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

Scientific Roadmap Document (SR)

Authors:
Matthias Schneider, Farahnaz Khosrawi, and Amelie Ninja Röhling: Institute of Meteorology and Climate Research (IMK-ASF), Karlsruhe Institute of Technology, Karlsruhe, Germany
Hartmut Bösch and Tim Trent: Department of Physics and Astronomy, University of Leicester, Leicester, United Kingdom
Iris Thurnherr and Harald Sodemann, Geophysical Institute, University of Bergen, Bergen, Norway

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1 Introduction

The goal of this project has been to develop, validate, assess and document the water isotopologue retrieval from the TROPOMI satellite mission. The developed retrieval retrieves XHDO/XH$_2$O (or XδD) column integrated data from the SWIR spectral range with an algorithm described in detail in the Algorithm Theoretical Basis Document (ATBD 2020). The validation of the TROPOMI XHDO/XH2O (or XδD) data has been performed for the time period May 2018 to July 2019 with the TROPOMI L2 V0.9.1 version. Ground-based measurements made at seven stations within the Network for Detection of Atmospheric Composition Changes (NDACC) and Total Carbon Column Observing Network (TCCON) were used. The comparisons demonstrate the already good quality of the TROPOMI L2 V0.91 XδD data product developed in this project (see Validation Report (VR 2021) for details). The TROPOMI XδD mean bias with respect to the ground-based FTIR measurements is about -26 ‰. The scientific impact of the TROPOMI XHDO/XH$_2$O product was demonstrated in the Impact Assessment Report (IAR 2022). The high spatial resolution of the product allows for new ways of assessing isotopic model simulations on a spatial and temporal scale. Further, an Observation System Simulation Experiment (OSSE) showed that the assimilation of satellite retrieved total column δD (TROPOMI XHDO/XH$_2$O and/or MUSICA IASI) in the IsoGSM model improves the prognostic skills of the model by 5-45%, depending on the assimilated variables. The δD data from TROPOMI derived within this project is of high quality and alone or in synergy with the MUSICA IASI isotopologue data provides a valuable data set e.g. for the evaluation of climate and process models and for scientific studies.

This document will discuss further advances and possible evolutions that will be a move towards operational processing of the TROPOMI δD retrieval, that allow fully exploiting the scientific potential of the TROPOMI δD product and that addresses limitations in existing validation data.

1.1 Purpose and objective

This document provides guidance on potential future developments with respect to the development of the processing, validation and synergetic use with the MUSICA IASI isotopologue product building on the Impact Assessment Report (IAR 2022). Possible applications and usefulness of the S5P data for scientific studies will also be discussed.

1.2 Document overview

In Sect. 2 we describe the suggestions for the future TROPOMI water isotopologue processing. In Sect. 3 we discuss the additional validation needs that go beyond what has been done in the Validation Report (VR 2021) and in Sect. 4 we discuss the synergetic use with the MUSICA IASI isotopologue product. In Sect. 5 we provide some guidance for application of the data products for scientific studies. Finally, in Sect. 6 we give a summary and recommendations for the future.

2 Evolution to the TROPOMI stable water vapour isotopologue processing chain

2.1 Covariant retrieval of H_2O and HDO

The retrieval approach adopted for the generation of water vapour isotopologue products with UoL-FP is based on a scaler retrieval of HDO and H_2O profiles. This is a robust and efficient retrieval approach and the resulting δD product compares well against the ground-based validation data.

As part of the MUSICA project, a framework for a retrieval of H2O, δD has been developed for the IASI instrument (Schneider et al., 2016; 2022; Diekmann et al. 2021). In this IASI retrieval approach, H_2O and HDO are simultaneously retrieved and a joint covariance is used that gives a constraint on H_2O and HDO but also on the covariance between H_2O and HDO. This approach is needed as the degrees of freedom for H_2O and HDO differ and thus the averaging kernels. The MUSICA approach also retrieves H_2O and HDO mixing ratios as profiles in logarithmic space which allows conversion to independent parameters H_2O and δD and to infer error metrics and averaging kernels for δD which is not possible with the approach currently used for TROPOMI.

