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

Final Report (FR)

Authors:

Hartmut Bösch and Tim Trent

School of Physics and Astronomy, University of Leicester, Leicester and National Centre for Earth Observation NCEO, United Kingdom

Matthias Schneider, Farahnaz Khosrawi, Amelie Ninja Roehling and Christopher Diekmann

Institute of Meteorology and Climate Research (IMK-ASF), Karlsruhe Institute of Technology, Karlsruhe, Germany

Iris Thurnherr, Harald Sodemann

Geophysical Institute, University of Bergen, Bergen, Norway

Change log

Version	Date	Status	Authors	Reason for change
Draft v1.0	23-Mar-2022	Initial internal draft for project team	H. Bösch, T. Trent	New document
Draft v1.1	17-Jun-2022	Revised Draft	All	Review by team
Final v1.2	06-Jul-2022	Final	H. Boesch	

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1 Executive Summary

The water cycle is a key element of the Earth's climate system and the insufficient understanding of the links between clouds, circulation and climate sensitivity is one of the grand challenges in climate research. Water vapour isotopologues offer unique possibilities for investigating the tropospheric water cycle. With their ability to record the condensation and rain-out history of air masses, and to some extent "tag" moisture as it travels through the atmosphere, ocean, biosphere, and cryosphere, water isotopologue ratios provide insights into key processes of the past and present global water cycle. Global observations of water isotopologues from column sensors such as Sentinel-5P can be of great scientific value and provide complementary information to observations from infrared sounders such as IASI for which the peak sensitivity of water isotopologues retrievals lies in the free troposphere.

The S5p+I project on water vapour isotopologues aims at developing, documenting, and validating a TROPOMI water vapour isotopologues retrieval and to demonstrate its scientific impact. The project is led by University of Leicester in collaboration with Karlsruhe Institute of Technology and University of Bergen.

The main achievements of this project are:

- A new retrieval has been developed for the retrieval of water isotopologues from the SWIR bands of TROPOMI based on the UoL-FP retrieval. This retrieval has been embedded in a semi-automatic processing chain for large scale processing of TROPOMI data. This retrieval generates the water isotopologues data together with additional key parameters such as averaging kernels and error estimates.
- The TROPOMI water isotopologue retrieval has been validated against fiducial ground-based reference data. We found a small mean negative bias of around -20‰ and we estimate a single sounding precision of about 25-30‰. This is slightly above the target requirement of the precision so that some averaging in space and/or time will be needed. Comparisons of the TROPOMI water isotopologue data to MUSICA IASI data shows no significant bias of the TROPOMI data compared to IASI.
- The scientific impact of the TROPOMI water isotopologues has been assessed against isotope-enabled models, MUSICA IASI and aircraft profiles. The TROPOMI isotopologue dataset provides spatial and temporal coverage that is highly useful for deciphering the interrelation between weather situations and the isotopic state of atmospheric water vapour, in particular in combination with other (infrared) satellite products.

In the future, the synergistic use of the TROPOMI isotopologue retrieval with IASI should be further explored to enhance the scientific impact. This will also allow a seamless transition to full synergistic retrievals which will become possible with the launch of METOP-SG and its Sentinel-5 and IASI-NG instruments.

2 Applicable Documents, terms and acronyms

2.1 Applicable Documents

AD1	Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO) Requirements Baseline Document (RBD), version 1.1, URL: https://s5pinnovationh2o-iso.le.ac.uk/wp-content/uploads/2019/11/RBD_S5pI_H2O_ISO_v1.1.pdf
AD2	Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO) Auxiliary User Manual (AUM), version 1.2, URL: https://s5pinnovationh2o-iso.le.ac.uk/wp-content/uploads/2020/02/aum_s5p-i_iso_version_1.2.pdf
AD3	Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO) Algorithm Theoretical Basis Document (ATBD), version 1.4, URL: https://s5pinnovationh2o-iso.le.ac.uk/wp-content/uploads/2021/10/S5P-I_ISO_ATBD_Version1.4.pdf
AD4	Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO) Validation Report (VR), version 1.3, URL: https://s5pinnovationh2o-iso.le.ac.uk/wp-content/uploads/2021/10/S5p-I_VR_Version1.3.pdf
AD5	Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO) Product User Manual (PUM), version 1.0, URL: https://s5pinnovationh2o-iso.le.ac.uk/wp-content/uploads/2022/05/S5P-I_ISO_PUM_Version1.1.pdf
AD6	Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO) Impact Assessment Report (IAR), version 2.0, URL: https://s5pinnovationh2o-iso.le.ac.uk/wp-content/uploads/2022/05/S5p-I_IAR_Version2.0.pdf
AD7	Sentinel-5p+ Innovation (S5p+I) - Water Vapour Isotopologues (H2O-ISO) Scientific Roadmap (SR), version 1.0

2.2 Terms, definitions and abbreviated term

Term	Definition
AUM	Auxiliary User Manual
CAMS	Copernicus Atmospheric Monitoring Service
CCI	Climate Change Initiative

