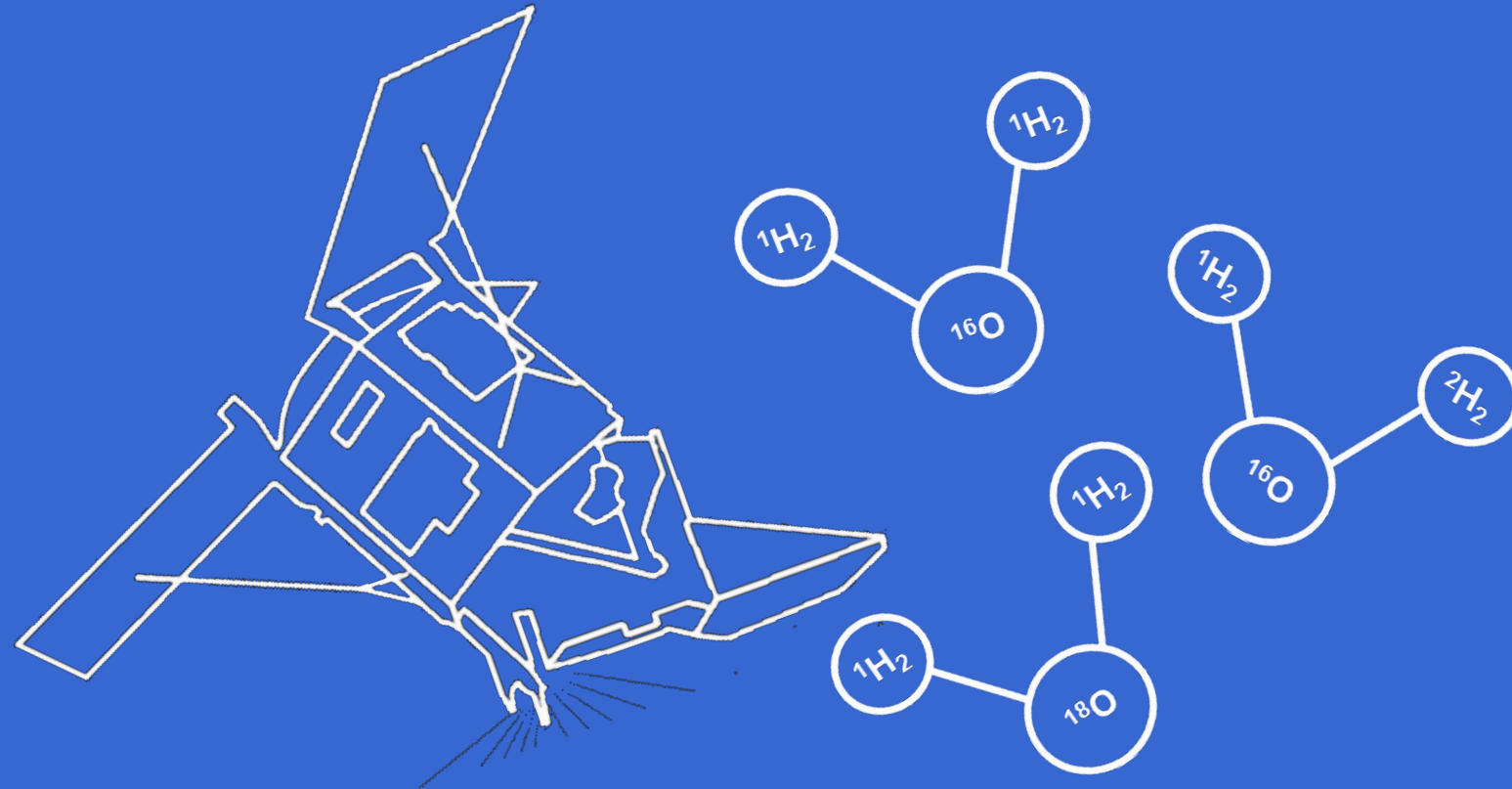


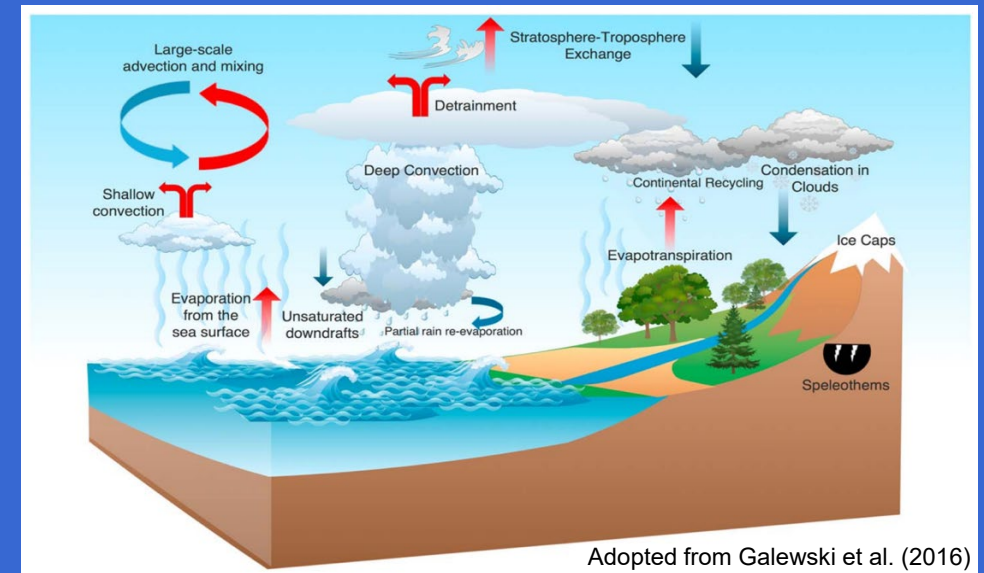
Observing the global distribution of water vapour isotopologues with the Sentinel-5P mission