An evolution of the developed TROPOMI water isotopologues retrieval will be to adopt the MUSICA retrieval approach. This approach is based on a simultaneous retrieval of H_2O and HDO in logarithmic space where a covariance linking H_2O and HDO is used. This approach allows to separate the retrieved H_2O and HDO into independent {H_2O, δD} pairs and to generate error characterization and averaging kernels for δD which is especially important if the degrees of freedom for the retrieval differs significantly between H_2O and HDO. This is the case for TROPOMI where the H_2O retrieval has many more degrees of freedom compared to the HDO retrieval. Another benefit will be that TROPOMI then uses the same retrieval approach to IASI which allows the synergetic combination of both (section 4) and subsequent separation between boundary layer and free troposphere.

The UoL-FP retrieval already has the capability to retrieve trace gas profiles in logarithmic space but UoL-FP assumes that each trace gas is retrieved independently and a priori covariances are assumed to be independent of each other. To adopt the MUSICA approach to allow covariances between different trace gases in the retrieval will require modifications to the UoL-FP processor used for this project. This would offer a clear enhancement of the capability that would offer great scientific value.

2.2 Migration to PAL

The TROPOMI water vapour isotopologue products are generated using the HPC system JASMIN at the Centre for Environmental Data Analysis. The processing chain consists of a pre-processing tool LRTP (Leicester retrieval preparation toolset) that prepares all required inputs for the retrieval sampled for a TROPOMI sounding, the UoL-FP spectral retrieval algorithm and a post-processor that generates the final data products. LRTP uses a range of meteorological and model data sets to generate the TROPOMI inputs. It also selects soundings that are clear and over land based on the VIIRS cloud products and a land-sea mask. LRPT is run on the granulation of the L1b radiance product. The UoL-FP is used for a spectral fit to the L1B data to estimate the HDO/H_2O ratio with a fast retrieval setup that uses a scaling retrieval of HDO and H_2O profiles. Aerosols are not included in the retrieval. The UoL-FP retrieval is run on a per-sounding basis using array scripts to execute hundreds of computations in parallel. The result of the retrieval is given as temporary ASCII files that are combined and converted into netcdf by the post-processor. The processing chain is detailed in the Auxiliary User Manual (AUM 2021) and Algorithm Theoretical Basis Document (ATBD 2020).

The Product Algorithm Laboratory (PAL) provides a state-of-the-art environment for supporting data product development from TROPOMI. Besides providing access to computational resources, a major advantage of PAL is that it provides access to TROPOMI L1 and L2 products, which eliminates the need for downloading the large L1B TROPOMI datasets. In general, the UoL-FP processing chain for the vapour isotopologue product has been configured to scale across large HPC systems and is used to process large datasets from TROPOMI and thus it is suitable for processing on PAL. However, there are differences in how the used HPC environment and PAL are managed. Therefore, to migrate the processing chain to PAL, modifications to the processing chain are required and some elements will have to be re-developed:

- The UoL-FP retrieval generates multiple temporary ASCII files per sounding which is not well suited for processing with a system like PAL. A new retrieval framework based on UoL-FP is under development at University of Leicester (FUSIONALP-UoL-FP) which rationalises I/O and all outputs are directly written into a single hdf file. The recommendation is to adopt this new framework for implementation in PAL.
- Switching the final output netCD4 format from 1D to 2D - format and naming convention already in line with operational products - will allow data to be used within PAL mapping tools (e.g. https://maps.ls5p-pal.com)
- If geophysical input products are available on PAL on a per TROPOMI-sounding basis, then the pre-processing code can be simplified and streamlined.

3 Validation needs

Validation is a continuous effort and it is important that reference data are made available for future validation exercises. Ground-based remote sensing reference data from the Network for the Detection of Atmospheric Composition change (NDACC), the Total Carbon Column Observing Network (TCCON) or the Collaborative Carbon Column Observing Network (COCCON) are important, because these platforms provide data for the entire atmosphere (similar to the TROPOMI/S5P data) and on a long term basis, usually over several years (i.e. are not limited to campaigns). In the framework of the MUSICA project a retrieval for the water isotopologues has been developed and applied to three NDACC stations (Kiruna, Karlsruhe and Izana/Tenerife). The MUSICA NDACC data have been calibrated with respect to fiducial standards (Schneider et al., 2016).

Another important component of reference data for validation are in-situ profile measurements. These data are very well calibrated and not affected by the sensitivity issues of the remote sensing data (the remote sensing references provide data according to the characteristics of the averaging kernels). Thus, these data provide key fiducial references. However, in-situ profile measurements are expensive and limited to a few days during specific measurement campaigns. In this context, taking into account the satellite overpasses and the meteorological situation for the planning of the campaigns is very important.

