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

Requirements Baseline Document (RB)

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Table of Contents

Abstract

Water vapour isotopologues offer unique possibilities for investigating the tropospheric water cycle. The aim of this S5p+I H2O-ISO project is the development and validation of a new S5p water vapour isotopologue product (the HDO/H_2O ratio or δD) with simultaneous consideration of the needs of the scientific community and of the potential future application within operational processing chains. For formulating realistic requirements on the project, the needs of the scientific community must be considered together with the tools/datasets that are currently made available by the scientific community.
A review on ongoing activities in the field of water cycle research and isotopologues revealed that an S5p product would suitably complement currently existing space-based remote sensing water vapour isotopologue datasets. In particular promising for scientific applications is the unique horizontal resolution and coverage (daily global over land), the multi-decadal data availability (S5p-like data are guaranteed until the 2040s), and the possibility for observing water vapour isotopologues in the boundary layer independently from the free tropospheric isotopologue composition (by a combination with IASI products).
For the development and validation of the new product comparisons to other observational water vapour isotopologue datasets of a well-documented high quality are needed and the impact of the new product on science could be demonstrated by cross comparisons to isotopologue enabled atmospheric models. A review on the existing in-situ and remote sensing observational datasets obtained from different platforms identified the datasets that will be decisive for the development and validation activities: the MUSICA NDACC, TCCON, GOSAT, and IASI remote sensing datasets and the LEMON aircraft-based in-situ data. From a review on model data made available within current research projects and considering the availability of the aforementioned decisive observational datasets, four geographical areas have been identified for the development, validation and impact assessment: Central Europe, West Africa, Iceland/Scandinavia, and the western Pacific Tropics.
Based on the aforementioned reviews and analyses realistic requirements on the project can be concluded as follows: The project should develop a S5p retrieval software with fully traceable retrieval settings. The product should be soundly characterised (with the leading errors being well identified) and a calibration should be achieved that is traceable to fiducial references. The product's scientific impact should be demonstrated in the context of selected ongoing research projects and a roadmap towards the future development of a $\{H_2O,\delta D\}$-pair product and of an S5p+IASI combined product should be elaborated. An operational processing scheme for the δD product should be developed which should consider the possibility for a future operational generation of S5p+IASI combined $\{H_2O,\delta D\}$-pair products. The risks for not achieving these requirements and thus the project's aim are relatively small, because the project's activities are focused on the carefully selected test areas causing strong synergies with related ongoing international research activities.
Harmonisation across the different S5p+I themes of retrieval input data streams (L1, re-analysis fields of temperature and humidity), of cloud detection algorithms, and of the used spectroscopic data should be considered for the organisation of a unified operational processing chain. Moreover, a harmonised data output is recommended for user friendliness.

1 Introduction

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). An example is the sensitivity of low-level clouds to humidity transport from the boundary layer into the free troposphere, whose understanding is essential for correctly estimating the cloud climate feedback (e.g. Sherwood et al. 2014). Another important question is how the large-scale atmospheric circulation systems (e.g. extratropical storm tracks, tropical rain belts) respond to different natural and anthropogenic forcings, where studies with paleoclimatic situations are very helpful by revealing the connections between large-scale circulation/precipitation patterns and different past climate states (e.g. Ortega et al. 2015). Furthermore, atmospheric models often do not well capture small-scale processes, responsible for instance for diurnal cycle, intensity and geographical distribution of cloud cover and rainfall, which then strongly affects tropospheric heating rates and thus large-scale circulation (linkage between small- and large-scale processes, e.g. Marsham et al. 2013).

With the ability to record the condensation history, 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. Divers water isotopologue observational data (measured in ice cores, rain, atmosphere, etc.) together with dedicated water isotopologue model tools offer promising opportunities for investigating different aspects of the past and present water cycle.