Hartmut Boesch, Tim Trent, Matthias Schneider, Farahnaz Khosrawi, Christopher Diekmann, Amelie Röhling, Harald Sodemann, and Iris Thurnherr

Background

- Atmospheric moisture is key component of Earth system responsible for most climate feedback mechanisms
 - What are physical processes responsible for cloud feedbacks and adjustments in models?
 - What are primary factors controlling modes of variability of large-scale atmospheric circulation and precipitation patterns?
 - What is the role of moist processes for major model biases (e.g., diurnal cycle of convection over continents)?
- Major challenge of World Climate Research Program (Clouds, circulation & climate sensitivity)



Background

- Water isotopologues allow to assess and improve model-based representations of moisture sources and pathways in climate (earth system) models

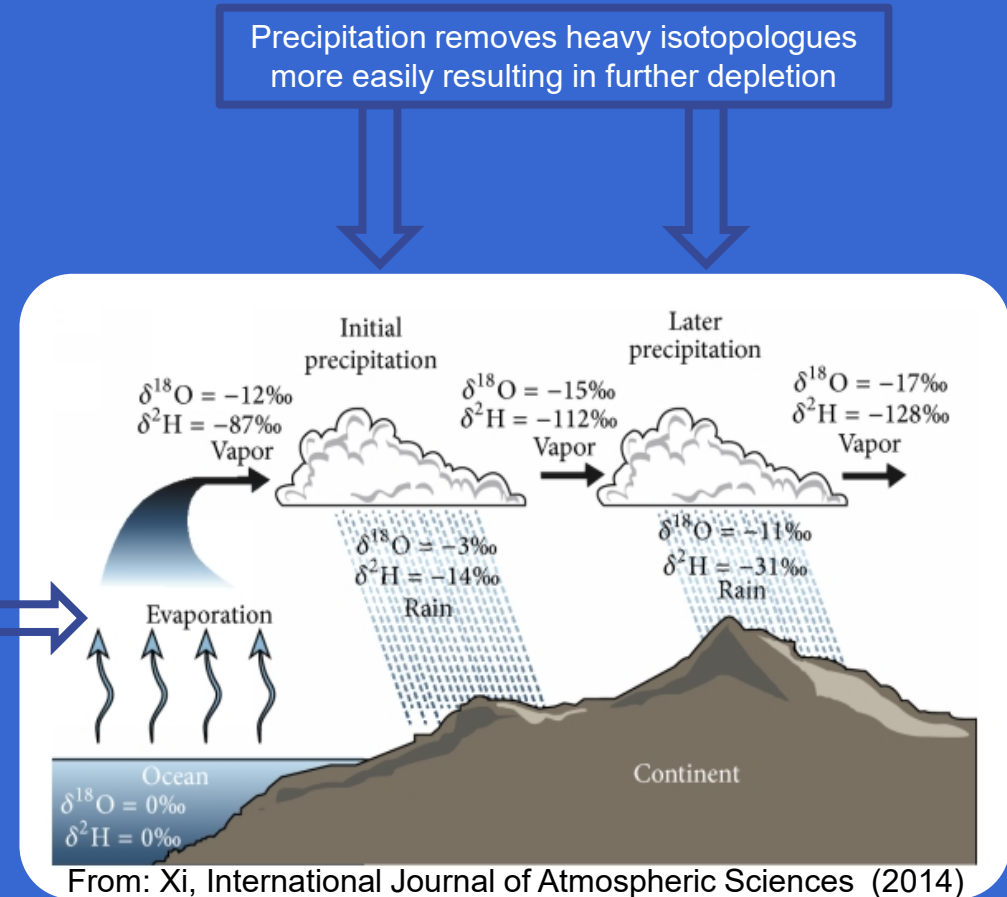
Water Isotopologues are given in δD [in ‰] notation:

$$\delta D = \frac{\text{HDO}/\text{H}_2\text{O}}{\text{VSMOW}} - 1$$

Reference: Vienna Standard Mean Ocean Water VSMOW

$$\text{VSMOW} = 3.1152 \times 10^{-4}$$

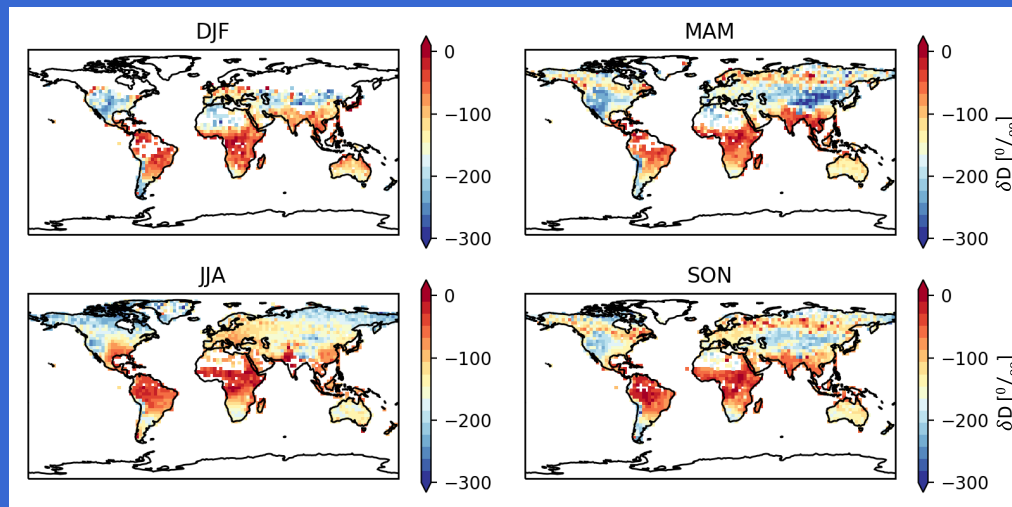
Isotopically lighter isotopologues evaporates more readily



