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

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Sentinel-5P Mission: 5 years anniversary

14th October 2022

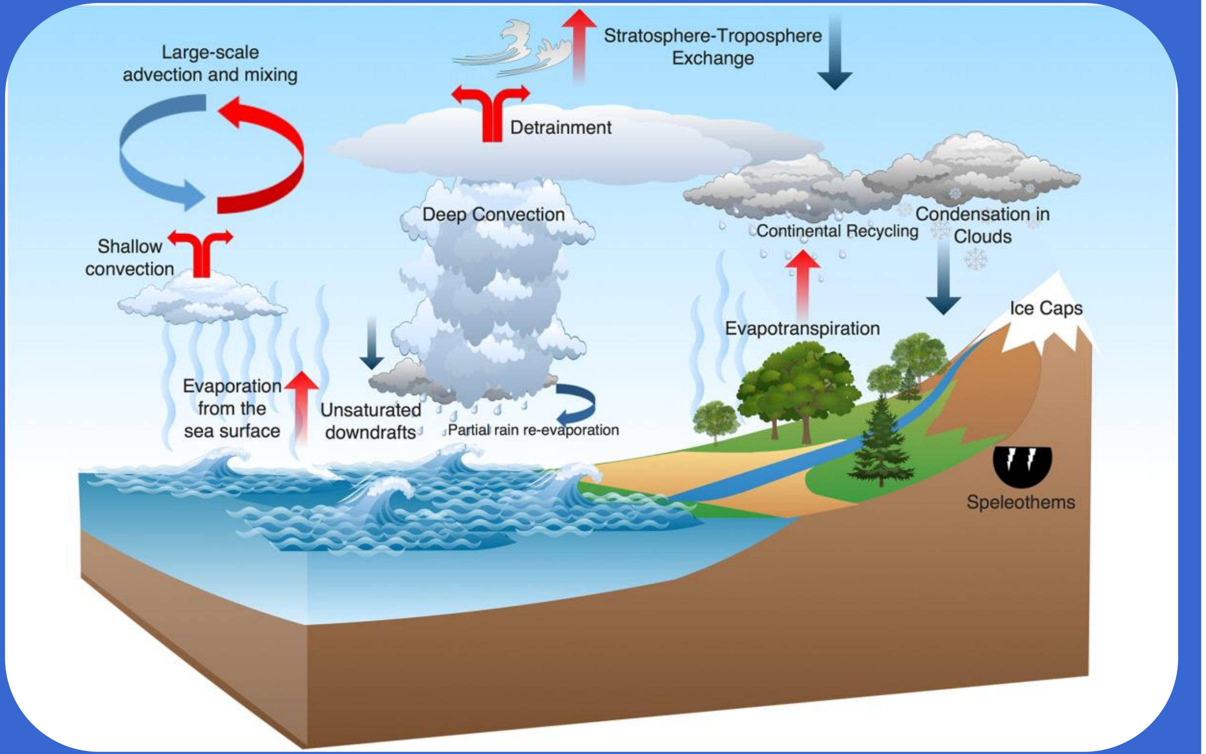
Outline

- Motivation – why do we care?
- Introduce the product – algorithm & validation
- Scientific case studies
- Outlook

Motivation

- Atmospheric moisture is key component of Earth system; however, missing knowledge of moisture pathways.
  - ➢ 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)?
- WCRP grand challenge

Atmospheric moisture pathways



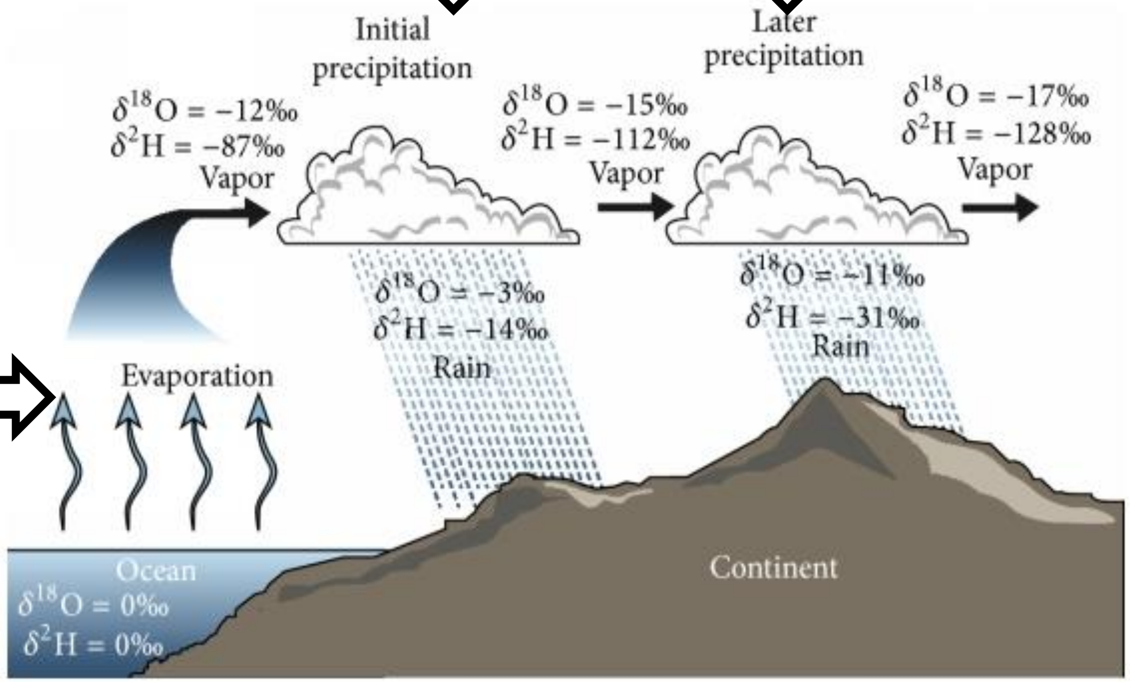
Adopted from Galewski et al. (2016)

Motivation

- Water isotopologues allow to assess and improve model-based representations of moisture sources and pathways in climate (earth system) models
- Water vapour pairs {H2O, δ} can provide information on evaporation, condensation, and precipitation.

Precipitation removes heavy isotopologues more easily resulting in further depletion

Depletion of deuterium (D) and O18 during evaporation from ocean surface (H2O16 -> isotopically lighter -> evaporates more readily)



(Figure taken from Xi, X., 2014.)

Motivation

- Water isotopologues allow to assess and improve model-based representations of moisture sources and pathways in climate (earth system) models
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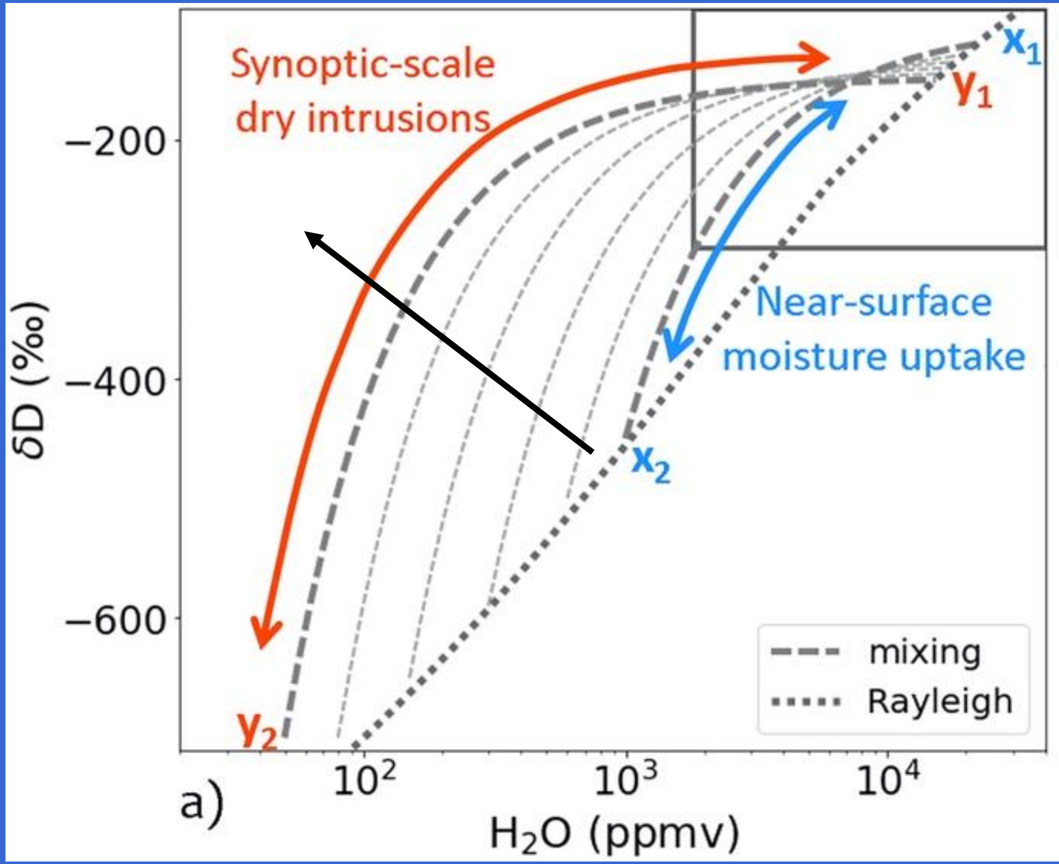
Mixing (no phase changes) causes distribution above the “Rayleigh line”.



Motivation

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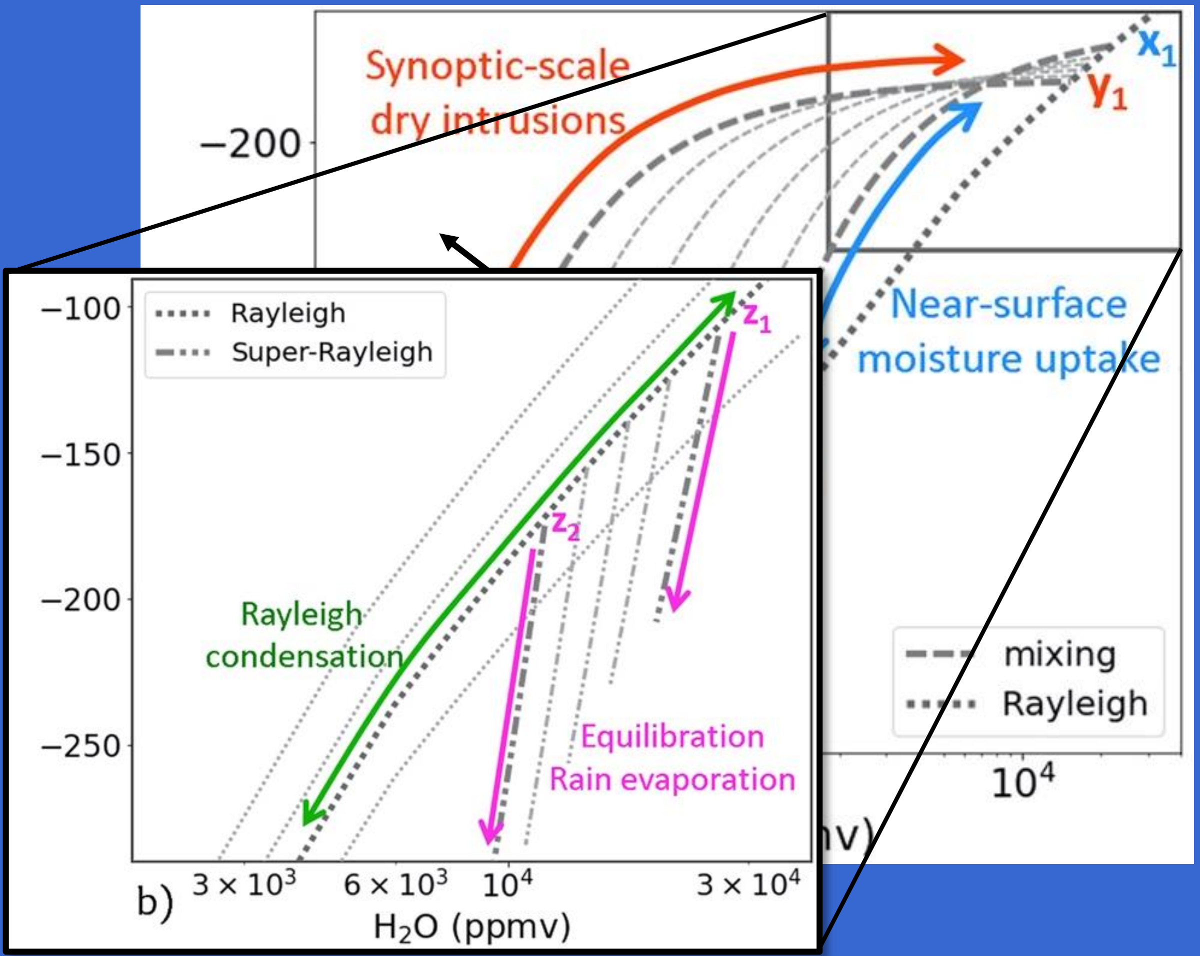