CEDA	Centre for Environmental Data Analysis
COSMO	Consortium for Small-scale Modelling
DEM	Digital Elevation Map
DLR	Deutsches Zentrum für Luft- und Raumfahrt
ECMWF	European Centre for Medium-Range Weather Forecast
ERA5	ECMWF 5th Reanalysis
EE8	Earth Explorer 8
ESA	European Space Agency
FTS	Fourier Transform Spectrometer
GHG	Greenhouse Gas
GOSAT	Greenhouse gases Observing Satellite
HAPI	HITRAN Application Programming Interface
GRUAN	Global Climate Observing System (GCOS) Upper Air Network
HITRAN	High Resolution Transmission
HTP	Hartmann-Tran-Profile
IASI	Infrared Atmospheric Sounding Interferometer
IASI-NG	IASI next generation
ICON-Art	ICOsahedral Nonhydrostatic weather- and climate model with Aerosols and Reactive Trace Gases
ILS	Instrument Line shape Function
IFOV	Instantaneous Field of View
ISS	International Space Station
L1b	Level 1b data product
L2	Level 2 data product
L4	Level 4 data product
LCC	Land Cover Change
LRPT	Leicester Retrieval Preparation Toolset
LSI	Low Streams Interpolation
LSM	Land Sea Mask
L-WAIVE	Lacustrine-Water vApor Isotope inVentory Experiment
METOP-SG	Metop Second Generation
MUSICA	MUlti-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water

NDACC	Network for the Detection of Atmospheric Composition Change
NWP	Numerical Weather Prediction
OCO	Orbiting Carbon Observatory
PCA	Principle Component Analysis
ROI	Region-of-Interest
RT	Radiative Transfer
RTE	Radiative Transfer Equation
S5p	Sentinel 5 precursor
S5p+I	Sentinel-5p+Innovation
SEOM-IAS	Scientific Exploitation of Operational Missions Improved Atmospheric Spectroscopy Databases
SIF	Solar Induced Fluorescence
SOLSPEC	SOLar SPECtrometer
SRTM	Shuttle Radar Topography Mission
Suomi-NPP	Suomi National Polar-orbiting Partnership
SWIR	Shortwave Infrared
TOA	Top-of-Atmosphere
TROPOMI	TROPOspheric Monitoring Instrument
TCCON	Total Carbon Column Observing Network
UoL-FP	University of Leicester Full Physics
VIIRS	Visible/Infra-red Imager and Radiometer Suit
VSMOW	Vienna Standard Mean Ocean Water
WCRP	World Climate Research Programme
XS	Cross Sections

3 Introduction and Overview over Activities

This report gives a summary of the activities carried out as part of the ESA Sentinel-5P+Innovation project on water vapour isotopologues by a consortium of researchers from University of Leicester, Karlsruhe Institute of Technology and the University of Bergen that bring together extensive expertise in satellite retrievals of water isotopologues, ground-based remote sensing, airborne in-situ observations and atmospheric modelling.

The water cycle is a key element of the Earth's climate system and the insufficient understanding of the links between clouds, circulation and climate sensitivity is one of the grand challenges in climate research (http://www.wcrp-climate.org/grand-challenges; Stevens and Bony (2013)). Water vapour isotopologues offer unique possibilities for investigating the tropospheric water cycle. With their ability to record the condensation and rain-out history of air masses, and to some extent "tag" moisture as it travels through the atmosphere, ocean, biosphere, and cryosphere, water isotopologue ratios provide insights into key processes of the past and present global water cycle. Tropospheric δD (the deuterium abundance in water compared to a reference) vapour data are particularly valuable if observed together with H_2O vapour concentrations because the {H_2O,δD}-pair distribution is directly linked to different moisture transport pathways (Noone 2012) (**Figure 1**). Continuous and simultaneous (but independent) global observations of water vapour isotopologues in the boundary layer and in the free troposphere are promising for different scientific applications (e.g. Risi et al., 2013, Risi et al., 2012, Yoshimura et al., 2014). More details on the scientific background and the requirements for a satellite product are given in [AD1].

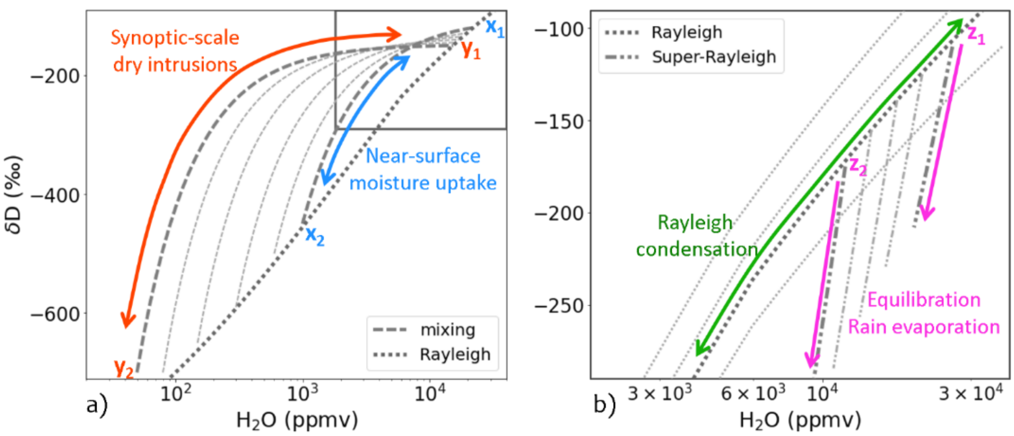

Figure 1: Overview of idealized process curves for paired distributions of H_2O and δD according to Noone (2012). An extensive discussion for these lines is given in Diekmann et al. (2021).