Validating the spatial patterns of satellite retrievals remains difficult, as no consistent large-scale, continuous in-situ water vapour isotope network is available. In-situ measurements of water vapour isotopes are still limited to specific sites, and the lack of a common, community-based calibration and post-processing protocol hinders an efficient combination and comparison of such measurements with satellite retrievals.

3.1 Ongoing in-situ profile observations

3.1.1 In-situ aircraft campaigns

The specific nature of aircraft observations demands a high measurement frequency and careful planning of flight patterns and installed instrumentation to account for memory effects in the measurement set up. An increasing number of aircraft campaigns incorporating in-situ water vapour isotope measurements in the past 10 years (e.g. HyMeX SPO1, MUSICA, ORACLES, IGP, L-WAIVE, LEMON, EUREC4A, ISLAS) improved the understanding of the specific needs for such measurements and are able to provide high quality aircraft-based water vapour isotopes measurements suitable for validation purposes. Nonetheless, aircraft-based in-situ measurements of water vapour isotopes are limited in their spatial and temporal coverage. Due to limitations in the in-situ measurements (e.g. complicated terrain at measurement site, time of the day of measurements) and the satellite overpasses and retrievals (e.g. no data over ocean surfaces or under cloudy conditions), the validation of satellite retrievals with aircraft-based in-situ measurements is often limited to a few profiles. Further, the campaigns had so far other specific objectives and were thus not focused on satellite validation. Therefore, the available profiles are not ideal for satellite validation purposes, for example in that they have a limited vertical extent. For an optimal satellite validation study, dedicated aircraft campaigns for this purpose are needed. Such dedicated campaigns should be designed to improve the collocation with satellite overpasses, target clear-sky conditions and include measurements to sufficiently high altitudes.

Recent aircraft campaigns (LEMON 2021 in the Rhone valley, ISLAS 2022 in Northern Sweden and the Barents Sea) provide new in-situ profiles for future validation studies. During ISLAS 2022, a dedicated satellite comparison flight is available which is collocated with satellite overpasses and ground-based remote sensing measurements in Sodankylä, Finland, and Kiruna, Sweden.

3.1.2 In-situ balloon campaigns

In the framework of another ESA project the instrument Water vapour Isotopologue Flask sampling for the Validation Of Satellite data (WIFVOS, https://eo4society.esa.int/projects/wifvos/) is developed. It is a balloon-borne flask-sampler. It autonomously samples atmospheric air in flasks during flight, the sampled air is analysed for isotopic composition of water vapour after landing and recovery using a cavity ringdown spectroscopy instrument. Per flight 8 flasks are sampled to represent to equal partial column of water vapour with the highest one at 95% of the total column, while there are two additional flasks for the detection of potential contamination. (The second generation of the sampler is planned with 7 flasks, 5 for atmospheric samples and two for standards).

Currently, two successful flights have been performed at Sodankylä with parallel TCCON observations. However, these first flights also showed the need for improvements of the instrument. To this end, a characterisation and minimisation of surface exchange effects in the sampler and the analysis system under simulated field conditions in the laboratory is required.

The ballon data are important for the calibration of the TCCON HDO data product which is currently missing. In addition, these in-situ balloon data can be used for validating the MUSICA

NDACC water isotopologue profile data for other sites than Tenerife (the validation for Tenerife with aircraft-based in-situ profile measurements are shown in Schneider et al., 2016).

3.2 Ongoing ground-based remote sensing observations

3.2.1 NDACC

NDACC is part of the Global Atmosphere Watch (GAW) program of the World Meteorological Organization (WMO). The network consists of about 20 globally distributed ground-based FTIR stations. In the framework of the MUSICA project a retrieval for the water vapour isotopologues $H_2{}^{16}O$, $H_2{}^{18}O$ and $HD^{16}O$ has been developed (Schneider et al., 2006, Barthlott et al., 2017). MUSICA NDACC data are unique in providing some profile information on δD in a continuous manner and over longer time periods. MUSICA NDACC is calibrated to a fiducial standard, but only for one NDACC site (Tenerife, Schneider et al., 2016). NDACC spectra used for the MUSICA NDACC retrievals are continuously measured. The MUSICA NDACC processing of these spectra has been carried out in the context of third party projects. Since these third party projects have ended, there has been no further generation of MUSICA NDACC data for recent dates. Currently, at most stations MUSICA NDACC processed data are only available until the end of 2015. In the framework of this project, processing until 2020 for the three stations in Tenerife, Karlsruhe, and Kiruna was possible.