Microphysical processes (convection, clouds) causes distributions below the “Rayleigh line” (“Super-Rayleigh”).

Motivation

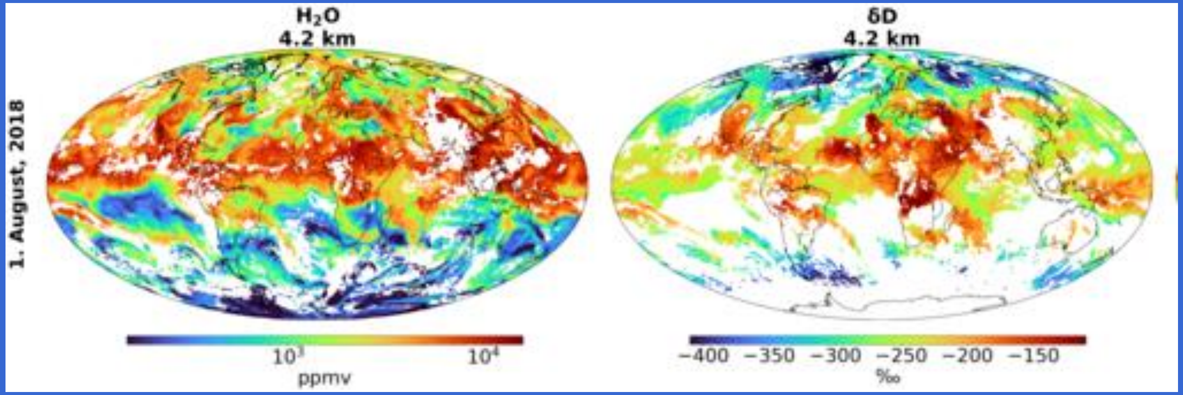
- Satellite observations of stable water Isotopologues can provide global information on the moisture pathways or add an additional constraint.
  - IASI (IR) – mid-tropospheric sensitivity
  - GOSAT and SCIAMACHY (SWIR) – column-averages with boundary layer sensitivity
- Water Isotopologues are given in δ (‰) notation:

$$\delta = \left[\frac{R_{satellite}}{R_s} - 1\right] \cdot 1000‰$$

$$R_s = \begin{cases} HDO/H_2O_{VSMOW} = 3.11 \times 10^{-4} \\ H_2O^{18}/H_2O_{VSMOW} = 2.0052 \times 10^{-3} \end{cases}$$

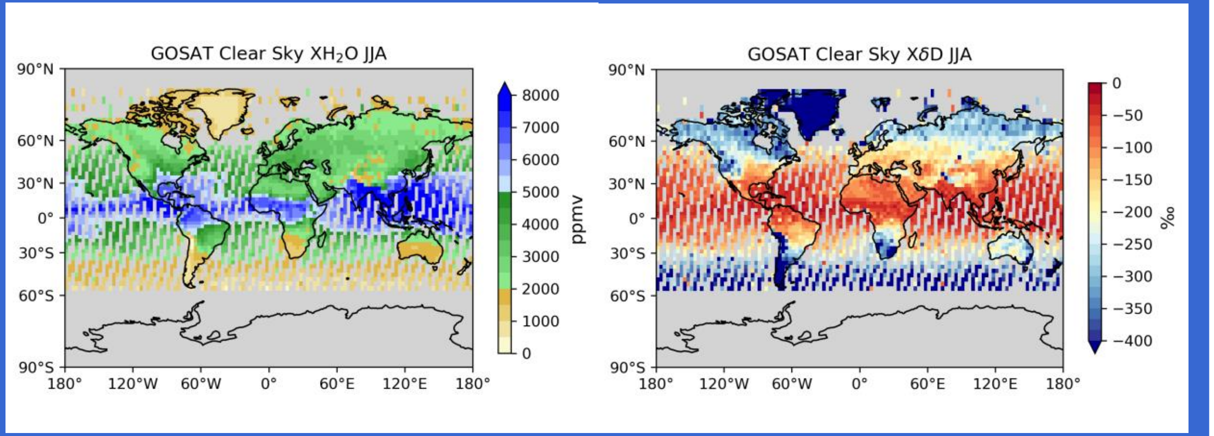
(VSMOW = Vienna Standard Mean Ocean Water)

IASI daily {H_2O, δD}



(e.g. Schneider et al. 2016)

GOSAT seasonal {H_2O, δD}



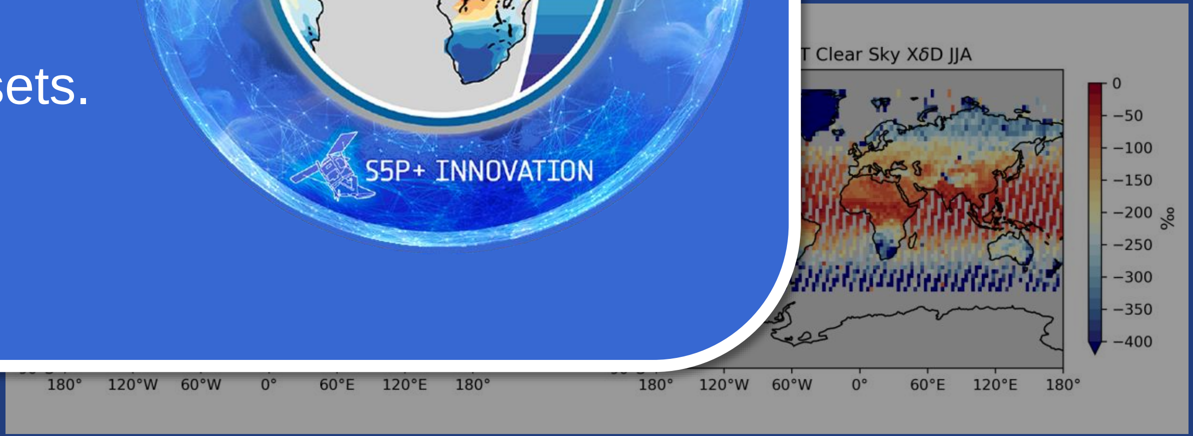
(e.g. Boesch et al. 2012 with updates from Trent et al. 2018)

Motivation

- To demonstrate the feasibility of measuring stable water isotopologues for S5P, specifically ratios of HDO/H2O.
- Characterisation of retrieval performance through validation studies against TCCON and MUSICA NDAAC reference datasets.
- Assess the impact of TROPOMI Isotopolgues through model intercomparison studies.

IASI daily {H_2O, δD}

(e.g. ... Schneider et al. 2016)



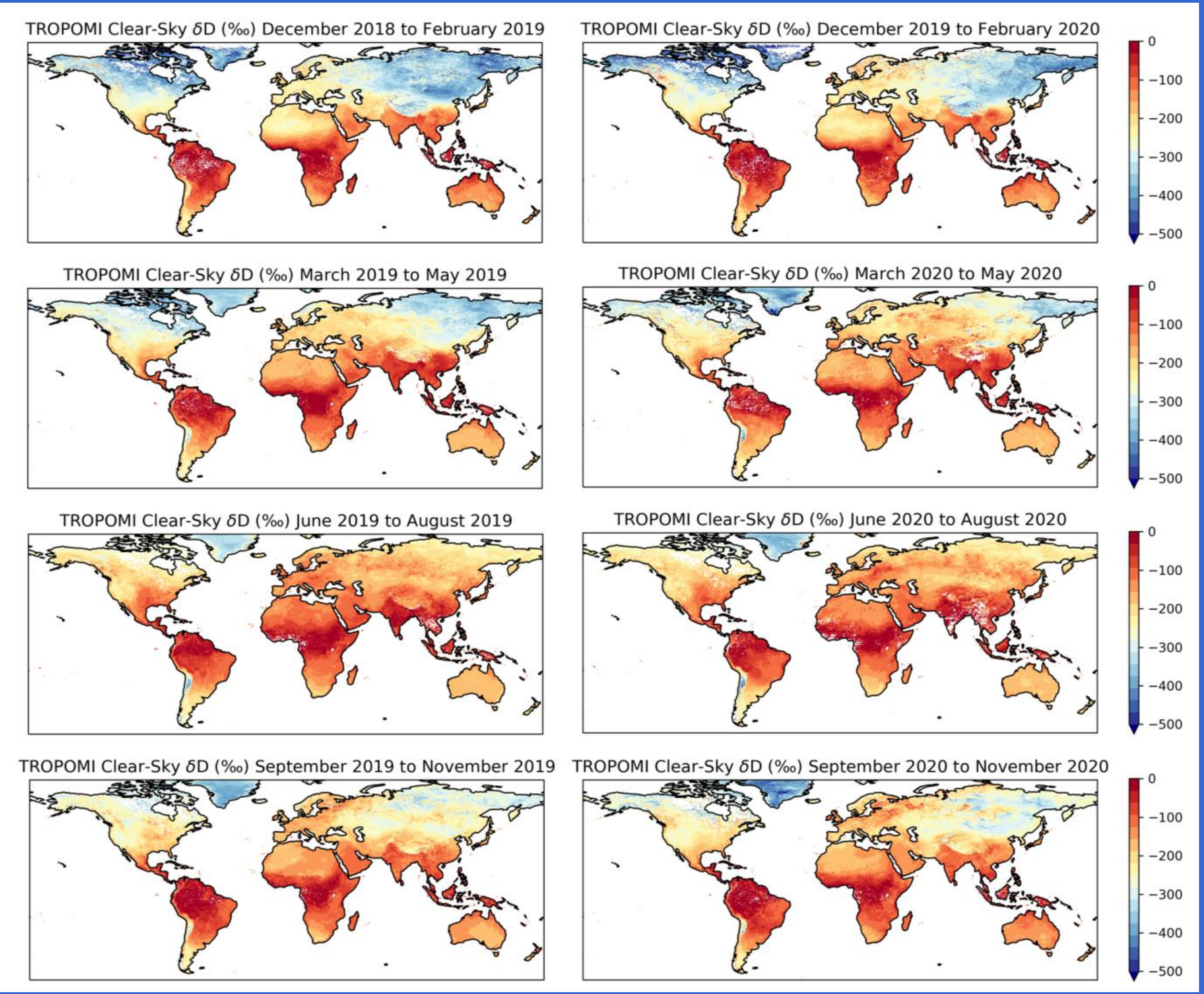
(e.g. Boesch et al. 2012 with updates from Trent et al. 2018)

$$R_s = \left\{ \frac{H_2O^{18}}{H_2O_{VSMOW}} = 2.0052 \times 10^{-3} \right.$$

(VSMOW = Vienna Standard Mean Ocean Water)

TROPOMI stable water vapour isotoplogue product

- Updated version of the UoL-FP algorithm (OE) which has previously used for XCO2, XCH4, XH2O, HDO/H2O, and SIF from SWIR platforms (SCIAMACHY, OCO-2, GOSAT, TanSat).
- Major updates include preprocessing, spectroscopy (SEOM-IAS) and solar model (SOLSPEC), qa_flag development.
- Current version of the L2 product (V1.0.1) currently spans from 1st May 2019 to 30th April 2021 and contains XH2O, XHDO and XδD.