Satellites provide global observations

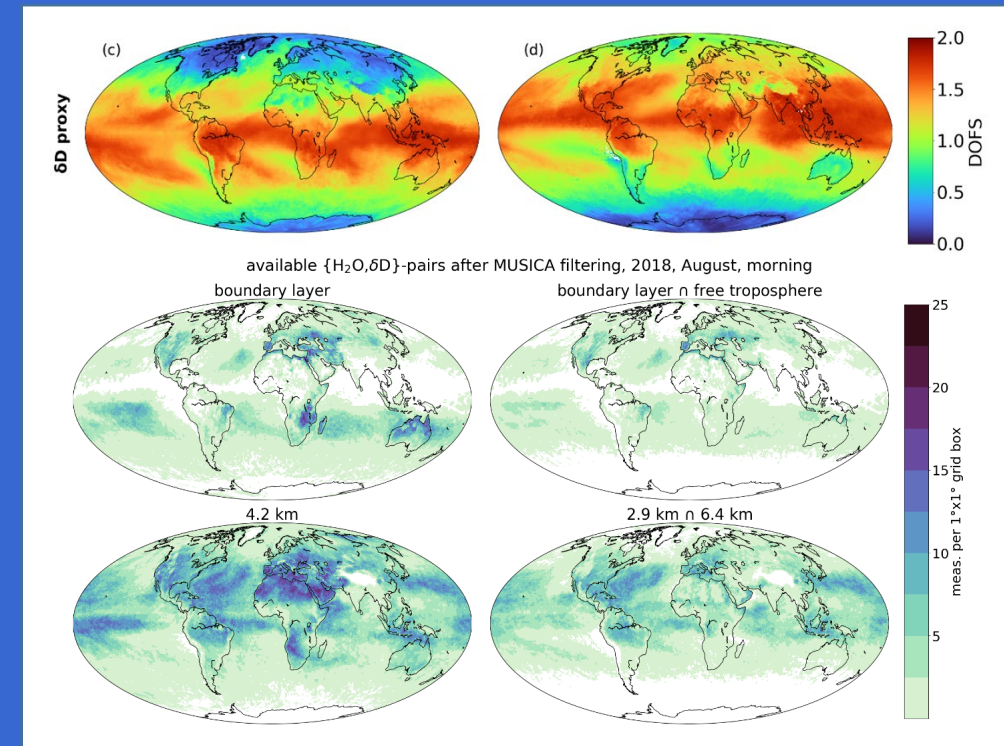
GOSAT

- Shortwave-infrared column retrieval
- Coarse coverage: 3-day repeat cycle with pixels separated by 200km
- Data generated by UoL



MUSICA IASI

- Infrared profile retrieval (peak sensitivity in mid troposphere)
- Coverage: Global twice daily with 12 km pixels
- Data generated by KIT



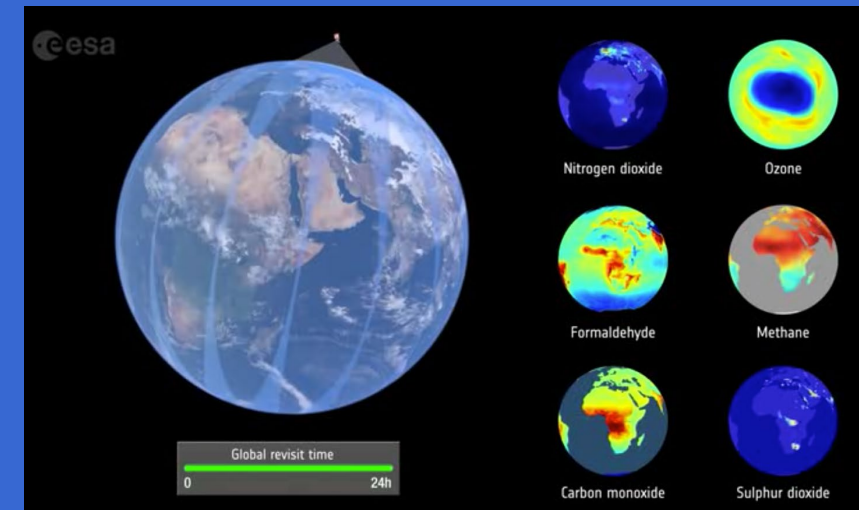
Sentinel-5P TROPOMI

- First atmospheric composition Sentinel, launched on 13 October 2017.
- TROPOMI provides daily global coverage with $5.5 \times 7 \text{ km}^2$ ground pixels
- SWIR bands well suited for water isotopologue retrievals
- Water isotopologue column product with much better coverage and precision compared to GOSAT



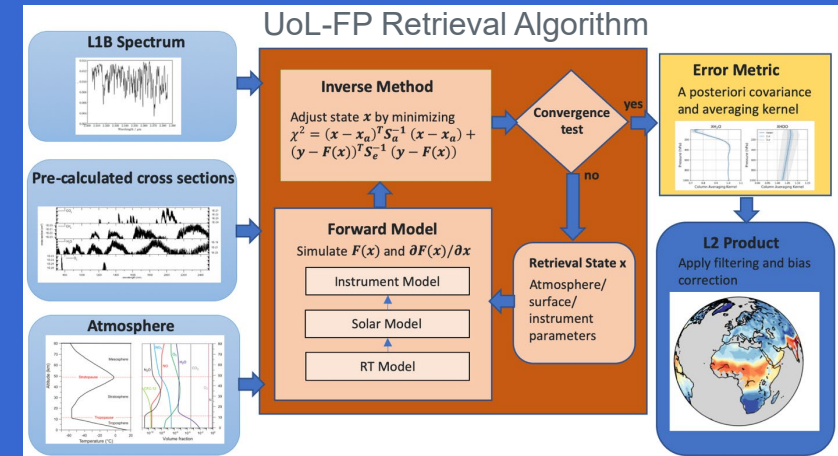
TROPOMI

- ▶ UV-VIS-NIR-SWIR nadir view grating spectrometer.
- ▶ Spectral range: 270-500, 675-775, 2305-2385 nm
- ▶ Spectral Resolution: 0.25-1.1 nm
- ▶ Spatial Resolution: $3.5 \times 7 \text{ km}^2$
- ▶ Global daily coverage at 13:30 local solar time.