To support the TROPOMI water isotopologue product (and other future missions) sustained MUSICA NDACC data generation from NDACC stations would be of great value which would require financial support. Furthermore, the recent development of the new balloon-borne observations can allow calibration at multiple sites and help to improve the calibration of the MUSICA NDACC water vapour isotopologue profiles.

3.2.2 TCCON

TCCON provides column averaged H_2O and HDO mixing ratios operationally, but referencing to fiducial standards is currently only possible for sites where NDACC measurements are made simultaneously to TCCON measurements.

The recent development of the new balloon-borne observations (see Sect. 3.1.2) of HDO and H_2O offer new possibilities for referencing the TCCON data to fiducial standards. Another possibility would be to use COCCON HDO and H_2O data as a travelling standard (see Sect.

3.2.3) and thus document and assure the consistency of HDO/H_2O between different TCCON stations.

3.2.3 COCCON

COCCON observations are made in the same spectra region as TCCON observations, but at a reduced spectral resolution and applying mobile instrumentation (EM27SUN). This instrument type has proven its high stability in various field campaigns and long-term studies (Frey et al. 2019). The good mobility makes the COCCON spectrometers perfectly suitable as a travelling standard (cheap intercalibration of ground-based stations, no need for dedicated profile observations at all sites). In the framework of the ESA project “Fiducial Reference Measurements for Green-House Gases II" the characteristics of the instruments are exploited to use it as a travel standard for TCCON. It is planned to visit sites in Japan, Canada, Germany and Australia to perform side-by-side measurements with the TCCON spectrometers. Between the visits, the stability of the travel standard will be monitored using the Karlsruhe TCCON site and the COCCON reference spectrometer (Benedikt Herkommer, private communication). Thus, by the comparison of the different TCCON stations to a common reference we will be able to verify the level of station-to-station consistency currently achieved by TCCON and support further improvements.

Furthermore, a COCCON EM27SUN can be installed at remote sites without the large logistic efforts needed for installing NDACC or TCCON experiments. This would facilitate the collection of reference data in remote regions like the Sahara, the Amazonas, or tropical Africa (e.g. Frey et al., 2021). Furthermore, COCCON could also provide reference data over oceans by its installation on ships (e.g. Klappenbach et al., 2015).

So far COCCON has mainly been used for measuring the total columns of CO_2, CH_4, and CO. Due to recent developments there is now a good possibility to use the COCCON spectra for observations of H_2O and HDO. In the following, we list these recent developments. The spectroscopy of water vapour is strongly improved in the HITRAN 2020 database (Gordon et al., 2022). Very important improvements have also been achieved for the spectroscopy of CH_4, which strongly reduces respective spectroscopic interferences for a HDO and H_2O retrieval. The good CH_4 spectroscopy is a self consistent line list that uses laboratory measurements performed by the Karlsruhe Institute of Technology (KIT) for a revision of the HITRAN 2020 parameters and includes empirical Rosenkranz first order line mixing parameters in TCCON and TROPOMI spectral range (Frank Hase, private communication). In addition, the solar spectrum has been improved (Geoffrey Toon, private communication).

4 Synergetic use of the TROPOMI (SWIR) and the IASI (TIR) isotopologue products

The thermal infrared (TIR) nadir spectra of IASI (Infrared Atmospheric Sounding Interferometer) are successfully applied for retrievals of different atmospheric trace gas profiles (e.g. Schneider et al., 2022). However, these retrievals offer generally reduced information about the lowermost tropospheric layer due to the lack of thermal contrast close to the surface. Earth surface reflected solar spectra observed in the short wave infrared, for instance by TROPOMI (TROPOspheric Monitoring Instrument), offer higher sensitivity near ground and are used for the retrieval of total column averaged mixing ratios of a variety of atmospheric trace gases.

Schneider et al. (2021a) present a method for the synergetic use of IASI profile and TROPOMI total column data. The method uses the output of the individual retrievals and consists of linear algebra a posteriori calculations. It has been shown that this approach is mathematically very similar to applying the spectra of the different sensors together in a single retrieval procedure, but with the substantial advantage of being usable together with different individual retrieval processors. Further advantages of this approach are that it is very time efficient, and of directly benefiting from the high quality and most recent improvements of the individual retrieval processors.