TROPOMI stable water vapour isotoplogue product

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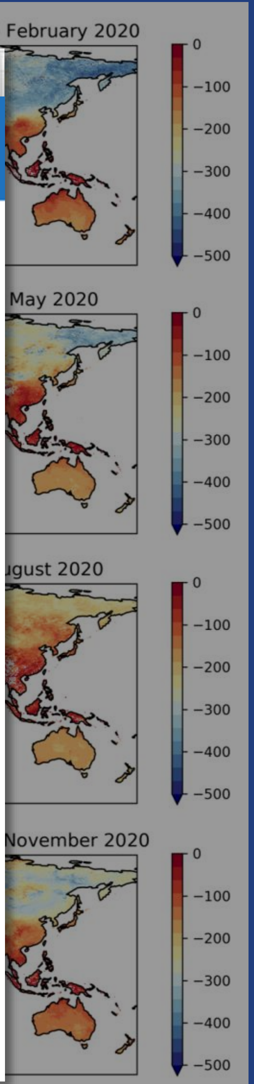

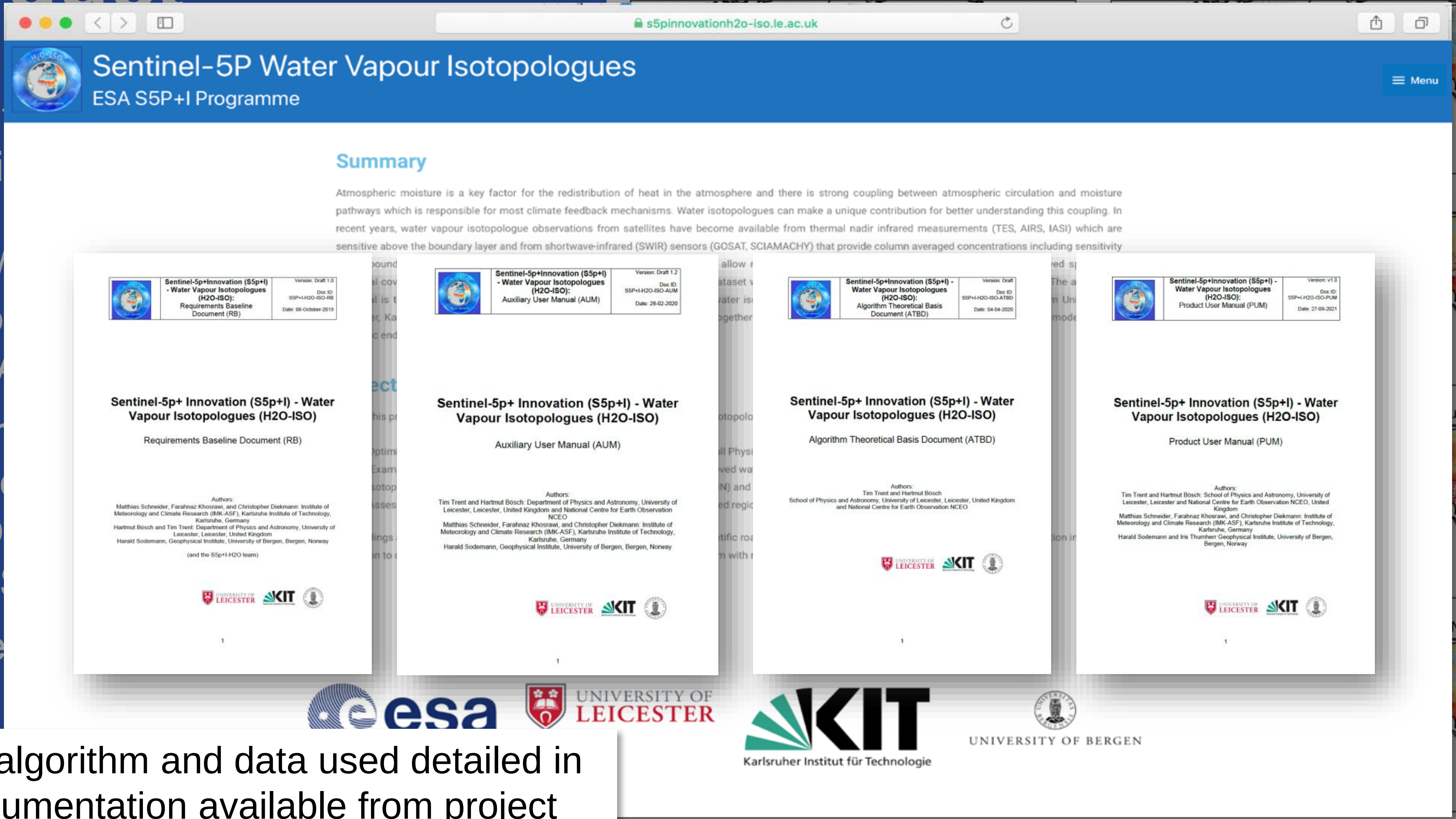

Details on algorithm and data used detailed in project documentation available from project website.

Validation and Study Regions

- Ground-based FTIR monitoring sites and areas identified for development and impact studies.
- TROPPOMI data over validation sites May 2018 – August 2020 was generated.
- MUSICA NDACC and TCCON remote sensing stations as fiducial references.
- Colocation criteria was investigated and set to TROPOMI pixels within a 50 km radius and ±3 hours of a NDAAC/TCCON measurement were used.

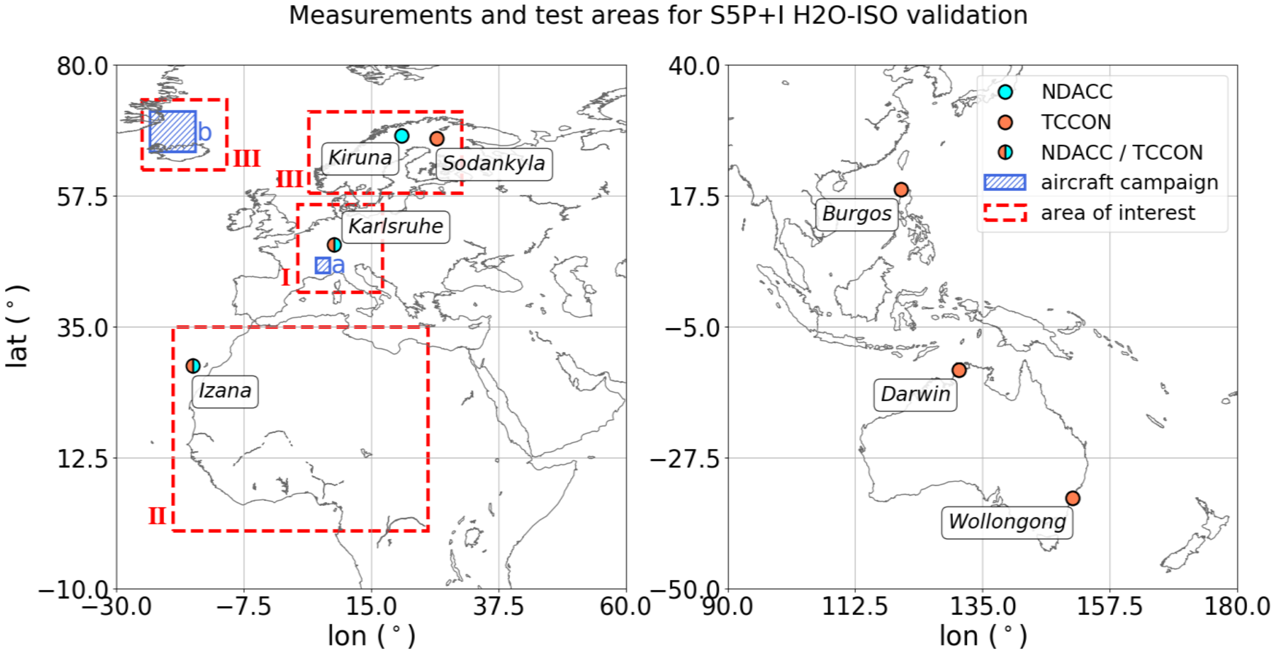

Table 3: Ground-based station, FTIR data availability, Code used for retrieving the FIR data and responsible team.

FTIR Station	Ground-based data availability	Code	Team
Karlsruhe	Apr 2010 – Apr 2021	PROFFIT	KIT-ASF
Kiruna	Mar 1996 – Apr 2021	PROFFIT	KIT-ASF; IRF Kiruna
Sodankylä	May 2009 - Oct 2020	GFIT	FMI
Burgos	Mar 2017 - Mar 2020	GFIT	NIES Tsukuba; U. of Wollongong
Karlsruhe	Apr 2010 – Oct 2020	GFIT	KIT-ASF
Darwin	Aug 2005 – Mar 2020	GFIT	U. of Wollongong
Wollongong	Jun 2008 – Mar 2020	GFIT	U. of Wollongong

Initial Validation Results

FTIR Station	# of colocated qa-filtered pixel (days) for 50 km	Mean bias [‰]	Uncertainty of mean bias [‰]	StdD of difference [‰]
Karlsruhe	46,950 (164)	-20.6 (-16.7)	0.2 (1.9)	31.9 (24.2)
Kiruna	14,567 (88)	-6.9 (6.6)	0.3 (3.0)	37.8 (27.7)
NDACC	**61,517 (252)**	**-17.3 (-8.6)**	**0.1 (1.8)**	**33.9 (27.8)**
Sodankylä	61,265 (241)	-10.2 (12.2)	0.2 (2.5)	39.6 (38.6)
Burgos	2,269 (85)	-52.7 (-41.1)	0.5 (3.2)	25.4 (29.8)
Karlsruhe	41,856 (170)	-26.5 (-21.9)	0.2 (2.3)	33.8 (29.4)
Darwin	22,437 (134)	-48.7 (-54.0)	0.1 (1.6)	18.3 (18.9)
Wollongong	15,987 (224)	-19.7 (-13.4)	0.3 (2.1)	36.8 (31.5)
TCCON	**143,814 (854)**	**-21.0 (-14.8)**	**0.1 (1.2)**	**36.5 (36.0)**
ALL SITES	**205,331 (1,106)**	**-21.1 (-15.1)**	**0.1 (1.1)**	**36.5 (36.8)**

Initial Validation Results

- The highest standard deviation values are found for the polar sites Kiruna and Sodankylä for solar zenith angles above 55°.
- Increased scatter for albedo values below about 0.07, especially at the high latitude sites Sodankylä and Kiruna.
- Strong dependency of the data quality with the total atmospheric water vapour content (1500 ppmv).
- Bias correction based XH2O dependence:
  -(-0.0112‰*XH2O + 1.03‰).