A water isotopologue product from Sentinel-5P can be of great scientific value. The goal of this project has been to demonstrate the feasibility of measuring stable water isotopologues from Sentinel-5P, to examining and to characterize the retrieval performance by validation of retrieved water isotopologues against satellite and reference data sets and to assess the impact of the datasets against models. This has been achieved in this project by first collecting scientific requirements (WP2) and datasets (WP3), followed by the algorithm development and validation (WP3), the prototype demonstration and impact assessment (WP4) and finally by drafting of a scientific roadmap (WP5).

The work of this project is summarised here according to product development, product validation, prototype demonstration, impact assessment and future developments. The detailed outputs and documents for each of the work packages are available from the project webpage (https://s5pinnovationh2o-iso.le.ac.uk).

4 Product Development

The algorithm to retrieve water isotopologues from TROPOMI is based on the University of Leicester Full Physics (UoL-FP) processor. This algorithm has been originally designed to retrieve column averaged CO_2 (XCO2) from spectrally-resolved near-infrared (NIR) and shortwave-infrared (SWIR) bands measured by the NASA Orbiting Carbon Observatory-2 (OCO-2) mission (Bösch et al., 2006, Boesch et al., 2011). The algorithm was designed to be highly adaptable to other trace gases and instruments and the algorithm has been used for a wide range of applications including XCO2 and XCH4 from SCIAMACHY, OCO-2, TanSat and GOSAT (Cogan et al., 2012; Parker et al., 2020; Somkuti et al., 2020; Yang et al., 2020), HDO/H_2O and boundary-layer XH2O from GOSAT or XCH4 from TROPOMI (Boesch et al., 2013; Trent et al., 2018).

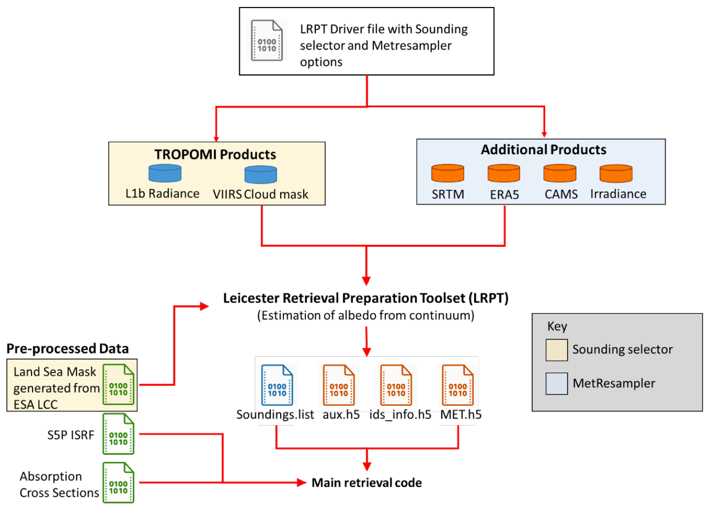

Figure 2: Flow of data in and out of the Leicester Retrieval Preparation Toolset (LRPT).

The fundamental approach of the UoL-FP retrieval algorithm is to use an iterative retrieval scheme based on a Bayesian optimal estimation to estimate a set of atmospheric/surface/instrument parameters, referred to as the state vector $\boldsymbol{x}$, from measured, calibrated spectral radiances. UoL-FP employs a forward model to describe the physics of the measurement process and to relate measured radiances to the state vector $\boldsymbol{x}$. It consists of a radiative transfer (RT) model coupled to a model of the solar spectrum to calculate the monochromatic spectrum of light that originates from the sun, passes through the atmosphere, reflects from the Earth's surface or scatters back from the atmosphere, exits at the top of the atmosphere and enters the instrument. The calculated top of atmosphere (TOA) radiances are then passed through the instrument model to simulate the measured radiances at the appropriate spectral resolution.

The full retrieval chain employed to the water isotopologue retrieval consist of a pre-processing step that prepares the input data for use in the UoL-FP retrieval, the main UoL-FP retrieval code and a post-processing step that generates the final output files. The details are given in [AD3].