TROPOMI Retrieval


- Based on UoL-FP Optimal Estimation retrieval algorithm modified for TROPOMI:
 - Fit window: 2.353 – 2.382 μm
 - Cloud clearing using VIIRS cloud flags
 - Updated solar model to solar spectrum measured by TROPOMI
 - Spectroscopy updated to use DLR SEOM-IAS data base
 - Offline calculation of scaler averaging kernels for HDO and H₂O



Description	Parameters	Number of Elements
Water Vapour (H2O)	Scaler or profile	1
Methane	Scaler	1
Carbon Monoxide	Scaler	1
Water Vapour Isotope (HDO)	Scaler or profile	1
Temperature	Scaler	1
Albedo	Slope and offset	2
Dispersion	Polynomial fit	4
Total		11




TROPOMI Water Isotopologue Data

- Generated and documented TROPOMI water isotopologue product for 2018 – 2020 globally (land only)

	Sentinel-5p+Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO): Product User Manual (PUM)	Version: v1.0 Doc ID: S5P+I-H2O-ISO-PUM Date: 27-09-2021
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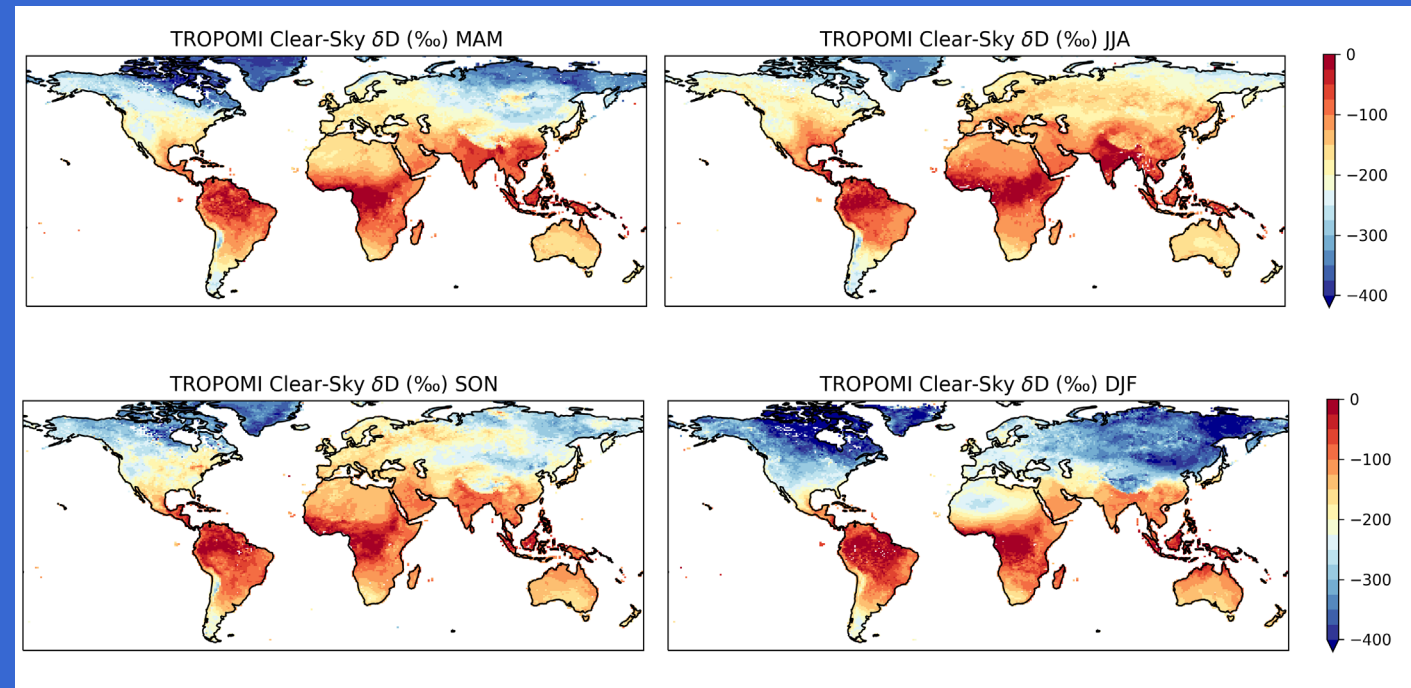
Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO)
Product User Manual (PUM)