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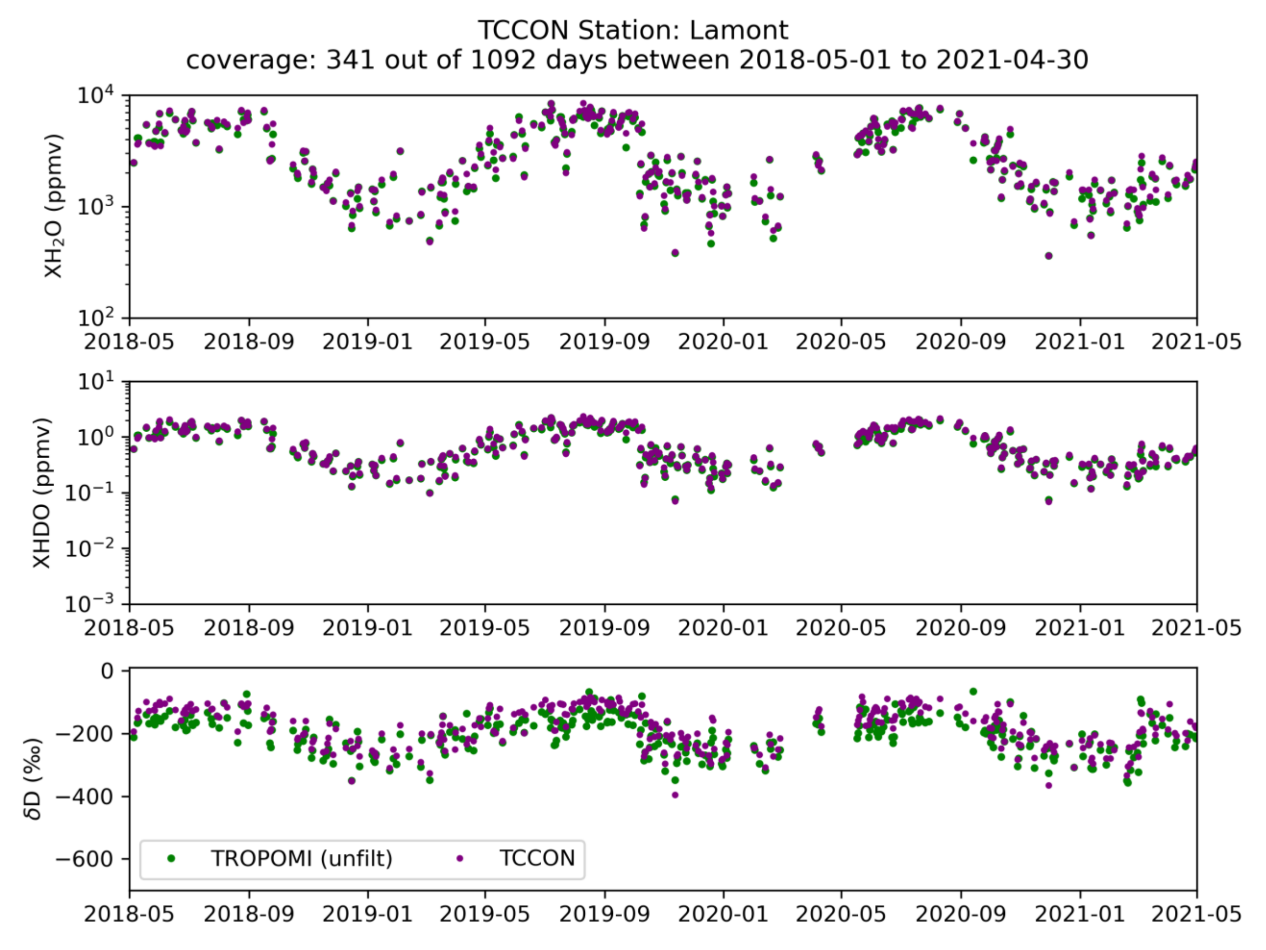
ALL SITES	205,331 (1,106)	-21.1 (-15.1)	0.1 (1.1)	36.5 (36.8)

Bias Corrected Results

FTIR Station	# of colocated qa-filtered pixel (days) for 50 km	Mean bias [‰]	Uncertainty of mean bias [‰]	StdD of difference [‰]
Karlsruhe	46,950 (164)	-0.9 (8.5)	0.0 (0.7)	32.5 (23.2)
Kiruna	14,567 (88)	13.0 (24.6)	0.1 (2.6)	37.5 (28.1)
NDACC	**61,517 (252)**	**2.4 (14.1)**	**0.0 (0.9)**	**34.3 (26.1)**
Sodankylä	61,265 (241)	13.4 (32.7)	0.1 (2.1)	38.4 (35.6)
Burgos	2,269 (85)	-7.2 (7.6)	0.2 (0.8)	26.3 (28.9)
Karlsruhe	41,856 (170)	-6.4 (3.8)	0.0 (0.3)	33.3 (25.2)
Darwin	22,437 (134)	-14.3 (-10.5)	0.1 (0.9)	18.6 (19.1)
Wollongong	15,987 (224)	2.8 (11.6)	0.2 (0.8)	35.4 (29.8)
TCCON	**143,814 (854)**	**2.0 (12.4)**	**0.0 (1.2)**	**35.3 (31.0)**
ALL SITES	**205,331 (1,106)**	**1.9 (12.6)**	**0.0 (0.2)**	**35.2 (31.3)**

Enhanced Validation and bias correction

- Uses full 3 year data set and collocations from 20 TCCON sites.
- Tighter collocation criteria,+/-30 mins, within 50 km, p_{surf} within 5 hPa and T700 within 2 K
- Calculate daily means.
- Utilize dependence on SZA, albedo, XH2O + others(?)
- Bias correction uses ML approach model build on extra-trees regressor



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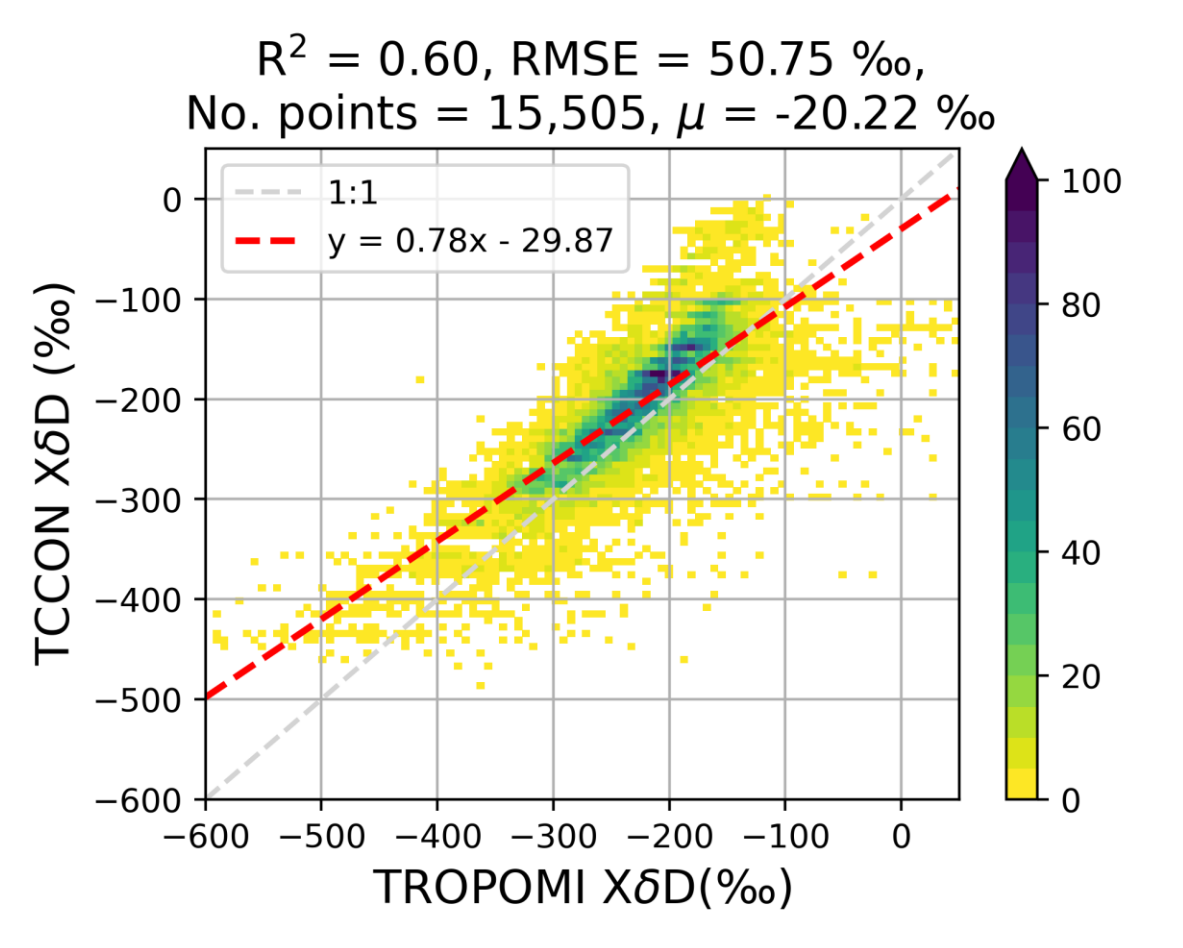