The preparation of data for use in the retrieval is processed through the Leicester Retrieval Preparation Toolset (LRPT) (**Figure 2**). The input datasets are detailed in [AD2]. LRPT will select soundings over sufficiently cloud-free land that are then passed to the UoL-FP retrieval. The cloud-screening is based on the VIIRS cloud mask data sampled to each TROPOMI sounding. This information is available for different spatial scales (between once and twice the TROPOMI ground pixel area). We require that the area of the ground pixel has to be 99% confidently clear which yields typically about twice the amount of data compared to a more conservative approach that would screen for twice the area of the ground pixel. We also screen for pixels over land using a land sea mask and we require soundings to have a land fraction of 99% or more . The meteorological regularly gridded reanalysis fields (surface pressure, water vapour, temperature, methane, carbon monoxide) are mapped to TROPOMI pixel footprints using trilinear interpolation of longitude, latitude, and time information. A validation against atmospheric radiosondes from the Global Climate Observing System (GCOS) Upper Air Network (GRUAN) has been performed as shown in Figure 3. For water isotopologue, we have adapted the approach from Scheepmaker et al. (2016a) to create atmospheric profiles. To obtain a representative surface elevation and its variability for a sounding, a Digital Elevation Model (taken from the Shuttle Radar Topography Mission (SRTM) provided by the U.S. Geological Survey) has been sampled for the whole footprint. This information is then used to infer the surface pressure and to estimate the contribution of surface topography to the error budget (see post-processing).

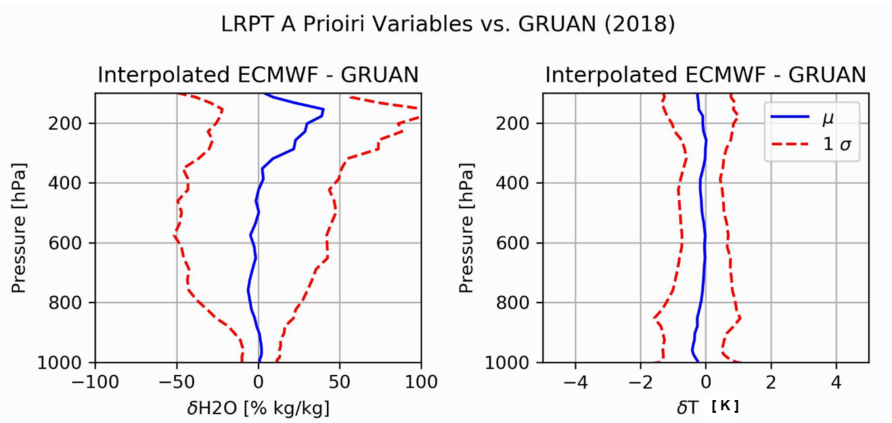

Figure 3: Comparison of the interpolated profiles from ECMWF against the GRUAN atmospheric sonde data**.**

The H_2O/HDO ratio is retrieved from TROPOMI SWIR spectra with UoL-FP in the spectral range of 2354.0 and 2380.5 nm as proposed by Scheepmaker et al. (2016b). Besides water vapour and HDO, interfering gases CO_2 and CH_4 and additional parameters temperature, surface albedo and instrumental shift are retrieved. For atmospheric gases, a multiplicative scaling factor is retrieved which scales an assumed atmospheric profile. For temperature, an additive temperature offset is retrieved that is applied to the assumed atmospheric profile. The main output of the retrieval is the H_2O/HDO ratio. Similar to the CH_4 proxy retrieval (Parker et al., 2020), light path variations from scattering effects will be similar for the retrieved H_2O and HDO columns and cancel in the H_2O/HDO ratio. Thus, aerosols are not included in the retrieval. Modifications to the UoL-FP retrieval itself include the applied solar model and the used spectroscopic database. The solar model parameters have been modified to represent the solar spectrum measured by TROPOMI. The spectroscopic tables for H_2O, HDO and CH_4 are computed from the Deutsches Zentrum Für Luft- und Raumfahrt (DLR) Scientific Exploitation of Operational Missions Improved Atmospheric Spectroscopy Databases (SEOM-IAS).

The post-processing step carries out the computation of averaging kernels and of error metrics. The averaging kernel is a key parameter to characterise the sensitivity of the retrieval and is generated by interpolation from a pre-calculated table (Figure 4). The error combines the a posterior error estimate from the retrieval with the estimate of the error from the variation in surface elevation (and thus surface pressure) based on DEM variability within footprint.

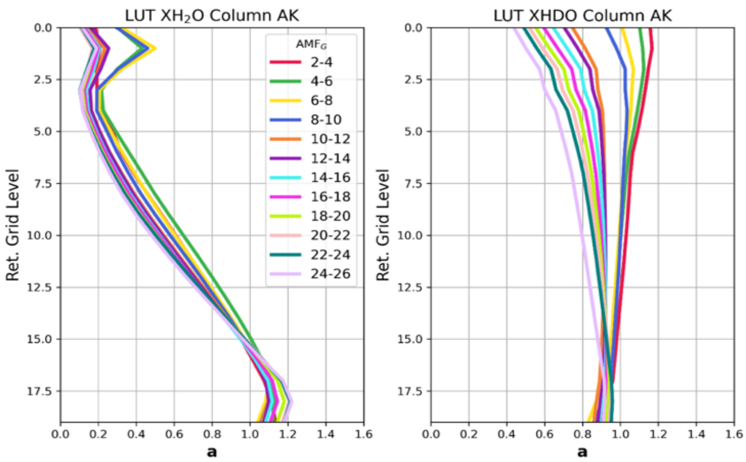

Figure 4: Example of normalised scaler averaging kernels for H_2O and HDO for the TROPOMI retrieval

5 Product Validation

The TROPOMI water vapour isotopologue product is a column integrated product. For the development and validation (including impact studies) of the TROPOMI isotopologue product, we need reference data sets with the following characteristics:

- They should cover the period of the prototype product
- They should be representative for different climate zones over land.
- They should be sensitive to water vapour throughout the troposphere.
- They should be traceable to fiducial references.