In the following section (Sect. 4.1), we investigate the synergetic use of TROPOMI and IASI, because of the perspectives given by the upcoming Metop-SG mission where both instruments will be on the same platform (https://www.eumetsat.int/metop-sg). Although IASI and TROPOMI are currently on different orbits (IASI is on an orbit with descending node equator crossing at 9:30 mean local solar time and TROPOMI is on an orbit with ascending node equator crossing at 13:30 mean local solar time), there is reasonable number of collocations within one hour and a few kilometres in the northern middle and high latitudes which makes a synergetic use feasible (Schneider et al., 2021a).

4.1 Synergetic use of Level 2 data

The Kalman filter based method has been demonstrated for methane (CH_4) in Schneider et al. (2021a). It requires the following TROPOMI/S5P Level 2 data: the retrieved total column, the column averaging kernel, the used a priori profile, and the noise uncertainty of the retrieved total column. All these data are operationally made available for the TROPOMI/S5P water vapour isotopologue products (H_2O and HDO). Furthermore, it requires the following MUSICA

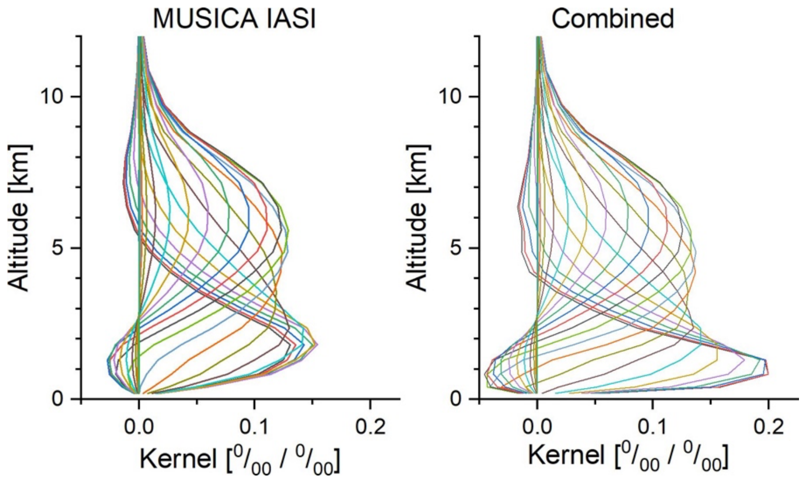

Figure 1: *HDO/H_2O ratio proxy row kernels. Left: Row kernel for a typical MUSICA IASI retrieval over the middle latitude site of Karlsruhe (49°N). Right: Row kernel for the same IASI observation, but with the additional synergetic use of the TROPOMI total column data by means of the Kalman filter approach.*

IASI Level 2 data: the retrieved vertical profiles, the profile averaging kernels, the used a priori profile, the noise uncertainty covariance of the retrieved profile, and the applied constraint matrix. All these data are made available for the MUSICA IASI water vapour isotopologue product.

The synergetic use for the water vapour isotopologue ratio can be made in analogy to the synergetic use of a simple trace gas product (like CH_4) by using the water vapour isotopologue ratio proxy state (ln[HDO]-ln[H2O]). For the MUSICA IASI data this proxy state method is described in detail in Wiegele et al. (2014) and Diekmann et al. (2021). For the TROPOMI/S5P total column product an analogue framework for an isotopologue ratio column proxy product has been developed in Sect. 4 of the Validation Report (VR 2021).

4.2 First test of synergetic use of HDO/H_2O data

First tests of a synergetic combination of the MUSICA IASI and the TROPOMI/S5P isotopologue ratio proxy products have been made for observations in the surroundings of the NDACC (and TCCON) station of Karlsruhe in south-western Germany. For this test we use the same collocation requirements as for the combination of the methane products (50 km, 6 hours and 50 hPa, see Schneider et al., 2021b). Figure 1 shows the effect of the combination on the