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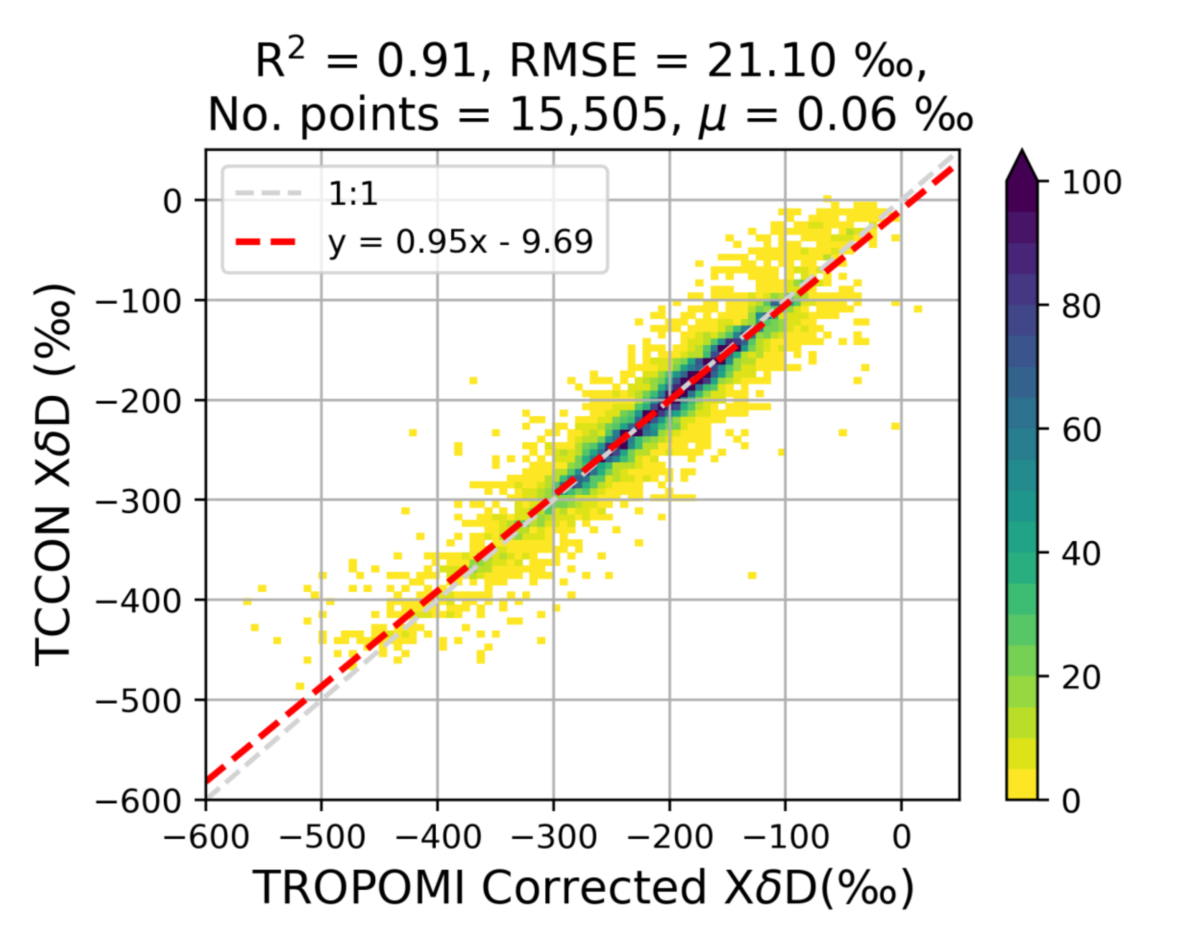

Enhanced Validation and bias correction

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- Utilize
  XH2O
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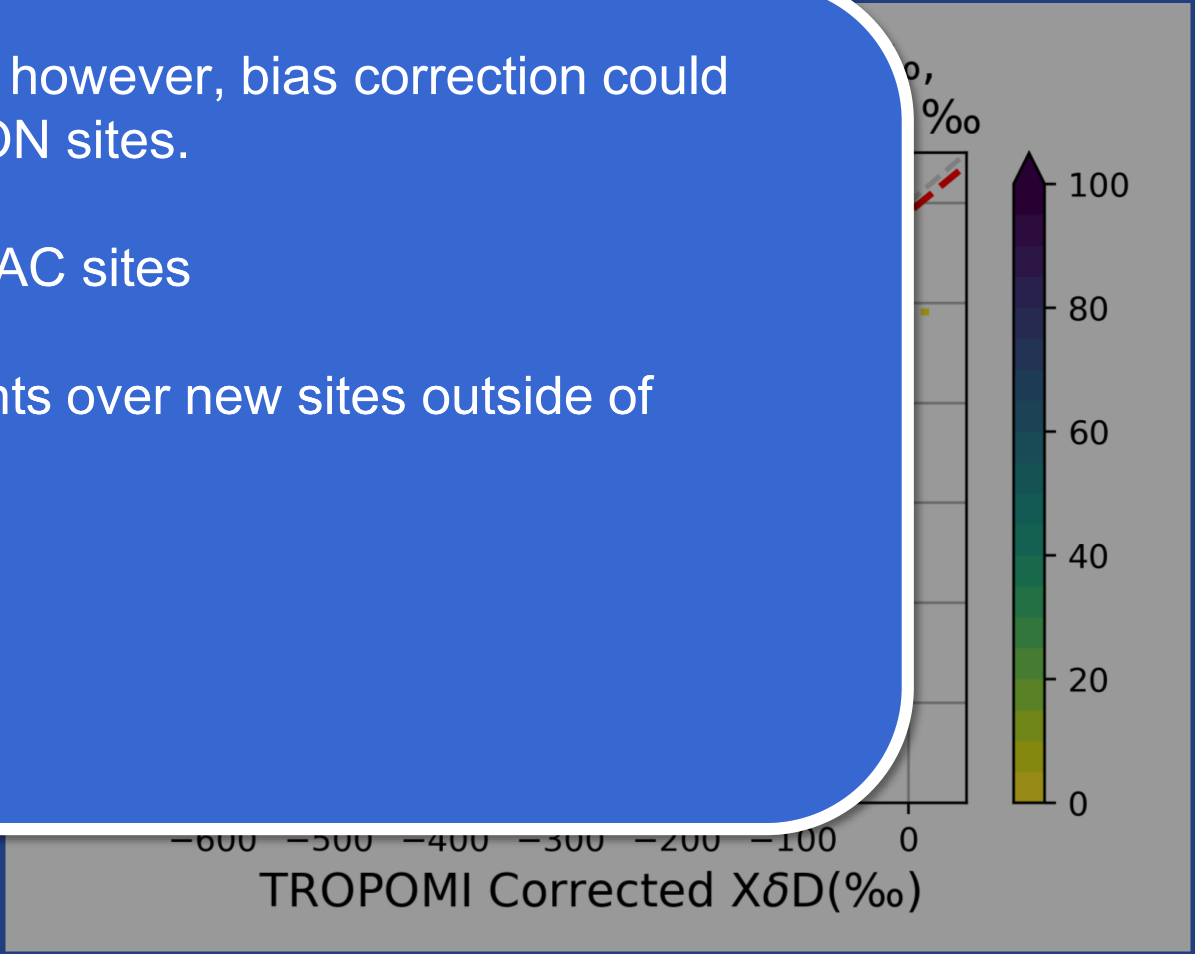
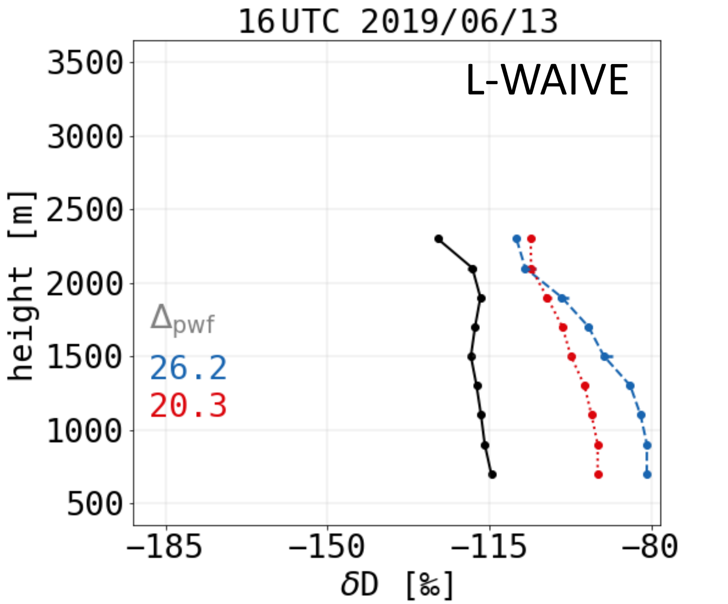
  model

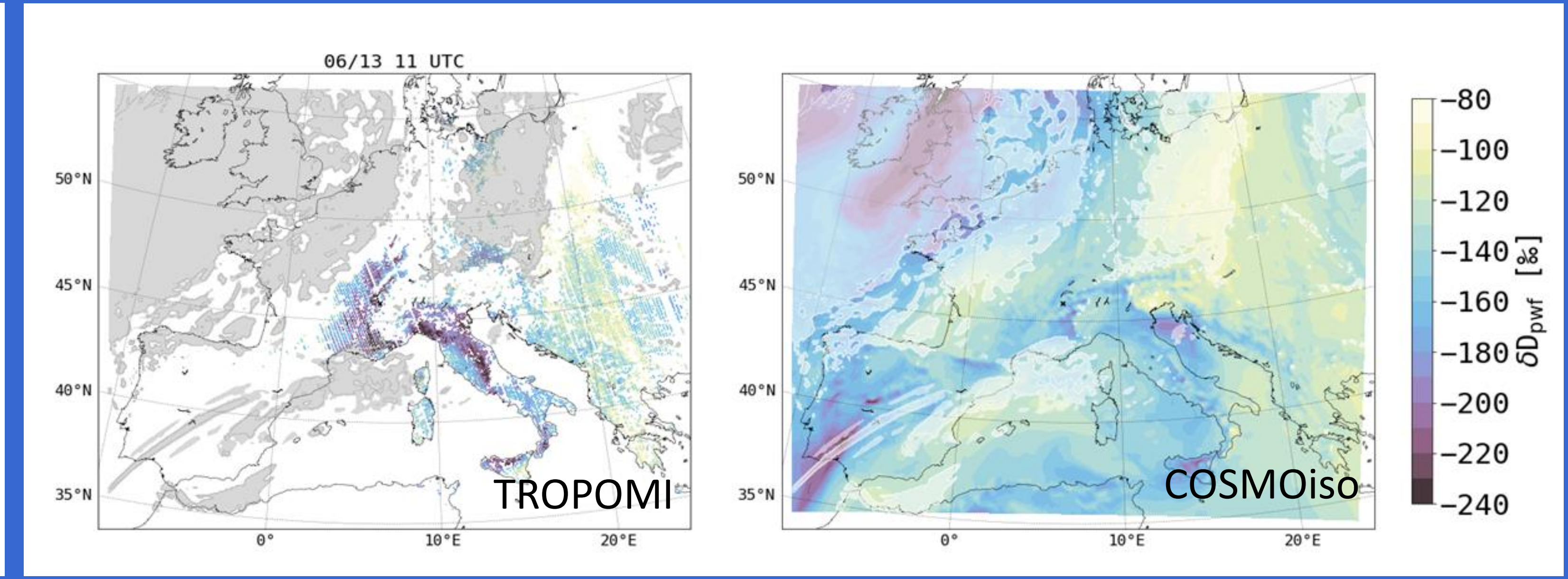
- Initial results look promising; however, bias correction could just perform well over TCCON sites.
- Can test over MUSICA NDAAC sites
- New COCCON measurements over new sites outside of current TCCON network.