Authors:
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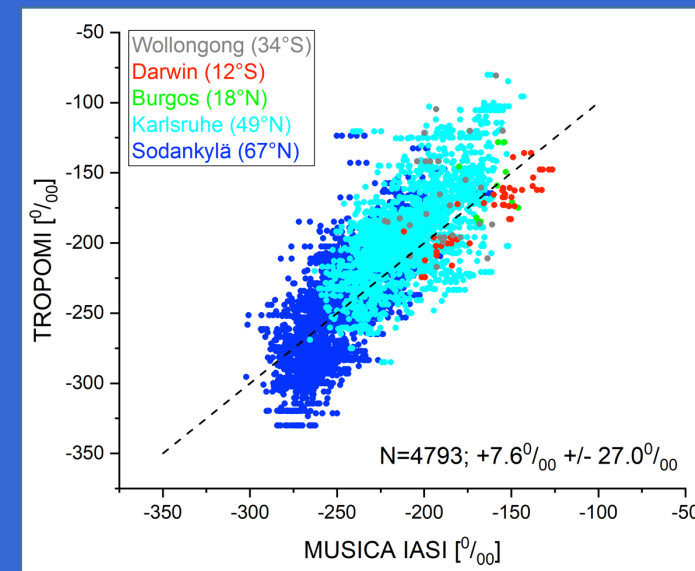
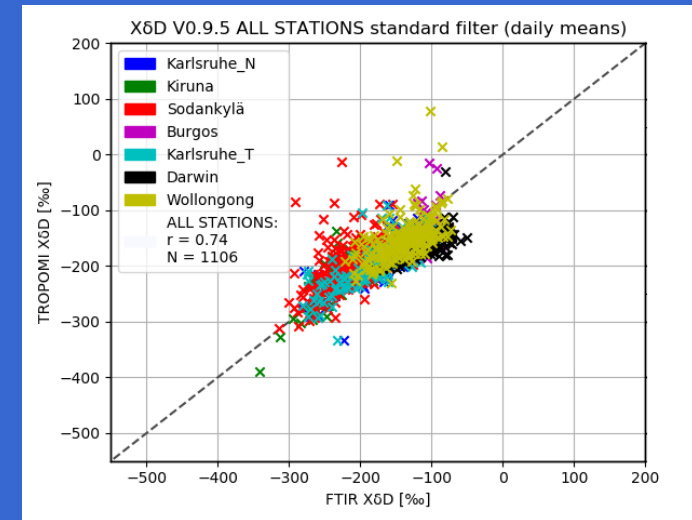
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https://s5pinnovationh2o-iso.le.ac.uk/wp-content/uploads/2022/05/S5P-I_ISO_PUM_Version1.1.pdf

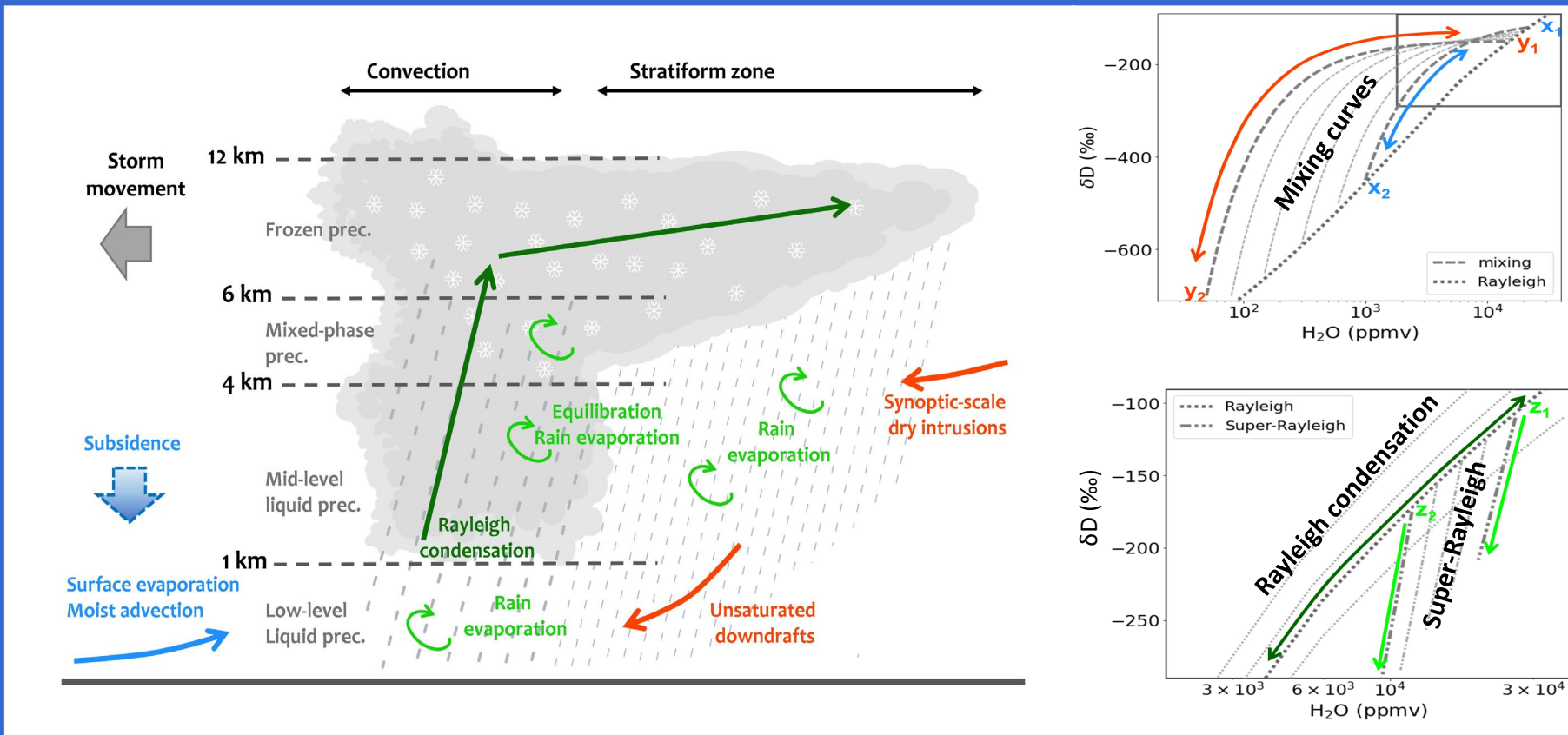


Evaluation of TROPOMI Retrieval

- Ground-based reference data:
 - MUSICA NDACC (calibrated against aircraft in-situ)
 - TCCON (calibrated against NDACC)
- TROPOMI – FTIR comparison:
 - Mean bias of -21‰ and scatter of 35 ‰
 - Largest differences in Tropics (high H₂O amounts)
- Good consistency with MUSICA IASI data with no significant bias