Figure 5 gives an overview on the reference products that fulfil some of these requirements. The MUlti-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water (MUSICA) Network for the Detection of Atmospheric Composition Change (NDACC) reference data is representative for the whole troposphere, calibrated with respect to fiducial references (Schneider et al., 2016). However, only at three stations (Kiruna, Karlsruhe and Izaña) data are currently available for the era 2018-2020 of TROPOMI observations. TCCON (Total Carbon Column Observing Network) data are also representative for the whole troposphere and available for the whole TROPOMI observation era; although, the TCCON isotopologue ratio data are not calibrated with respect to fiducial references. The aircraft-based in-situ observations from the Iceland Greenland Seas Project/Lidar Emitter and Multi-species greenhouse gases Observation instrument (IGP/LEMON project) represent a fiducial reference, but they are only available for short campaign periods, for a limited geographical region, and only cover the lowermost four kilometres of the troposphere. Comparisons is also possible against other space-based datasets. MUSICA Infrared Atmospheric Sounding Interferometer (IASI) space-based products are calibrated with respect to fiducial references (Schneider and Hase, 2011), available during the TROPOMI era on global scale; however, they are only representative for the free troposphere (thus not well representative for the boundary layer). Greenhouse Gases Observing Satellite (GOSAT) space-based observations are total column data and thus contain boundary layer information but are not calibrated against fiducial references.

For the validation of the TROPOMI XHDO/XH2O (or δD) column integrated data we use the ground-based direct sun measurements made within the NDACC (MUSICA NDACC) and TCCON networks at seven different stations as the primary reference. These stations represent different climate zones (polar, mid-latitude, subtropics, and tropics) of the northern and southern hemisphere. Comparisons to these primary references are used for a detailed investigation of the TROPOMI quality (bias, dispersion, dependence on solar zenith angle, albedo, and total atmospheric water vapour content). A detailed description of the validation approach and its results are given in [AD4].

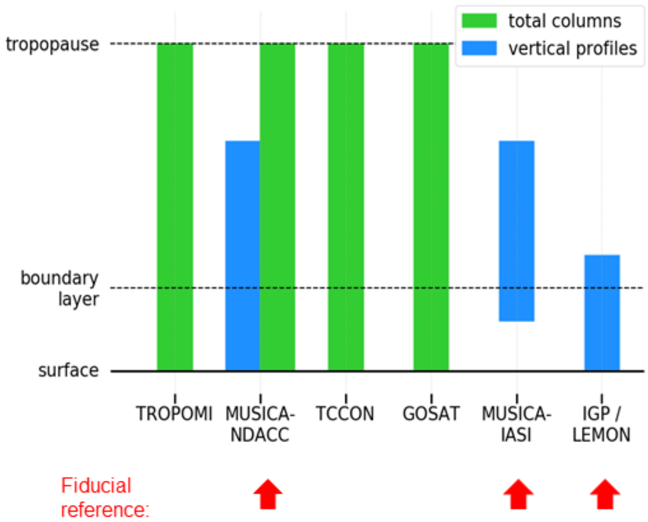

Figure 5: Vertical representativeness of TROPOMI data and of the associated data. Green colour means column integrated data and blue means data containing some information about the vertical distribution. Note: generally, more than 50 % of the total water vapour resides in the boundary layer.

The TROPOMI soundings have been co-located to ground-based NDACC and TCCON measurements using a colocation criteria of 50 km and Δt = 3 h. From these comparisons (Figure 6), we found a mean negative bias of -17.3‰ and -21.0‰ for NDACC and TCCON, respectively. A larger mean bias is observed for the comparison to the tropical sites Burgos and Darwin due to the higher water columns observed at these sites and we have investigated the possibility of a water-vapour-dependent bias correction. We found that it widely reduces the bias and most importantly it removes the inconsistency in the bias between low and high latitudes to a large part.

The dispersion for the comparison to MUSICA NDACC data is 33.9 ‰ and to TCCON it is 36.5 ‰. If we exclude very dry conditions, e.g. by requiring XH2O values larger than 1500 ppmv the dispersion can be significantly reduced and remains generally below 30‰. If we consider a 10-15 ‰ uncertainty of the reference data and assume an uncertainty of another 15‰ due the different vertical sensitivities, a ~35‰ dispersion means that the uncertainty of the TROPOMI data is about 25-30‰. This is slightly above the target requirement of the precision (that has been set to 20 ‰). Nevertheless, this estimated uncertainty of 30‰ is for an individual observation (single TROPOMI pixel). In this context, the target value of 20‰ can be achieved by calculating averages over several individual pixels.