Scientific case study 1: Scale analysis

- **Datasets of different spatial and temporal resolution:**
  - In situ measurements during the LWAIVE campaign in Annecy 2019 (Chazette et al. 2021)
  - Sentinel 5-P retrieval of total column δD
  - COSMOiso (Pfahl et al. 2012) simulations during the L-WAIVE campaign

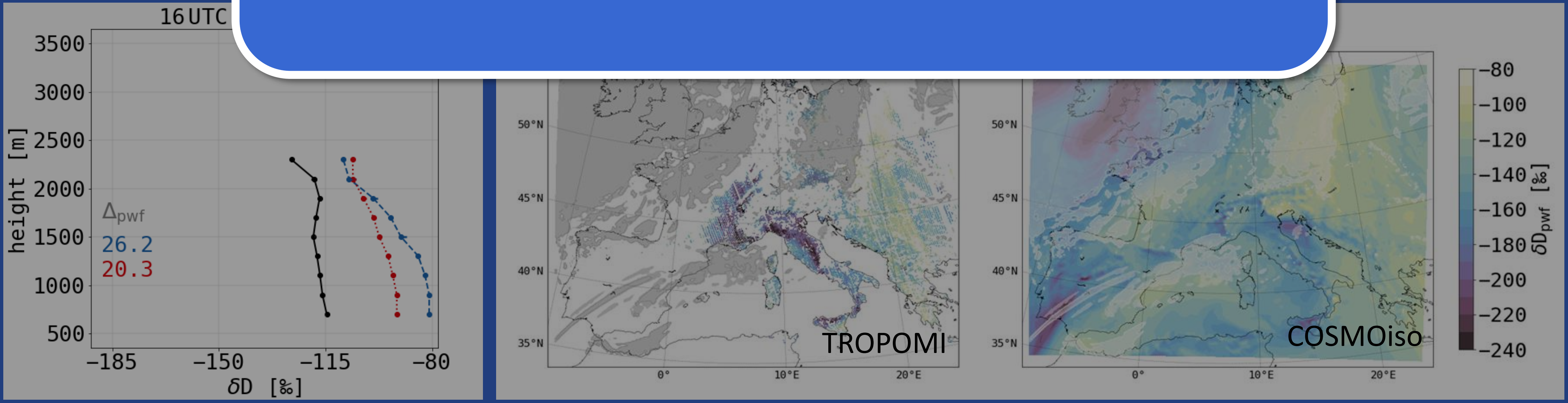




Scientific case study 1: Scale analysis

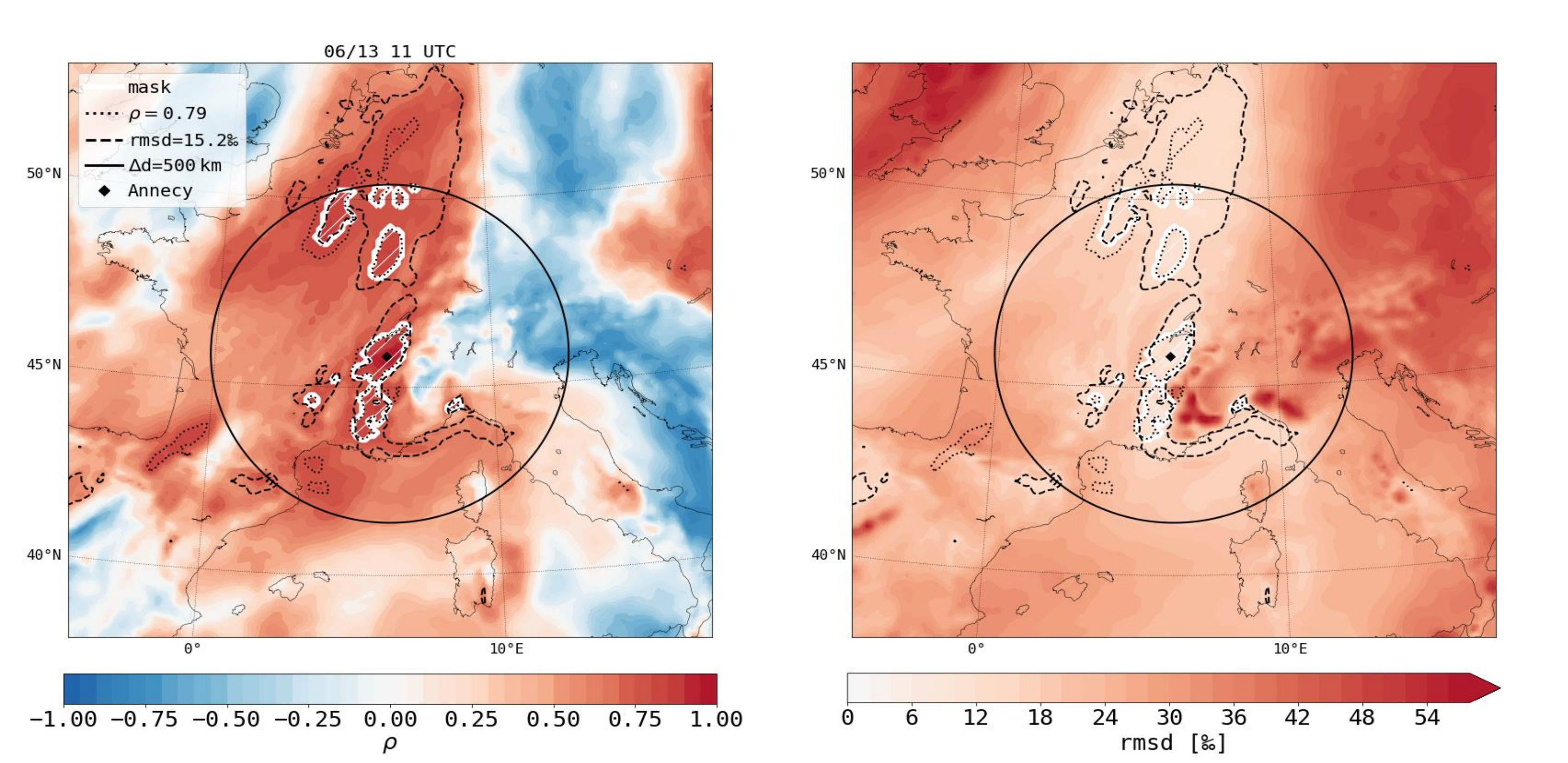
- **Datasets**
  - In sit... tte et al. 2021)
  - Sent...
  - COS...

- How representative are in situ measurements for large-scale δD patterns?
- How to use regional COSMOiso simulations to enable a comparison between in-situ and satellite observations?



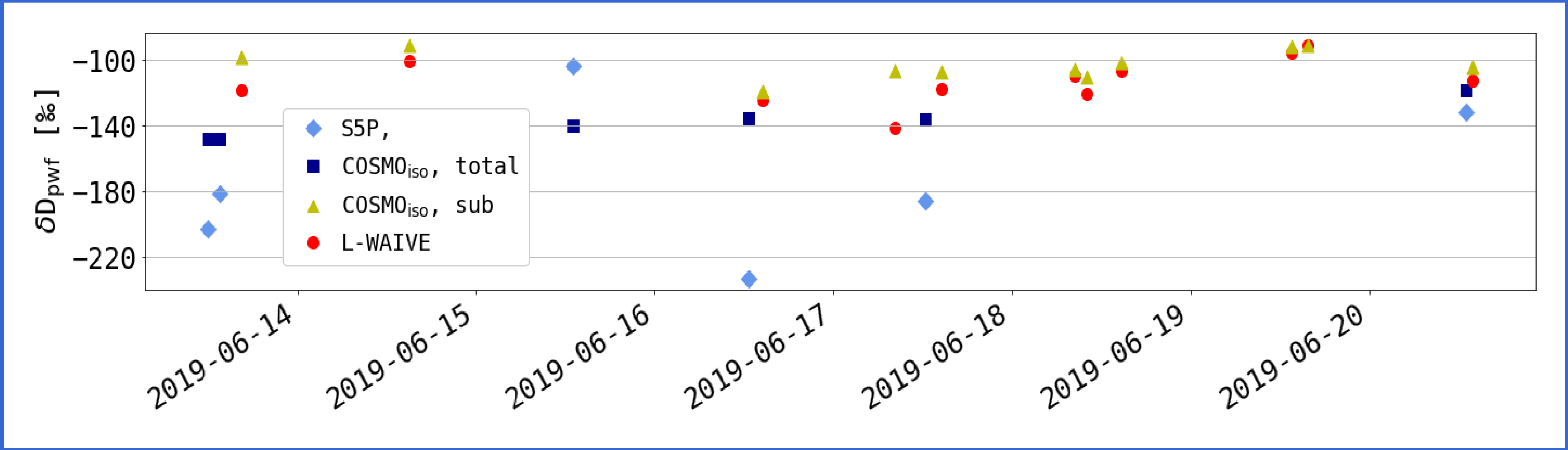
Scientific case study 1: Scale analysis

- **With COSMOiso:**
  - Definition of collocation regions
  - Comparison of total and subcolumn δD



Scientific case study 1: Scale analysis

- COSMOiso agrees well with in situ measurements and subcolumn value in boundary layer.
- TROPOMI total column values lower than COSMOiso: underestimation of δD at high altitude by COSMOiso.

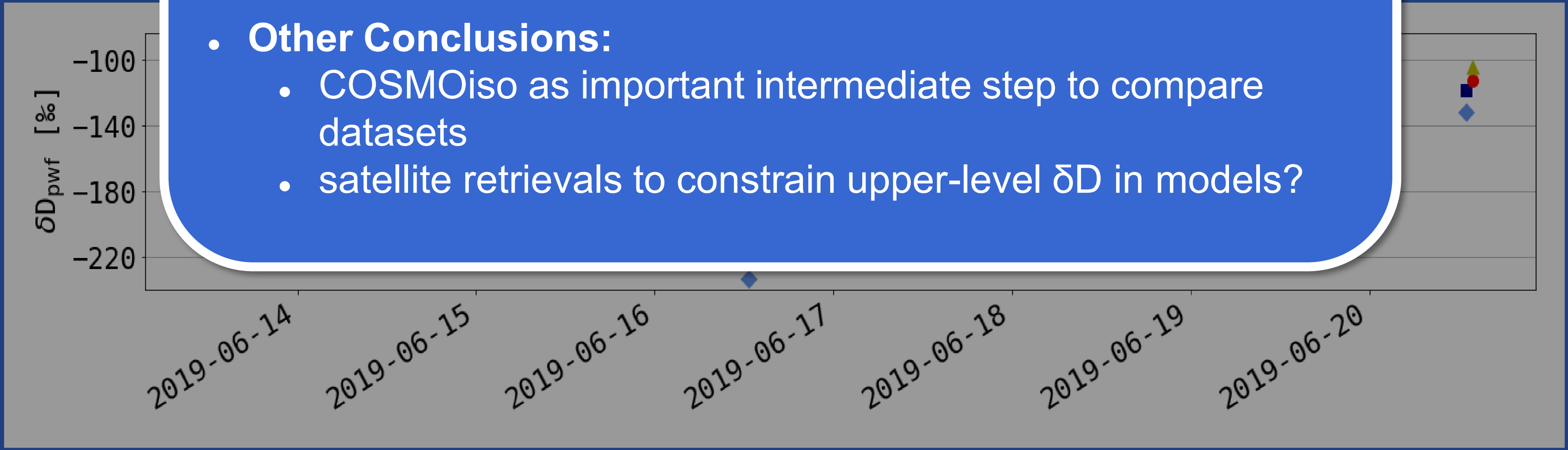


Scientific case study 1: Scale analysis

- COSMOiso … ndary layer.
- TROPOM … igh altitude by …

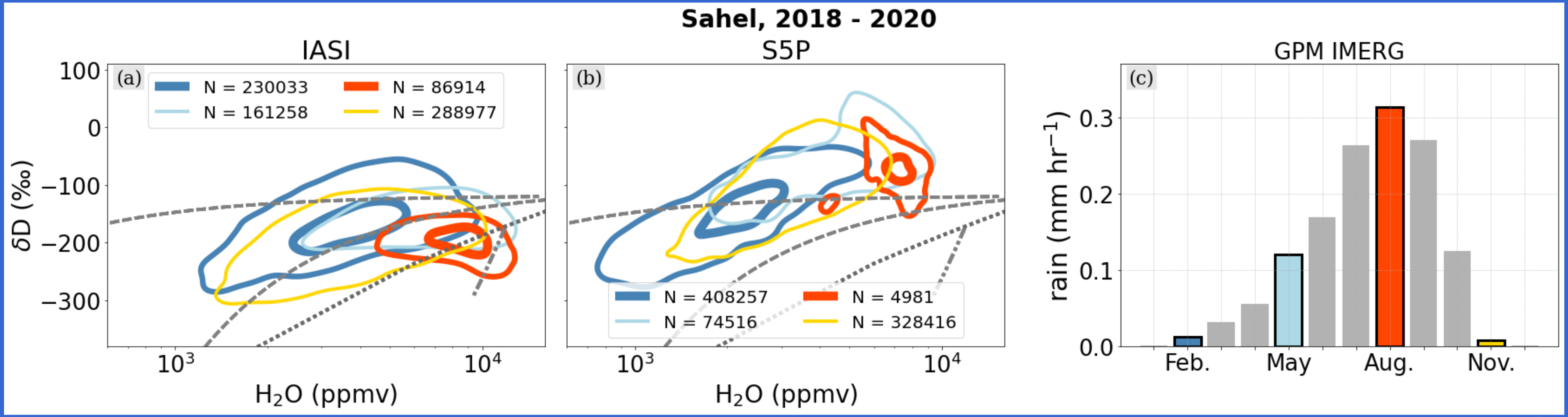
- **Learnings for future campaigns:**
  - flat terrain vs. topography
  - synchronize flights with satellite overpasses (if possible w.r.t to campaign goals)

- **Other Conclusions:**
  - COSMOiso as important intermediate step to compare datasets
  - satellite retrievals to constrain upper-level δD in models?