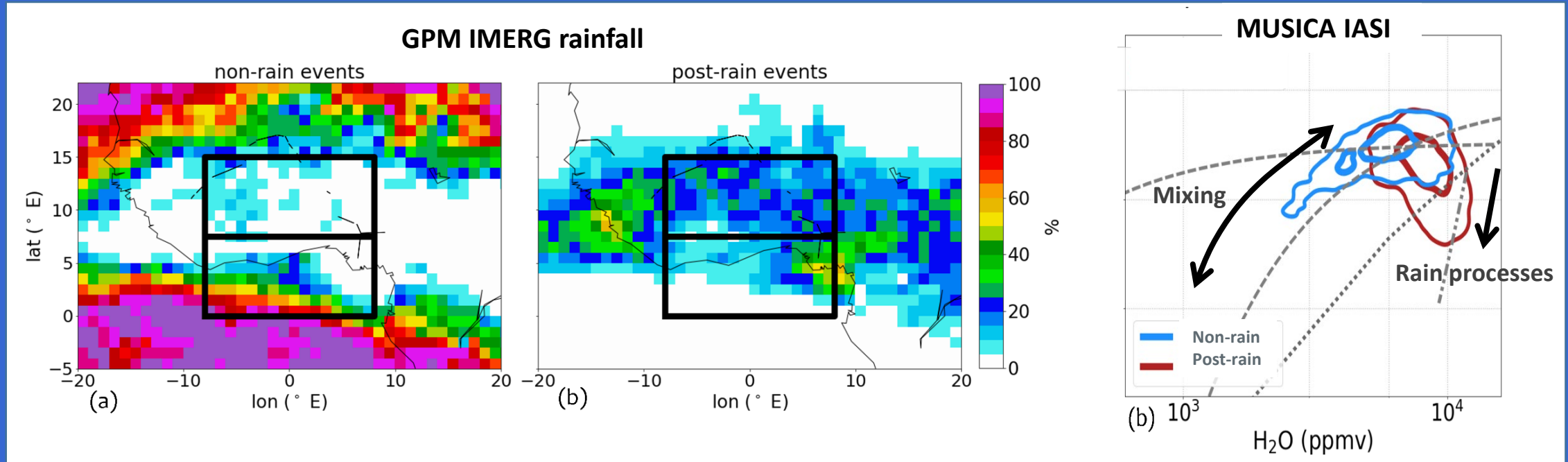
Case Study: {H₂O, δD}-pair distributions during the West Africa Monsoon season



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

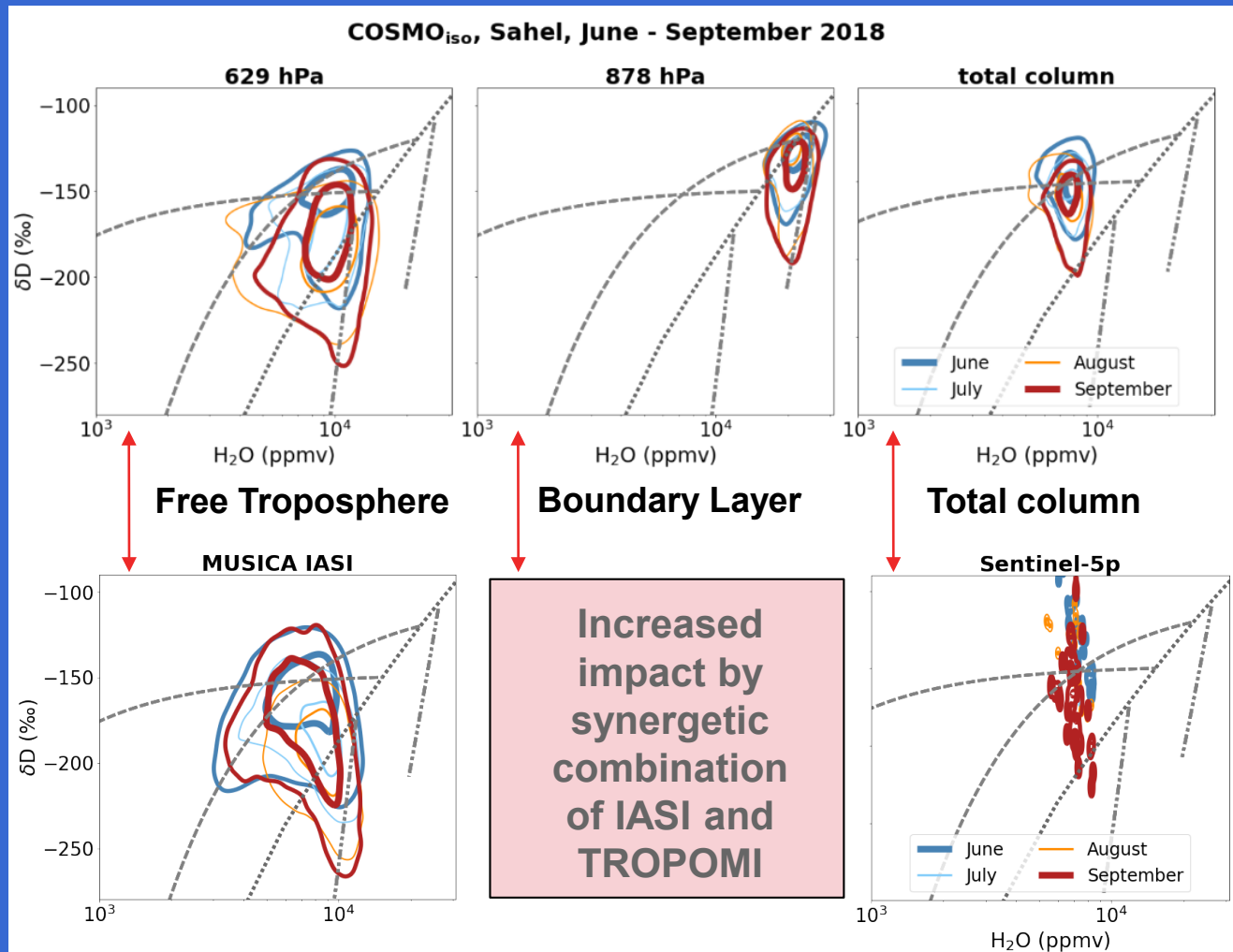
- Mixing (no phase changes) causes distribution above the “Rayleigh line”
- Microphysical processes (convection, clouds) causes distributions below the “Rayleigh line” (“Super-Rayleigh”).