Historically water isotopologues were measured in paleo archives and in surface rain samples and were therefore mainly representative of the isotopic composition of past and present precipitation events. More recently the activities have been expanded to the observation of water isotopologues in the gas phase. The vapour data show a larger isotopologue variability than precipitation data and are not limited to precipitation events. Concerning vapour data, the HDO/H_2O ratio (or $\delta D=1000*\{(HDO/H_2O) / VSMOW - 1\}$ with $VSMOW = 3.1152*10^{-4}$; Vienna Standard Mean Ocean Water) is very interesting, because it can be detected by remote sensing instruments (for an overview see Schneider et al. 2016). It has been shown that tropospheric δD vapour data are particularly valuable if observed together with H_2O vapour concentrations in form of $\{H_2O,\delta D\}$-pairs, because the $\{H_2O,\delta D\}$-pair distribution is directly linked to different moisture transport pathways (Noone 2012). Continuous and simultaneous (but independent) global observations of water vapour isotopologues in the boundary layer and in the free troposphere would be very promising for different scientific applications (e.g. Risi et al, 2012a; Risi et al, 2013; Field et al. 2014; Yoshimura et al. 2014).

In this document the requirements on a TROPOMI S5p water vapour isotopologue product are developed. These requirements result from the needs of the scientific community. However, the requirements must also be realistic and achievable within this two-year project, which is only possible by a close linkage to currently ongoing related activities. In Section 2 we give a review on such related activities. Section 3 gives very detailed information on currently available isotopologue observation and model data. In Section 4 the data needed from the scientific community for development and validation are discussed. In Section 5 we present the test areas selected for the development, validation and impact assessment of the new S5p product. The risks for achieving the objectives of the project are discussed in Section 6. Section 7 concludes on the achievable and realistic scientific and operational requirements. Finally, in Section 8 harmonisation possibilities between different S5p+I themes are briefly discussed, and Sections 9 and 10 list acronyms, abbreviations and references.

2 Related Activities

In this section we provide a brief insight into important currently ongoing activities related to this S5p+I H2O-ISO project and discuss the value that can be added by this project.

2.1 Currently ongoing activities

The scientific community working with atmospheric water vapour isotopologue observations and modelling is relatively small, but at the same time spread over many different institutions. In this section we cannot address all the details of the many different individual activities. Instead we focus on the activities related to important international collaborations, on ongoing research activities working on successfully evaluated research proposals, and on the activities in the field of satellite-based remote sensing with a focus on tropospheric water vapour isotopologues.

2.1.1 Community efforts

The PAGES (Past Global Changes, http://pastglobalchanges.org/) project is an international effort to coordinate and promote past global change research. The PAGES Iso2k project is creating a global database of paleo-δ^{18}O and δD records (standardised ratios of $H_2{}^{18}0/H_2{}^{16}O$ and $HD^{16}O/H_2{}^{16}O$, respectively) for the past 2000 years. The database integrates a diversity of archives, such as glaciers, ground ice, speleothems, corals, sclerosponges, trees, lake and marine sediments, with a wide range of resolutions. The Iso2k database is compared to climate simulations produced with models that include the treatment of stable water isotopologues (in the following called as isotope-enabled models). The objective is to understand to what extent the past regional- and global-scale features in hydroclimate and atmospheric circulation are reflected in the water isotopologue data.

A further very important international effort is GNIP (Global Network for Isotopes in Precipitation, https://www.iaea.org/services/networks/gnip). In the framework of GNIP, initiated in 1960 by the International Atomic Energy Agency (IAEA) and the World Meteorological Organization (WMO) (https://www.iaea.org/services/networks/gnip), the water isotopologue composition of precipitation is measured at more than 1000 different globally distributed sites. Depending on station and time period GNIP data are available for single precipitation events or as a mean of all precipitation events taking place during an extended time period (e.g. during one month). The GNIP data provide integrated information about many different relevant atmospheric processes: surface evaporation, moisture transport, condensation and precipitation. The GNIP data have been used as a major source for validating atmospheric water isotopologue models. The GNIR (Global Network for Isotopes in Rivers, https://www.iaea.org/services/networks/gnir) was initiated in 2002 to complement GNIP. GNIR is a global environmental observation programme dedicated to the compilation of isotopic assays of river waters.