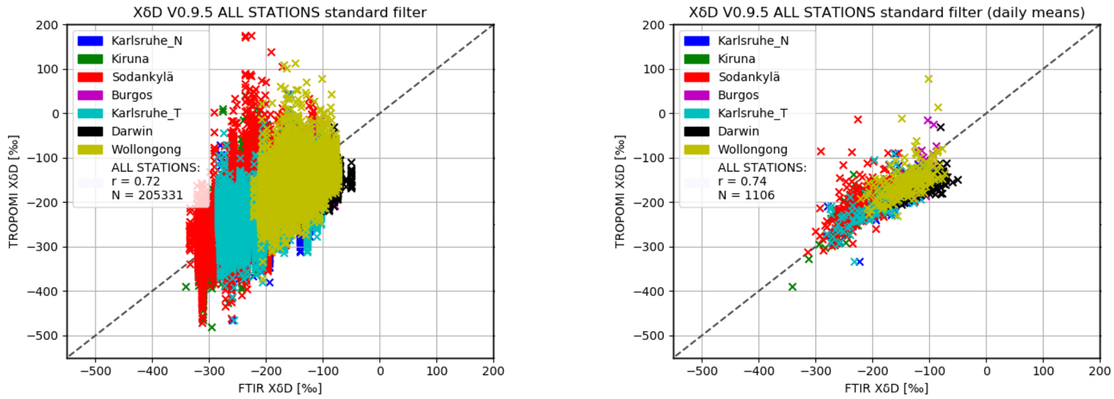

Figure 6: Correlation of FTIR and TROPOMI XδD single pixel measurements (left) and daily means (right) with standard filtering around the FTIR stations.

To show the consistency (and complementary) between the MUSICA IASI and the TROPOMI product, we compare the TROPOMI and MUSICA IASI data co-located to five ground-based sites (Figure 7). We find no significant offset (mean difference) between both datasets and a dispersion (1-σ standard deviation around the mean difference) of about 27‰. While the dispersion is in the range of the dispersion found for the comparison between the TROPOMI and the ground-based network data, the bias is significantly smaller and by about 25‰ more positive. Similar to the comparison to the ground-based network data we found a dependence of the dispersion on the total atmospheric water vapour content (XH2O, right panel of Figure 7).

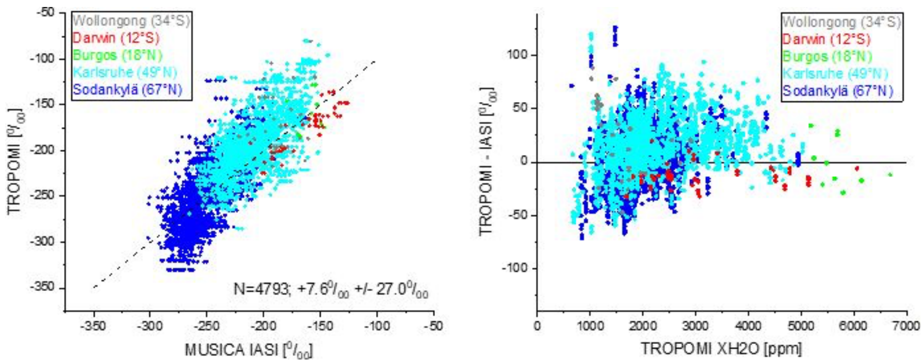

Figure 7: Comparison of TROPOMI and MUSICA IASI XδD with the latter fulfilling the lower tropospheric sensitivity criterion. Data belonging to different locations are marked by different colours. Left: correlation plot; Right: Dependence of the TROPOMI-IASI difference on TROPOMI XH2O

6 Prototype Product

Using the developed algorithm, a prototype TROPOMI water isotopologue dataset (v1.0.0) has been generated from TROPOMI soundings for May 2018 to February 2020. This product contains XH2O, XHDO and XδD columns over land, along with quality-flags, uncertainty estimates, averaging kernels and a priori profiles for validation studies. This dataset contains only observations over land. The adopted quality flag for v1.0.0 flags desert areas as 'poor' resulting in data gaps over desert regions. Production of version v1.0.1 is underway which includes a modified quality-filter that avoid these data gaps. This data product is shown in (Figure 8) from June 2018 to May 2019. The content structure, variable names and definitions of the data product are described in the Product User Manual [AD5] with a description of quality filters given in the ATBD [AD3].