Observations: GPM IMERG rainfall and MUSICA IASI {H₂O, δD} pair distributions (FT), June and July



- Air masses without rain impact: mixing signals in {H₂O, δD} pair distribution
 - Air masses with rain impact: super Rayleigh signals in {H₂O, δD} pair distribution
- {H₂O, δD} pair distribution can identify FT moistening by convective processes

Observations and model (COSMOiso): additional value of TROPOMI column integrated $\{H_2O, \delta D\}$ -pair data



Reasonable model – observations agreement, increasing depletion from June to September:

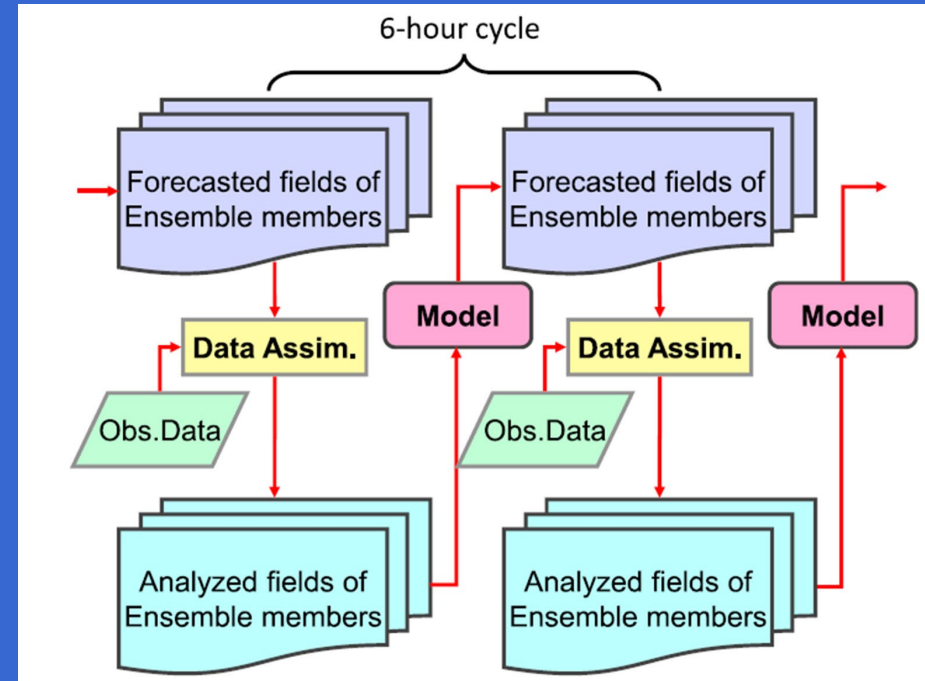
- Free Troposphere (model and IASI observations): mixing and microphysical processes
- Boundary layer (only model): mainly microphysical processes, potential of observation by synergetic combination of IASI and TROPOMI
- Total column (model and TROPOMI observations): data mock a vertically mixed atmosphere, microphysical processes

Data assimilation of water isotopologues

- Assimilation of TROPOMI and IASI q and δD data into the isotope incorporated model (IsoGSM)
- Observation Simulation Experiment (OSSE)
- Data assimilation with an Local Ensemble Transform Kalman Filter (LETKF)
- Impact assessment of the idealized assimilation experiments done by using the Root-Mean-Square Deviation (RMSD) and Skill