SWING (Stable Water Isotope Intercomparison Group) is an international effort of comparing water-isotopologue enabled Atmospheric General Circulation Model results across different modeling groups. Via this initiative different atmospheric water isotopologue model data are made available mostly for the time period between 1980 and the mid-2000s. More details on available models, the model settings and data availability can be found on the SWING Phase 2 webpage: https://data.giss.nasa.gov/swing2/

ESA CCI+ Water Vapour (European Space Agency, Climate Change Initiative, Water Vapour, http://cci.esa.int/watervapour) is an initiative for generating new global high-quality climate data records of both total column and vertically resolved water vapour, which are homogeneous in space and time, work towards fulfilling GCOS (Global Climate Observing System, https://gcos.wmo.int/en/home) requirements, and respond to the user needs of the climate research community in the best possible way. The generation of a product by combining information from different satellite sensor is one topic of this initiative. Phase 1 of ESA CCI+ Water Vapour started in May 2018 and as a first step a user requirements survey has been performed (see respective User Requirement Document, available on the webpage, http://cci.esa.int/sites/default/files/Water_Vapour_cci_D1.1_URD_v1.1.pdf). The survey reveals that there is a substantial interest in having climate data records of water vapour together with water vapour isotopologues. This user requirement can be hopefully soon considered and water isotopologues can be included in the ESA CCI+ Water Vapour activities.

GEWEX (Global Energy and Water Exchanges, https://www.gewex.org/) is a core project of the WCRP (World Climate Research Programme, https://www.wcrp-climate.org/). GEWEX is dedicated to understanding Earth's water cycle and energy fluxes at the surface and in the atmosphere. In the framework of the GEWEX activity G-VAP (GEWEX Water Vapor Assessment, http://gewex-vap.org/) water vapour products that are important for the generation of globally consistent water and energy cycle products are identified. The recently updated list of G-VAP recommendations states: "Given the various applications, there is a need for the sustained provision of tropospheric water vapour isotopologue data." This recommendation can hopefully help to improve the funding situation of the different activities dedicated to the global observation of tropospheric water vapour isotopologues.

SPARC (Stratosphere-troposphere Processes And their Role in Climate, https://www.sparc-climate.org/) is another WCRP core project and WAVAS-II (https://www.sparc-climate.org/activities/water-vapour/), the follow-up project of WAVAS is SPARC's water vapour activity. Following the recommendations of the WAVAS report published in 2000, climatological measurement programmes have continued, new campaigns to investigate UTLS water vapour have been carried out, new satellite observation programmes have been launched, and many model and laboratory studies have been made. WAVAS-II has its main focus on water vapour and its isotopologues between the upper troposphere/lower stratosphere (UTLS) and the lower mesosphere. The main objective is to document the quality of the different data products and to derive long-term stability assessments in order to be able to reliably assess long-term trends in water vapour and its isotopologues in the UTLS and stratosphere. This is essential to investigate the reasons and implications of long-term changes of water vapour for atmospheric radiation, dynamics, chemistry, clouds, and the climate.

2.1.2 Scientific projects

EUREC^{4}A, (Elucidating the role of clouds-circulation coupling in climate, http://eurec4a.eu/), is an international initiative with support from the European Research Council. The aim is to better understand the response of clouds to global warming, i.e. it directly supports the World Climate Research Programme's Grand Science Challenge on Clouds, Circulation and Climate Sensitivity. It is investigated how shallow cloud amount depends on convective mixing, surface turbulence and large-scale circulation; and vice versa, how the radiative effects of water vapour and clouds influence shallow circulations and convection. The project works with different modelling tools and during a dedicated field campaign between 20 January and 20 February 2020 in the surroundings of Barbados water isotopologues will be measured from ground, ship and aircraft together with other meteorological parameters.