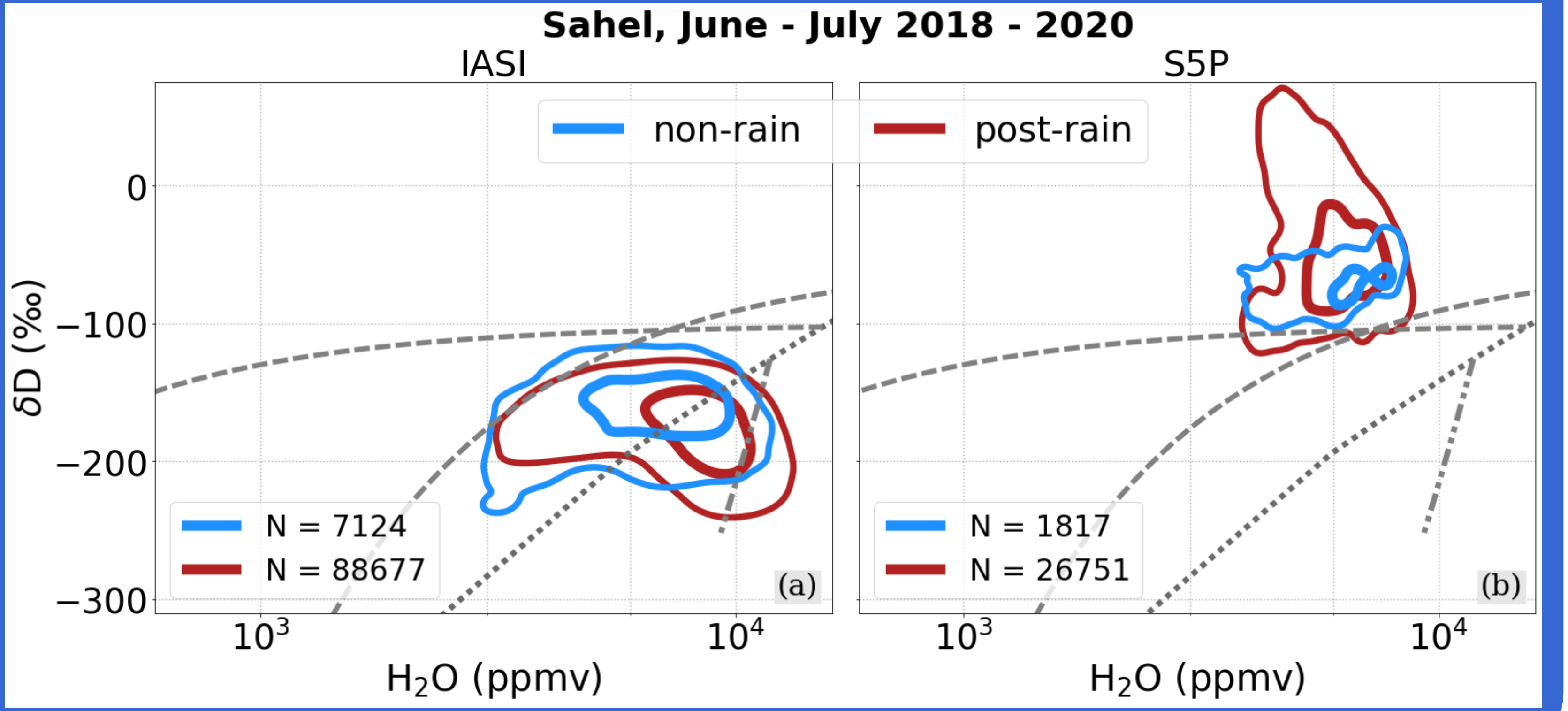
Scientific case study 2: Complimentary observations

- Quantitative differences in both H2O and δD, which arise from different vertical sensitivities of IASI and TROPOMI.
- IASI and S5P show an overall similar annual cycle, from a dry and depleted winter to a moist monsoon summer. Both sensors record an enhanced depletion in δD during summer, which is a result of cloud and rain processes associated with the monsoon convection.
- In addition to that, we observe strongly enriched values in S5P during May and August, which is not reflected in IASI.



Scientific case study 2: Complimentary observations

- For IASI, we observe a pull towards moister and more depleted H2O-δD regimes if the observed air masses were affected by convective rain. These features again result from microphysical processes like rain evaporation.
- Interestingly, for S5P we observe some opposite effects: here, convective precipitation has a strongly enriching effect.
- S5P captures effects from the boundary layer, where surface evaporation has strong impact (e.g. convection lifts moisture from the ground).

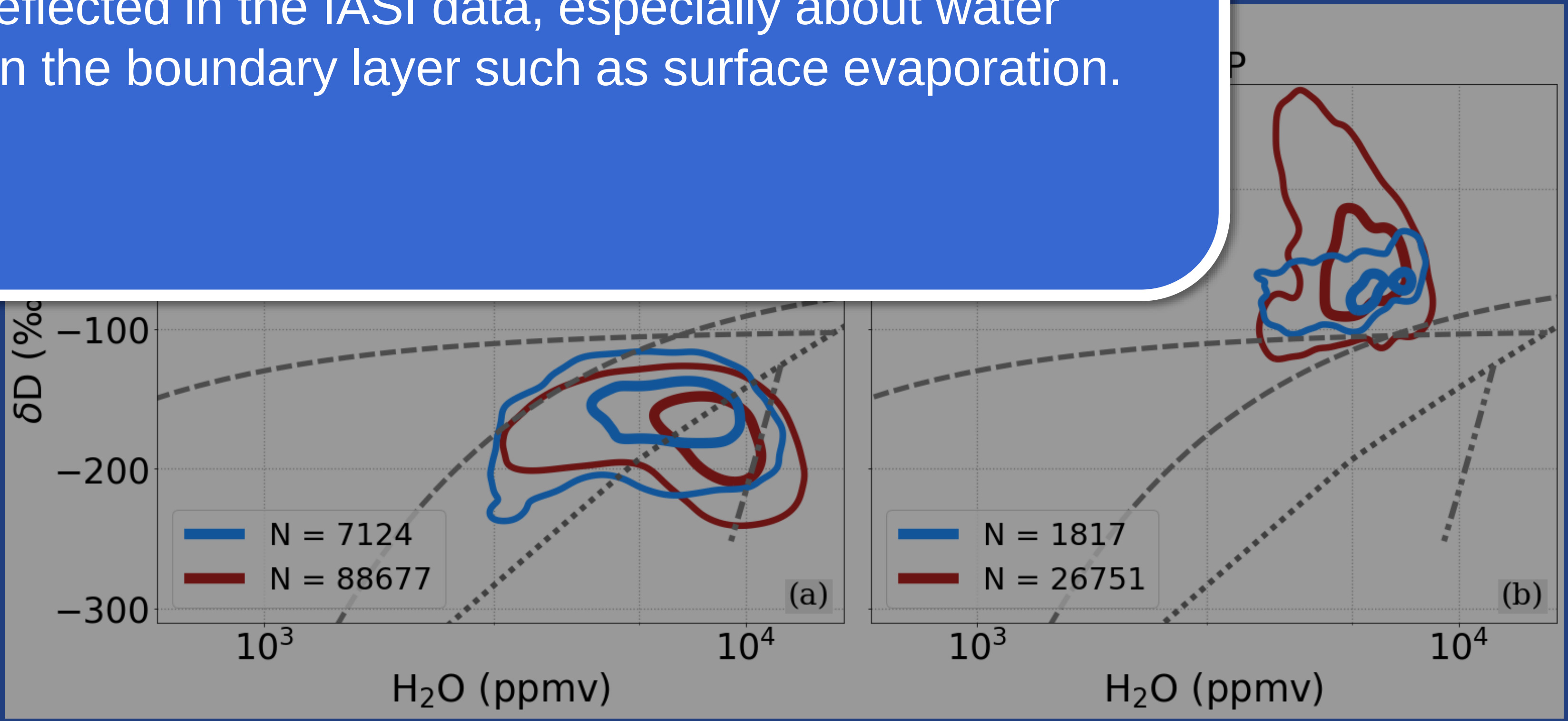


Scientific case study 2: Complimentary observations

- For IASI, w… if the observed … lt from microphys…
- Interesting… observe s… effects: he… precipitati… strongly en…

- S5P captures effects from the boundary layer, where surface evaporation has strong impact (e.g. convection lifts moisture from the ground).

- clearly see that TROPOMI adds complementary information that is not reflected in the IASI data, especially about water processes in the boundary layer such as surface evaporation.