$$RMSD = \sqrt{\frac{1}{N} \sum_{i=t_1}^{t_N} (\bar{x}_i - x_n)^2}$$

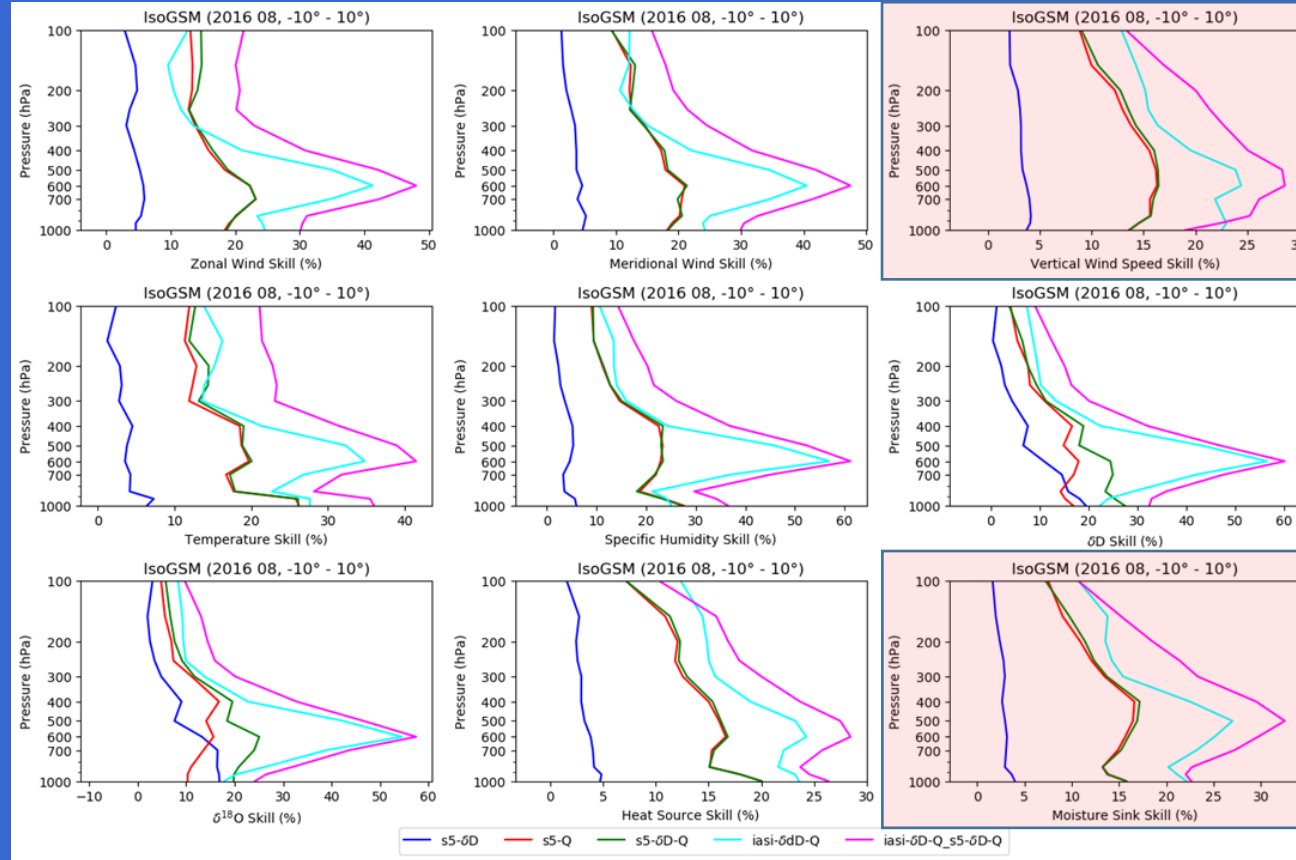
$$skill = \frac{RMSD_{CTRL} - RMSD}{RMSD_{CTRL}}$$



From: Yoshimura et al. (2014)

Data assimilation of water isotopologues

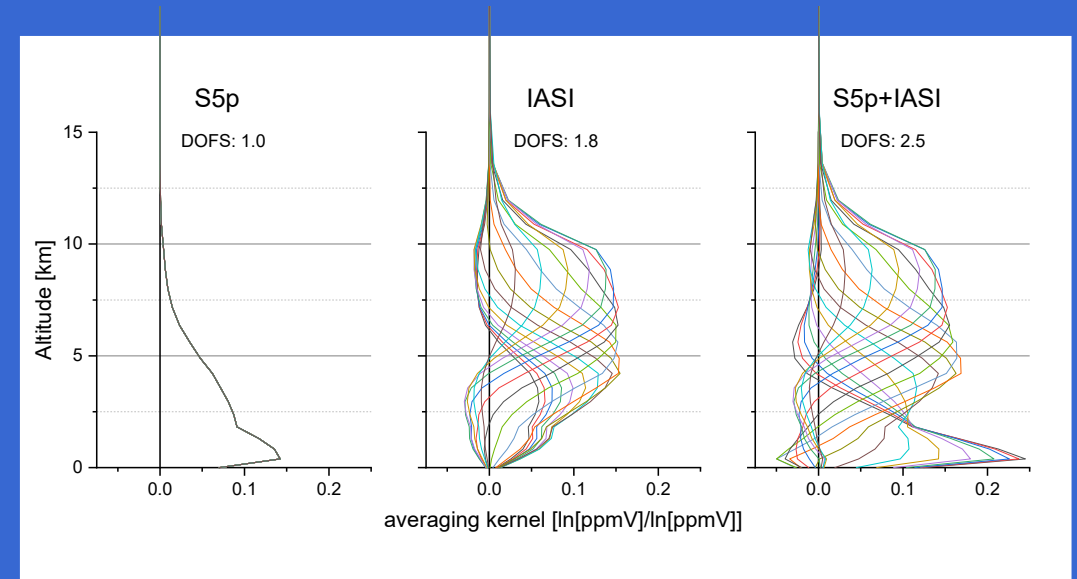
- Skill for the tropics (-10 to 10)



- For all meteorological parameters about 5% improvement is derived when only SP-5 δD is assimilated
- Higher improvements (20-40%) can be derived when S5P q or S5P δD and q are assimilated
- Highest improvements of about 35-45% are derived when S5P δD and q are assimilated together with MUSICA IASI δD and q

Summary and Outlook

- We have developed and validated (wrt fiducial references) a new global TROPOMI water isotopologue retrieval product
- Thanks to its high spatial and temporal coverage of TROPOMI, this dataset is highly useful for deciphering interrelation between weather and isotopic state of atmospheric water vapour
- The new data complements existing free tropospheric data (MUSICA IASI): comparison to model, positive assimilation impact.
- Largest benefit of TROPOMI is realised when used in conjunction with MUSICA IASI data and we plan adoption of synergetic combination of TROPOMI and MUSICA IASI retrievals to extract vertically resolved information.
- The future Sentinel 5 and IASI-NG on METOP-SG-A will offer ideal platform for such a combined approach



Combining TROPOMI with IASI offers unique potential for generating isotopologue profile information

Thank you for Listening.



Further information can be found at:
<https://s5pinnovationh2o-iso.le.ac.uk/>



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