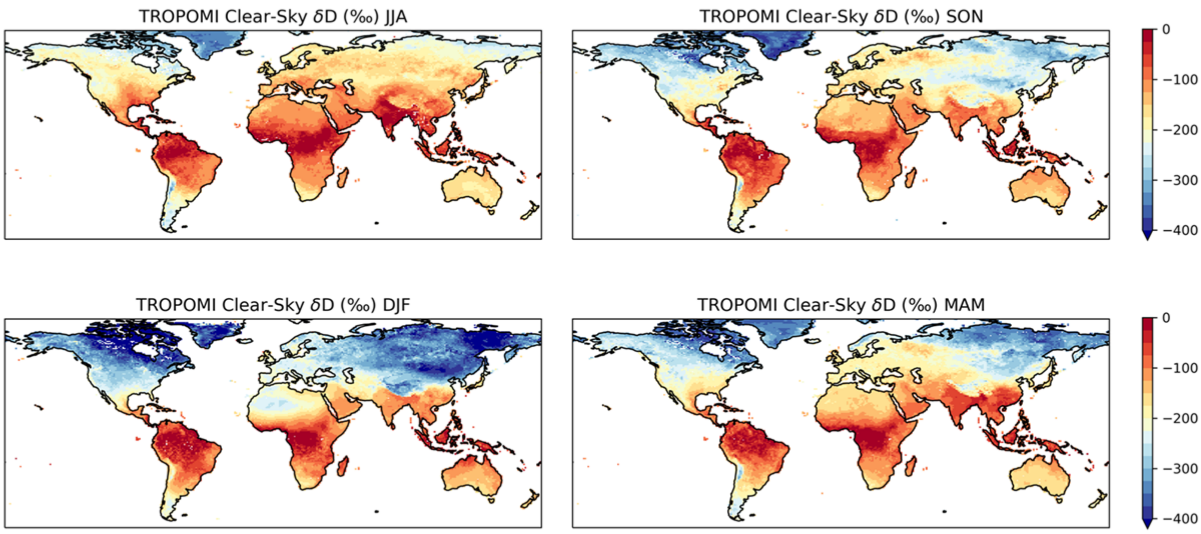

Figure 8: TROPOMI prototype product (v1.0.1) between June 2018 and May 2019 shown as 3-month averages after quality-filtering.

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7 Impact Assessment and Future Development

To assess the impact of the TROPOMI stable water vapour isotopologues product a variety of datasets have been used [AD6]. This includes in situ vertical δD profiles from the Lacustrine-Water vApor Isotope inVentory Experiment (L-WAIVE) campaign in June 2019 (Chazette et al., 2021), the MUSICA IASI stable water isotopologues product and model simulations with the isotope-enabled numerical weather prediction (NWP) models COSMOiso (Consortium for Small-scale Modelling) and ICON-ART-Iso (ICOsahedral Nonhydrostatic weather and climate model with Aerosols and Reactive Trace Gases)

We pursued four goals during the data assessment: (1) assess the ability and conditions of in-situ measurements to serve as ground-truth for satellite observations, (2) assess the insight offered by S5P total column data to supplement information available from MUSICA IASI in West Africa, and (3) a preliminary investigation in the context of data assimilation. From these partial goals, we more generally assess (4) the additional value of the TROPOMI satellite data product compared to other data

Spatial and temporal scales are important factors for the comparison between satellite, in-situ, and NWP model data. The measurement location of in-situ data critically determines on what scales a meaningful comparison can be made. Hereby, local topographic effects combined with the weather situation need to be assessed for the relevant scales based on a so-called complete proxy (here, regional isotope-enabled NWP model simulations). Cloud cover, shifts in weather pattern, and varying topography can limit comparison efforts, as was the case for the Alpine region investigated during L-WAIVE. Apart from such adverse effects, these factors create variability of the signal, and thus provide the structure in the data set that enables meaningful interpretation. To the extent feasible, measurements should be planned to balance these counteracting demands by choosing a measurement site and time which represents the regions' isotopic variability without shortcutting on the data coverage. For best possible aircraft – satellite comparison, the flights and satellite overpasses should be synchronized (if possible, considering overall campaign objectives). This is most important in regions with a strong daily cycle in vertical δD profiles or in situations with a high temporal variability in large-scale forcings. The design of flight patterns for optimal in-situ comparisons is challenging, and restricted by the measurement platform and endurance, air traffic restrictions, and the weather situation. To allow for a larger degree of overlap, sampling patterns should cover horizontal scales of 50 km and more, and cover vertical levels from the ground to above about 5000 m. The ultralight aircraft employed in the L-WAIVE campaign were focused on smaller scales and boundary-layer characteristics in complex terrain. Despite the overall value of the L-WAIVE data, measurements from aircraft that cover larger horizontal scales would be more suitable for the comparisons targeted here.

The value offered by TROPOMI total column data to complement information available from MUSICA IASI has been assessed with a focus on West Africa. As a basis for all comparisons in the target region West Africa, we note that the large-scale circulation patterns in the Sahel region strongly vary with altitude, inducing vertical wind shear. In the free troposphere, the air mass origins are rather different from the air mass origins in the boundary layer. Such differences can strongly impact both total column and vertically resolved satellite observation products. The MUSICA IASI {H_2O, δD} pair data are able to capture signals well that are due to the large-scale circulation in the free troposphere and signals of convective processes. The basis for this conclusion is that the {H_2O, δD} pair distribution is in accordance with Super-Rayleigh lines. The TROPOMI total integrated column data reflect a mix of the different altitudes with different circulation patterns. Air masses from different origins and different transport processes determine the total column signals. Such differential advection is a substantial obstacle to the use of the S5P data for atmospheric water pathway studies in this region. Combining TROPOMI with MUSICA IASI offers the potential for separating the boundary layer from the free tropospheric signals (Schneider et al., 2022). Testing such a boundary layer isotopologue separation for our region, we found strong indications that the distribution of boundary layer {H_2O, δD}-pairs is different for ocean or land evaporation sources.