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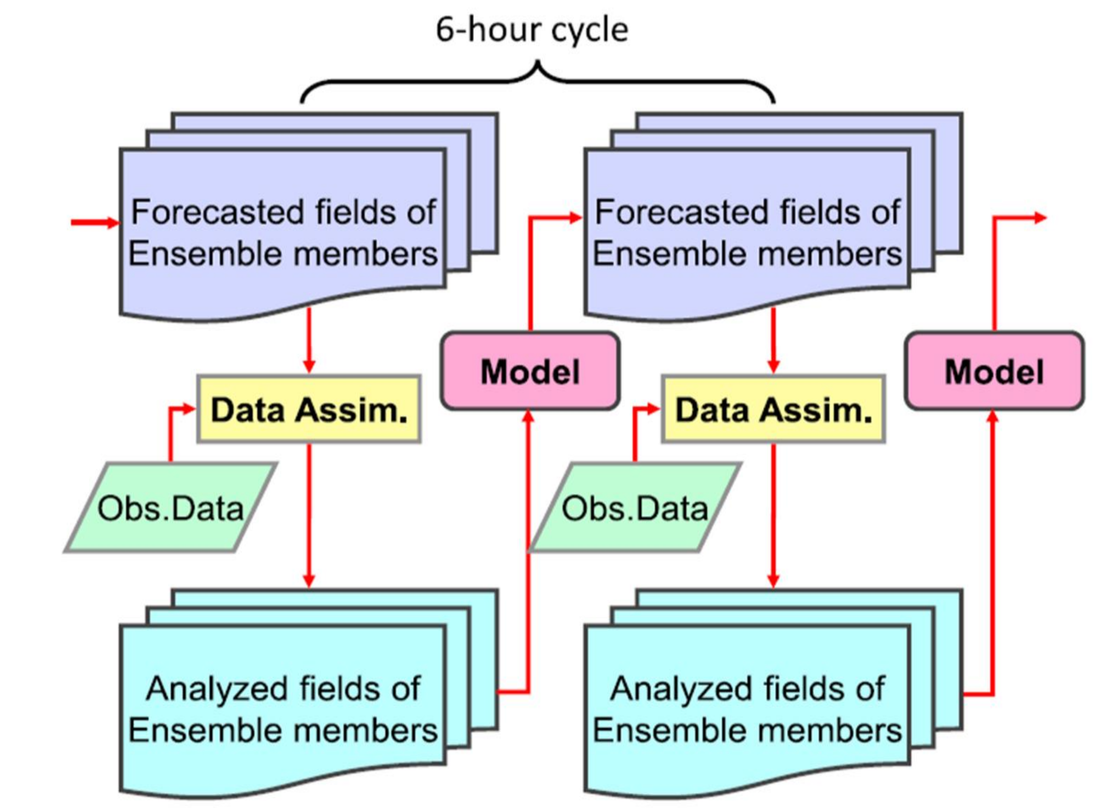
Scientific case study 3: Data assimilation

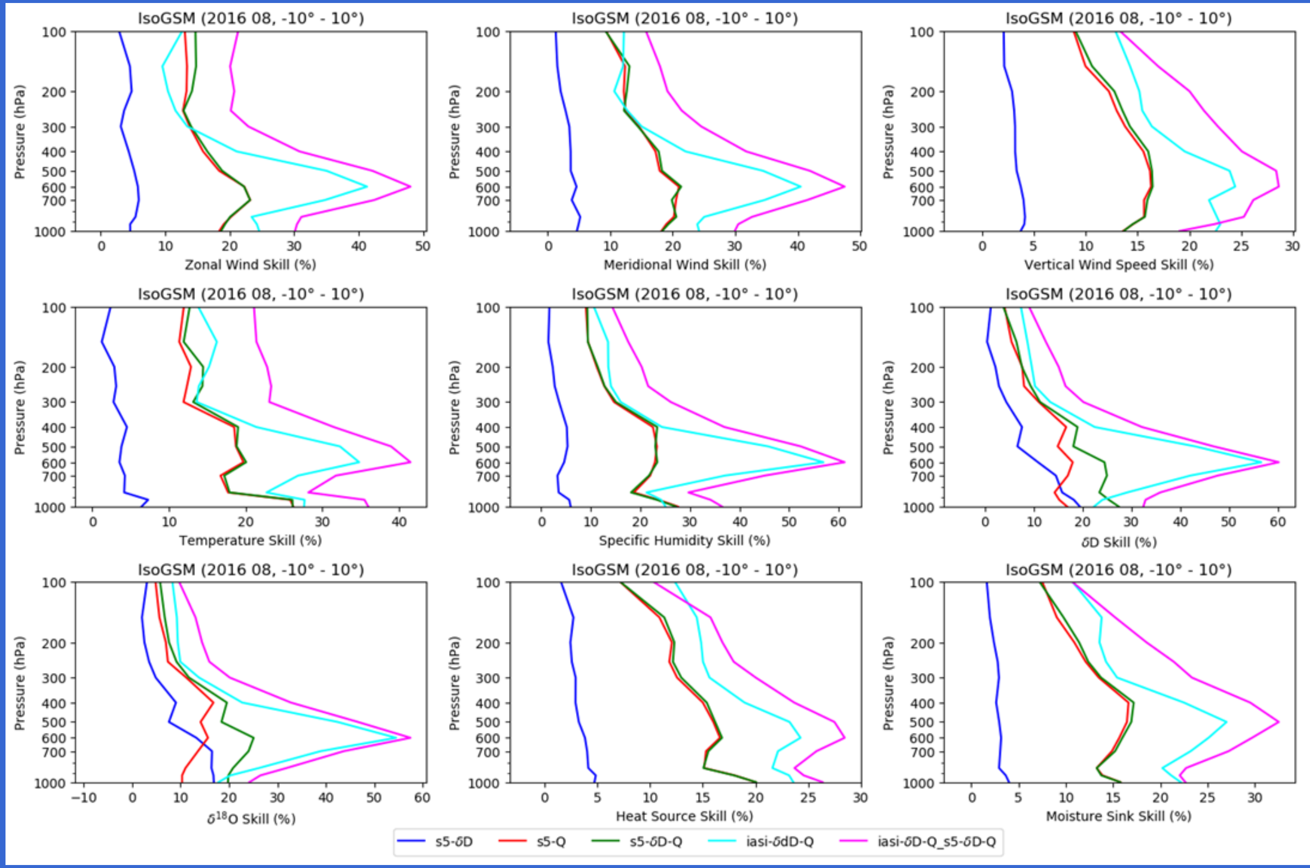
- Assimilation of TROPOMI and IASI q and δD data into the isotope incorporated model (IsoGSM)
- Observation Simulation Experiment (OSSE)
- Data assimilation with an Local Ensemble Transform Kalman Filter (LETKF)
- Impact assessment of the idealized assimilation experiments done by using the Root-Mean-Square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



From: Yoshimura et al. (2014)

Scientific case study 3: Data assimilation

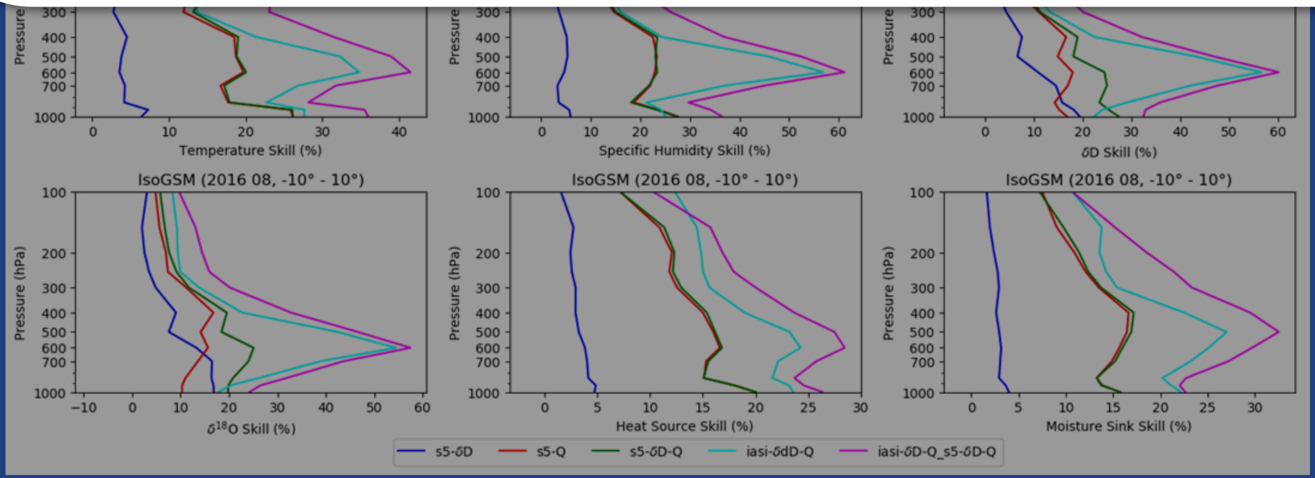
- Skill for the tropics (-10 to 10)

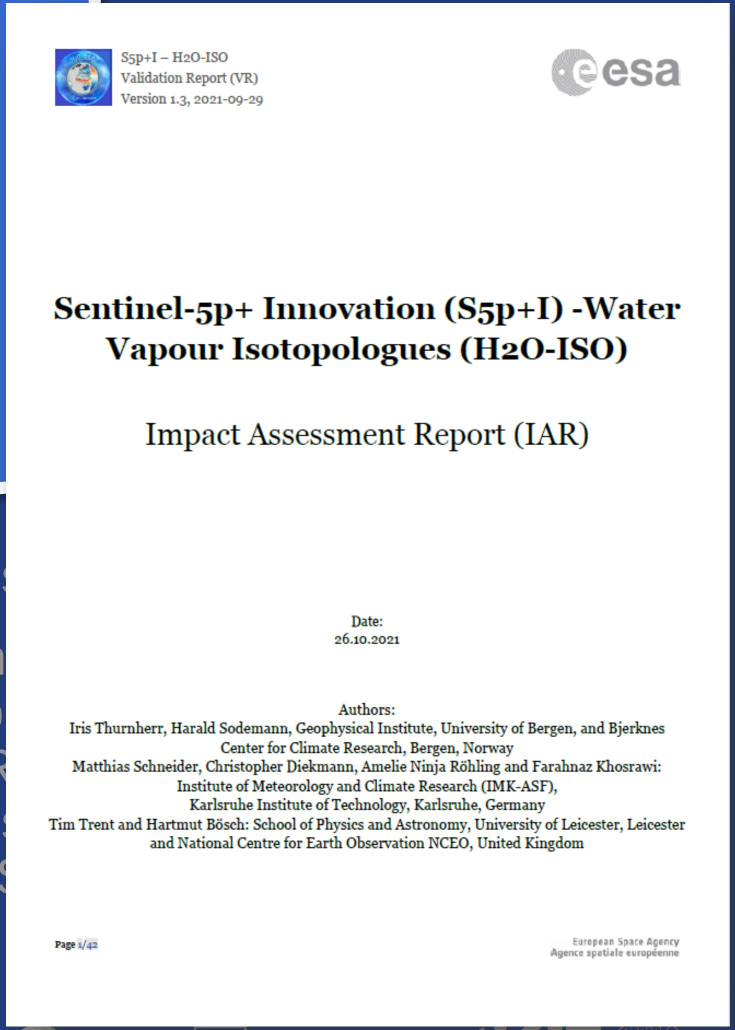


- For all meteorological parameters about 5% improvement is derived when only TROPOMI δD is assimilated.
- Higher improvements (20-40%) can be derived when TROPOMI q or TROPOMI δD and q are assimilated.
- The highest improvements of about 35-45% are derived when TROPOMI δD and q are assimilated together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

Scientific case study 3: Data assimilation

- Combination of IASI and TROPOMI q and δD information clear benefit for NWP.
- Future work will focus on merging MUSCIA IASI and TROPOMI isotopologue products.
- All case study results can be found in the impact assessment report




S5p+I – H2O-ISO
Validation Report (VR)
Version 1.3, 2021-09-29

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Sentinel-5p+ Innovation (S5p+I) -Water Vapour Isotopologues (H2O-ISO)

Impact Assessment Report (IAR)

Date:
26.10.2021

Authors:
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Summary

- Now produced 3 years of UoL prototype TROPOMI stable water vapour isotoplogue product.
- The TROPOMI XδD mean bias with respect to the ground-based FTIR data is about -21 ‰ ± 36.5 ‰ and -1.9 ‰ ± 35.2 ‰ after bias correction.
- Different dependencies on influence quantities can be observed (e.g. water vapour content in the atmosphere and albedo).
- Simulations with isotope-enabled NWP models are a key asset during such validation studies, and provide both larger spatial and temporal context, serve as verification target, and enable synthetic verification studies.
- S5P spatial and temporal coverage highly useful for deciphering the interrelation between weather situations and the isotopic state of atmospheric water vapour.
- Potential for the assimilation of data from both instruments together for improving meteorological analysis and thus weather forecasts.

Thank you for Listening.

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