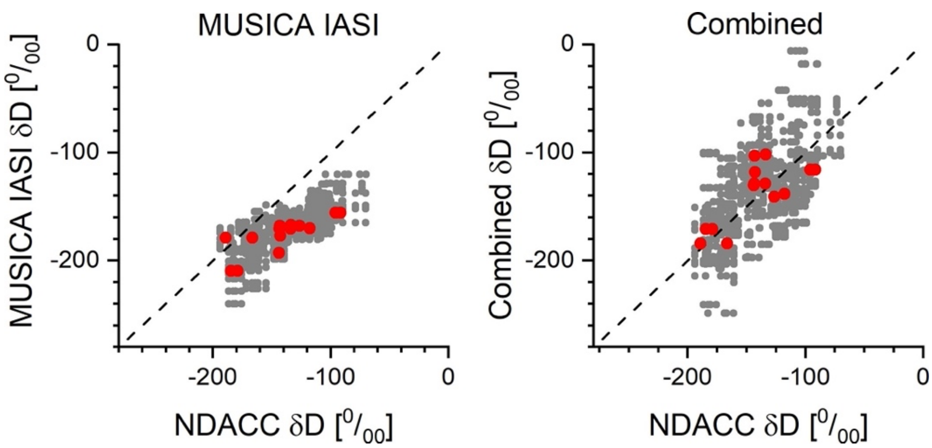

Figure 2: *Correlation between collocated MUSICA NDACC δD data (representative for 1000 m a.s.l.) and two different satellite δD products (representative for 1000 m a.s.l.) in the surroundings of Karlsruhe (49°N). Left: MUSICA IASI satellite data. Right: MUSICA IASI data optimally combined (using the Kalman filter approach) with the TROPOMI/S5P total column data. Grey dots present all daily mean data, red dots only the daily mean data when more than 20 different TROPOMI/S5P observations contribute to the daily mean.*

vertical sensitivity. Only using the IASI observation there is a lack of sensitivity close to ground (low values of the averaging kernels, left panel of Fig. 1). If we optimally combine the information provided by the TROPOMI/S5P total column data with the MUSICA IASI profile data by using the Kalman filter approach, we can significantly improve the sensitivity close to ground (right panel of Fig. 1).

We tested this combination for collocated IASI and TROPOMI/S5P observations between June 2018 and August 2019 over Karlsruhe. At Karlsruhe FTIR measurements are made from ground in the 2000 – 4200 cm^{-1} region (in addition to the TCCON near infrared measurements above 4000 cm^{-1}). These spectra are used for the MUSICA NDACC retrieval, which generates a water vapour isotopologue ratio product that has some profile information (Barthlott et al., 2017). Here we use this MUSICA NDACC water isotopologue ratio product from the Karlsruhe station as a reference for the satellite based lower tropospheric water isotopologue ratio data. Figure 2 shows the correlation between the collocated MUSICA NDACC references and the satellite data (for data representative for 1000 m a.s.l.). We observe a good correlation already between the MUSICA IASI and the MUSICA NDACC δD values; however, the slope of the regression line is significantly lower than unity (left panel of Fig. 2). The combined data product shows more scatter, but the data group very well around the one-to-one diagonal. The increased scatter is due to the uncertainty of the TROPOMI/S5P data (uncertainty in the TROPOMI total column data is seen by a factor of more than two as an uncertainty in the lower tropospheric combined data, see Schneider et al., 2021a). We can significantly reduce the scatter by using only the daily mean when more than 20 individual TROPOMI/S5P observations contribute to the daily mean (red dots in Fig. 2).

4.3 Perspectives for Metop-SG

In the context of an already approved Metop-SG mission the IASI and TROPOMI/S5P successor instruments (IASI-NG and Sentinel-5) will be on board of the same three satellites whose operations will be guaranteed until the 2040s. These missions offer unprecedented potential for climate and weather research; however, also serious challenges in the field of data processing. The developed water isotopologue processor can be well adapted to Sentinel-5 which will allow extending TROPOMI data sets with Sentinel 5 but the processing chain will need optimizations to deal with the large data volume. Furthermore, the MUSICA IASI retrieval will be suitable for processing of IASI-NG data.

The fact that IASI-NG and Sentinel-5 will be on the same platform (Metop-SG, https://www.eumetsat.int/metop-sg) and spatially and temporally co-located measurements are performed is an ideal opportunity for optimally combining the IASI-NG and Sentinel-5 Level 2 data. Here we showed that this combination can be done with the respective level 2 products in a computationally very efficient way (see Sect. 4.2), i.e. the development of a dedicated (computationally expensive) combined retrieval is not needed. We already have a well elaborated theory for exploiting the unique water vapour isotopologue observing possibility offered by Metop-SG.