We have also carried out a preliminary investigation of benefit of TROPOMI isotopologue data for data assimilation. In the tropics, the assimilation of TROPOMI specific humidity (q) and TROPOMI δD and q combined leads to almost the same improvement. In other words, little additional gain is derived from assimilating column δD additionally to column q. This limited gain indicates that column δD holds less detailed information on moisture processes than if δD observations are obtained for a specific altitude in the mid-troposphere. The assimilation of both IASI δD and q additionally to TROPOMI δD and q leads to the highest improvement for all meteorological parameters (tropics and Africa). This improvement shows the potential for the assimilation of data from both instruments together for improving meteorological analysis and thus weather forecasts. For capturing the precipitation and thus latent heating pattern correctly a higher horizontal and vertical resolution as the one used here for the data assimilation could be beneficial (the data assimilation experiment was performed with IsoGSM with a horizontal resolution of 200 x 200 km^2 and a vertical resolution of 28 pressure levels up to 2.5 hPa). We expect that assimilation experiments using e.g. a different model, a higher model resolution and/or a different number of ensemble members might give different results.

In summary, the isotopologue retrieval from TROPOMI provides spatial and temporal coverage that is highly useful for deciphering the interrelation between weather situations and the isotopic state of atmospheric water vapour, in particular in combination with other satellite products, as demonstrated from preliminary data assimilation experiments. Similar additional value became evident from the analysis of isotopic signatures in the large-scale circulation in West Africa, where a combination of the TROPOMI data with the MUSICA product may allow to extract vertically resolved information. Vertical atmospheric differences are also a key challenge for the use of in-situ validation, which generally benefit more from high-reaching profiles than from high vertical resolution. Complex terrain influences both the correlation length scales and the vertical structure, which therefore need to be taken into account during the design of in-situ aircraft measurement campaigns and the comparison of total column retrievals with in-situ data. 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.

To maximise the impact from the TROPOMI isotopologue data developed here, the following recommendations are made [AD7]:

- to further evolve the TROPOMI water isotopologues retrieval towards a covariant H_2O-HDO retrieval that will allow to explore the synergistic use with IASI TIR data and thus will enhance the scientific impact. This will then also allow a seamless transition to full synergistic use of Sentinel-5 and IASI-NG on METOP-SG
- to adopt a sustained validation concept based on a small number of fiducial reference supersites (with regular NDACC, TCCON, COCCON and balloon-born in-situ profile observations and the use of the portable COCCON instruments as travel standard to cross-reference the wider network). This will require the development of a COCCON δD retrieval and support for continued processing of NDACC δD data. Furthermore, a few dedicated aircraft in-situ campaigns are recommendable for generating fiducial profile reference data at high vertical resolution from ground to the upper troposphere.
- to conduct further satellite comparison studies with isotope-enabled model simulations to study modes of δD variability and to characterise the spatial and temporal scales of δD variations. Furthermore, data assimilation experiments with isotopic data should be performed using e.g. different isotope enabled models with higher model resolution than previous studies to better estimate the benefits of satellite δD and H_2O data for meteorological analyses and weather forecasts.
- To foster a stronger engagement with GEWEX by contributing results of this project on stable water vapour isotopologues to the 2nd Water Vapor Assessment (G-VAP) report due in Q1 2023, by submitting a GEWEX newsletter by Q4 2022 to highlight the progress on satellite remote sensing of stable water vapour isotopologues within this TROPOMI project and to increase ESA and GEWEX interaction in the longer term by submission of a new project idea under the GEWEX Data Assessment Panel (G-DAP) focussing on the assessment of isotopologues from models, satellite and ground based measurements, helping to bring together a number of existing communities. A first step will be to hold a global workshop to bring communities together and decide on the objectives of the proposed project. Such an activity will require funding from ESA as GEWEX itself does not provide funding

8 Promotion

To promote the work of this project and to engage with the wider community interested in water vapour isotopologues, we have presented the project at a number of scientific conferences. This includes the EUMETSAT Meteorological Satellite Conference 2021, where presentations have been given by M. Schneider, C. Diekmann and F. Khosrawi. At this conference, C. Diekmann has received the Early Career Scientist Initiative Award. Futhermore, at the ESA ATMOS Conference with pesentations given by H. Boesch and I. Thurnherr, the EGU General Assembly 2021 with presentations given by M. Schneider, T. Trent and C. Diekmann and at the ESA Living Planet Symposium with a presentation given by M. Schneider (on behalf of H. Boesch). The project has also been included in a presentation by M. Schneider at the US CLIVAR Water Isotopes and Climate Workshop. Team members (T. Trent) have also engeged with the the GEWEX project to ensure that a summary of water vapour isotopologue records will be included in next GEWEX Water Vapour Assessment (G-VAP) report to WRCP. The project has contributed to the publication by Diekmann , C. J., Schneider, M., Knippertz, P., de Vries, A. J., Pfahl, S., Aemisegger, F., et al. (2021). Three further publicaitons are in preparation on the TROPOMI water isotopologes product and its validation, the impact assessment using high-resolution models and aircraft observations and on the science exploitation in combination with IASI data.

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