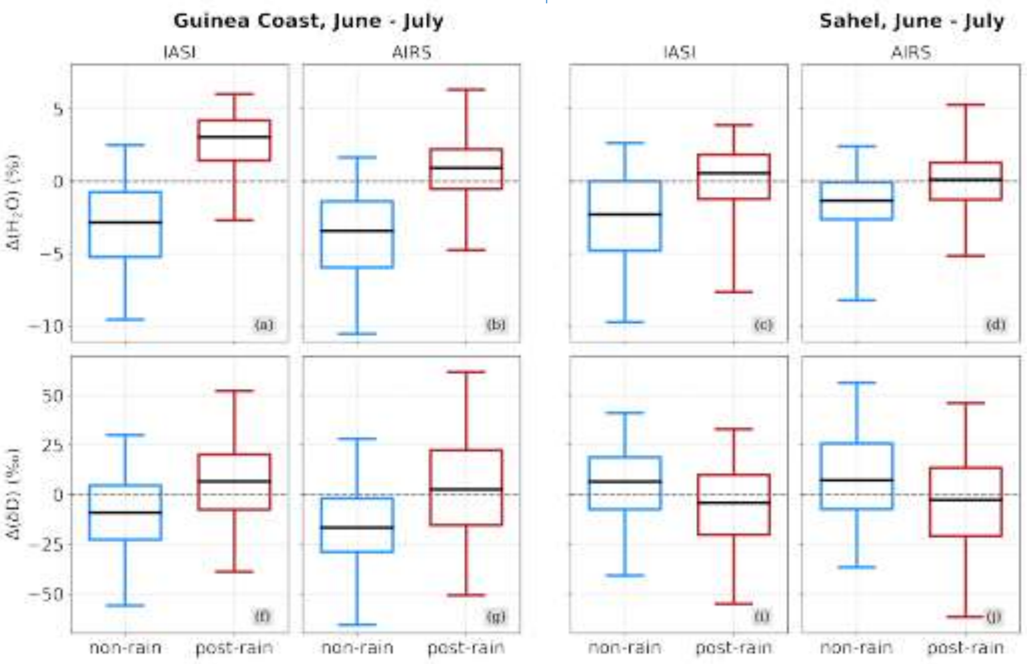
Moisture transport

Example West African Monsoon, Diekmann et al., 2024

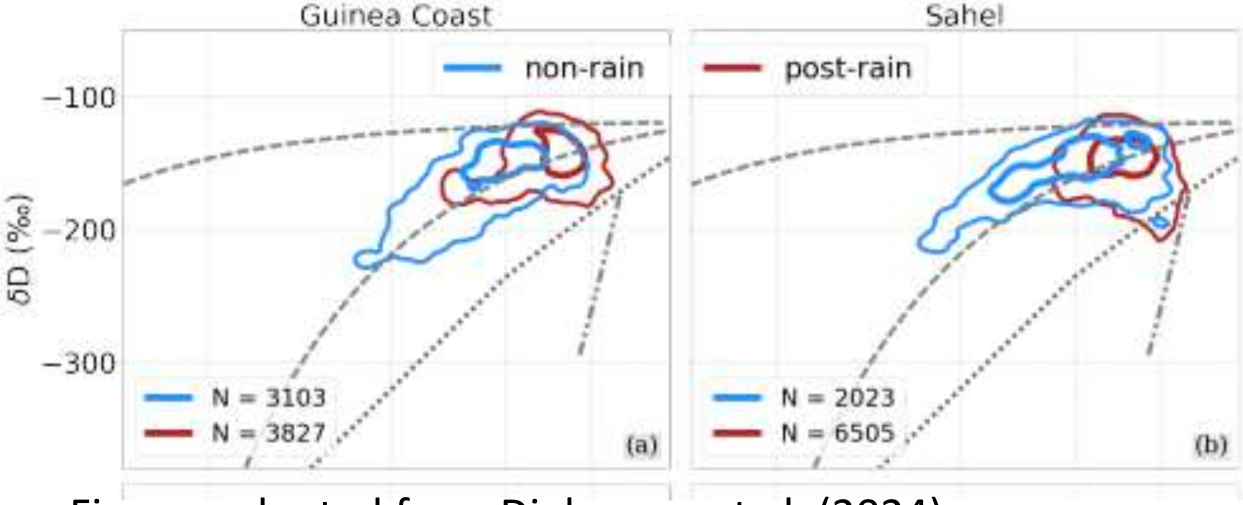
Classification: rain versus non-rain (IMERG)



Anti-correlation between H_2O and δD



$\{H_2O, \delta D\}$ distribution: rain versus non-rain



Figures adopted from Diekmann et al. (2024)

<u>Guinea Coast:</u> generally positive correlation between H_2O and δD

<u>Sahel:</u> super-Rayleigh $\{H_2O, \delta D\}$ distribution significantly more frequent after rain events.

-> Anti-correlation between H_2O and δD.