5 Scientific Impact

The high spatial and temporal coverage of the TROPOMI observations allows for a wide range of applications of the TROPOMI water vapour isotope retrievals. A further development of the UoL-FP retrieval, especially in combination with IASI retrievals, will have a scientific impact on the understanding of atmospheric moisture cycling in the boundary layer and free troposphere, of spatial isotopic patterns of weather system and on the modelling of water vapour isotopes from global climate models to regional weather prediction models.

There are still inconsistencies between global climate models (GCMs) and process models (as e.g. Large-Eddy Simulation (LES) and Single Column Models (SCM)). For example, climate models predict that the area covered by shallow cumuli at cloud base is very sensitive to changes in environmental conditions, while process models suggest the opposite, namely that the cloud-base fraction of trade-wind cumuli appears to be much more resilient to changes in environmental conditions (Bony et al., 2017). Therefore, field campaigns as well as satellite data are essential to quantify physical properties of trade-cumuli (e.g. cloud fraction and water content) as function of the large-scale environment. The resulting data sets can then be used for evaluating the convective parameterisations of the climate and process models. Further, with these data sets the role of ocean mesoscale eddies in air-sea interaction and convective organisation can be assessed.

As an example, recent dedicated research campaigns incorporating water vapour isotopes aim to investigate the efficiency of the water cycling in subtropical (EUREC^{4}A campaign) and polar (ISLAS campaign) regions and provide datasets for evaluation and comparison studies with satellite retrievals.

The EUREC^{4}A (ElUcidating the RolE of Clouds-Circulation Coupling in ClimAte) field campaign was performed in early 2020 in the western tropical Atlantic near Barbados. During the campaign seven water vapour isotopic analyzers on two aircraft, on three ships, and at the Barbados Cloud Observatory (BCO) were deployed. The field observations were complemented with satellite observations of water isotopologues from AIRS, IASI and TROPOMI covering the respective area of interest. While the EUREC^{4}A's in situ isotopic measurement network provides the opportunity to assess the spatial variability of the isotopologues in the trade wind environment, routine satellite retrievals of δD over the study region provide additional large-scale context, as well as compositional information about air masses upstream of the target measurement region (Bailey et al., 2022).

The Isotopic links to atmospheric water's sources (ISLAS) project aims on characterising the vertical air mass mixing and the efficiency of cloud processes during cold-air outbreaks and warm air intrusions from in-situ water isotope measurements. In total, three field campaigns including aircraft profile measurements were performed in Northern Scandinavia between 2020 and 2022. The TROPOMI data will be a valuable complement to the aircraft and ground-based data, and will help to put the in-situ results in a larger context and to evaluate climate and process models. Furthermore, one research flight was dedicated to remote sensing comparison by overflights over the two FTIR sights Kiruna and Sodankylä in collocation with satellite overpasses.

These on-going efforts to combine in-situ and remote sensing datasets show the usefulness of satellite retrievals by adding a large-scale perspective to localised in-situ measurements by other means than modelling of water vapour isotopes.

A weakness of current atmospheric modelling is the difficulty to validate water vapour transport in model simulations due to a lack of Lagrangian measurements for validation. Isotope-enabled numerical models overcome this problem by explicitly representing stable water isotopes in the model to act as tracers of microphysical processes in the water cycle. Satellite retrievals provide datasets to validate large- to meso-scale isotopic patterns in isotope-enabled atmospheric models. Such comparison studies have the potential to validate numerical weather and climate models and to improve our understanding of the specific isotopic signature of weather systems and the spatial representativeness of in-situ measurements.

The data assimilation experiments presented in the Impact Assessment Report (IAR) show that assimilation of TROPOMI or TROPOMI together with IASI has the potential to improve meteorological analyses and thus weather forecasts and climate predictions. So far only theoretical experiments with an Observation System Simulation Experiment (OSSE) have been performed. Performing assimilation experiments with real data and with a variety of isotope-enabled numerical weather and climate models could be the focus of current research to assess the potential of isotope data assimilation in operational weather forecasting.

A continuous retrieval of TROPOMI H_2O and δD will further be beneficial for the ESA Water Vapour Climate Change Initiative (CCI). The ESA CCI project aims at the generation of new global high-quality climate data records of both total column and vertically resolved water vapour (https://climate.esa.int/en/projects/water-vapour/about/). A long-term record of the isotopic variability of atmospheric water vapour adds an important climate variable to this record by providing integral information on the total column water vapour history not available from conventional water vapour measurements.

6 Summary and Recommendations

In this Scientific Roadmap Document, we have reviewed and discussed future development needs and activities in the area of processing, validation and scientific exploitation.

In this project, a successful TROPOMI vapour isotopologue retrieval has been developed and characterised. A future evolution of the TROPOMI water vapour isotopologue processing chain should focus on advancing the retrieval to take into account the covariance of H_2O and HDO adopting the approach developed for the MUSICA IASI retrieval and on the migration to the PAL system to allow large-scale and automated processing.

Validation against a fiducial reference standard as developed for the MUSICA project for the ground-based NDACC instruments plays an important role for assessing the performance of space-based water isotopologue retrievals. In this project, data from three MUSICA sites have been processed and applied but there is no sustained effort to generate these dataset limiting the ability to validate water vapour isotopologue data from satellites in the future. Additional validation data is provided by the TCCON network but calibration against in-situ standards is needed. This can ideally be achieved by comparisons to new balloon-borne in-situ profilers. Portable COCCON instruments can provide observations at locations not covered by TCCON or NDACC and they could in addition act as a travelling standard between sites. In-situ aircraft campaign data can provide high quality and high frequency measurements and such data from ongoing projects (e.g. LEMON2021) has already been used. However, to better exploit such data will require dedicated aircraft campaigns that should be ideally collocated with satellite overpasses.

Water isotopologue data is also measured by IASI in the thermal-infrared (TIR) with peak sensitivity in the free troposphere facilitating synergistic use with the TROPOMI SWIR column product. A method for combining the IASI TIR profile and TROPOMI SWIR column level 2 products has been presented in Schneider et al. (2021a) for methane and here we showed that this method can also be applied for HDO/H_2O (first combination results and their validation with MUSICA NDACC HDO/H_2O profile references at the Karlsruhe site are promising). Unprecedented perspectives of such synergistic use are offered by the launch of Metop-SG which provides perfectly collocated observations from IASI-NG and Sentinel-5.

The high spatial and temporal coverage of TROPOMI observations allows for a wide range of scientific applications, especially when used in combination with IASI. An operational TROPOMI water isotopologue product will help to advance our understanding of atmospheric moisture cycling in the boundary layer and free troposphere and on the modelling of water vapour isotopes from global climate models to regional weather prediction models as part of current and future projects such as EURECA^{4}A or ISLAS.

The specific recommendation for future activities and projects are:

- 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 higher model resolution than previous studies to better estimate the benefits of satellite δD and H_2O data for meteorological analyses and weather forecasting.

7 Acronyms and Abbreviations

Acronym	Meaning
AIRS	Atmospheric Infrared Sounder
COCCON	Collaborative Carbon Column Observing Network
CCI	Climate Change Initiative
EUREC4A	ElUcidating the RolE of Clouds - Circulation Coupling in ClimAte
GAW	Global Atmospheric Watch
GCM	Global Climate Models
FTIR	Fourier Transform Infrared spectroscopy
HITRAN	High-resolution TRANsmission molecular absorption database
HyMeX SOP1	Hydrological cycle in Mediterranean Experiment Special Observation Period 1
IASI	Infrared Atmospheric Sounding Interferometer
IASI-NG	IASI Next Generation
IGP	Iceland Greenland Seas Project
ISLAS	Isotopic Links to Atmospheric Water's Sources
KIT	Karlsruhe Institute of Technology
L-WAIVE	Lacustrine-Water vApor Isotope inVentory Experiment
LEMON	Lidar Emitter and Multispecies greenhouse gases Observation instrument project
LES	Large-Eddy Simulation
Metop-SG	Meteorological Operational Satellite - 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
ORACLES	ObseRvations of Aerosols above Clouds and their intEraction
OSSE	Observation System Simulation Experiment
PAL	Product Algorithm Laboratory

TCCON	Total Carbon Column Observing Network
SCM	Single Column Model
TIR	Thermal InfraRed
TROPOMI	Tropospheric Monitoring Instrument
UoB	University of Bergen
UoL	University of Leicester
UoL-FP	University of Leicester Full Physics
WIFVOS	Water Vapour Isotope Flask sampling for the Validation Of Satellite data

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