The European Horizon 2020 project LEMON (Lidar Emitter and Multi-species greenhouse gases Observation iNstrument, https://lemon-dial-project.eu/) is addressed by a consortium of eight partners coming from France, Germany, Norway and Sweden. It aims at developing a Lidar emitter for airborne and future space applications to monitor greenhouse gases and water vapour isotopologues. The objectives are to perform the first range resolved (vertically and/or horizontally resolved) water vapour isotopologue Lidar measurements and to validate the observations through an aircraft profile measurement campaign. Furthermore, a roadmap for integrating the Lidar instrument in a future space mission is elaborated. LEMON is closely related to the French national project WaVIL (differential absorption lidar for monitoring water vapour isotope HDO in the lower troposphere, https://anr.fr/Project-ANR-16-CE01-0009). More than 10 research flights with water vapour isotopologue measurements, reaching an altitude of up to 3500 m a.s.l. have been performed in June 2019 in the Annecy valley, France.

The project SNOWISO (Signals from the Surface Snow: Post-Depositional Processes Controlling the Ice Core Isotopic Fingerprint, https://steenlarsen.w.uib.no/erc-stg-snowiso/) is funded by the European Research Council. The ice core water isotopologue signals depend on the isotopologue composition of the precipitated water, and post-depositional exchange of the snow/ice with the atmosphere. Disregard of the latter is an important deficit in current climate reconstruction studies. SNOWISO's aim is to reduce this deficit by working on a quantification of the post-depositional exchange mechanisms and on developing a respective parameterisation to be used in models. For this purpose, in-situ snow and water vapour isotopologue observations are performed in the laboratory and in Greenland and Antarctica. The observational data are then used to benchmark a coupled snow-atmosphere isotopologue enabled model and ensure a more realistic simulation of the ice cores' isotopologue signals.

The project ISLAS (Isotopic links to atmospheric water's sources, https://www.uib.no/en/rg/meten/112875/isotopic-links-atmospheric-waters-sources-islas) is a Consolidator Grant funded by the European Research Council. It investigates compensation of parameterisation errors regarding small-scale processes associated with the water cycle in atmospheric models. Mutual compensation of these errors makes their detection difficult and led to a limited understanding of hydrological extremes, the response of the water cycle to a changing climate, and the interpretation of paleoclimate records. The project uses recent technological advances in isotopologue measurements and in-situ sample collection for acquiring high-resolution, high-precision isotopologue observational data from ground and aircraft (between about 0 and about 3500 m a.s.l.). In March 2018, during the run-up to the ISLAS project, in-situ profiles have been measured during 10 research flights around Iceland within the IGP campaign (Renfrew et al. 2019). Sophisticated model tools are used to decipher, synthesize and exploit these observations, and to identify compensating errors between different water cycle processes in the models.

In the context of the European Research Council project MUSICA (MUlti-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water, funding phase 2011-2016) the MUSICA research group (http://www.imk-asf.kit.edu/english/musica.php) started its activities. The focus of the group is towards consistent ground- and space-based remote sensing retrievals, the comprehensive documentation of the remote sensing data (in particular of the complex nature of isotopologue ratio data), and the integration of remote sensing data with well-calibrated reference measurements. A particular focus is {H_2O,δD}-pair data, because the {H_2O,δD}-pair distribution is directly linked to different moisture transport pathways (Noone 2012). Recently, the group optimised the data flow involved in the processing of spectra from the satellite instrument IASI (Infrared Atmospheric Sounding Interferometer) and 1 orbit with IASI cloud free spectra can now be processed per computing node and 12h. Currently massive MUSICA IASI retrievals of H_2O, {H_2O,δD}-pairs, CH_4, N_2O, and HNO_3 are performed. The MUSICA NDACC (Network for the Detection of Atmospheric Composition Change) retrieval processor developed for generating tropospheric water vapour isotopologue profiles from the NDACC FTIR (Fourier-Transform InfraRed) solar absorption spectra is currently not operative due to funding reasons; however, the FTIR spectra are measured continuously at the different NDACC sites and the MUSICA group can perform MUSICA NDACC retrievals as soon as the funding situation permits.

The German-Swiss project MOTIV (MOisture Transport pathways and Isotopologues in water Vapour, https://gepris.dfg.de/gepris/projekt/290612604?language=en) is supported by German and Swiss national funds. The aim of the project is to establish global tropospheric water vapour isotopologue satellite observations (observation of {H_2O,δD}-pairs) as a tool for testing model-based representations of moisture pathways from source to sink. Tropospheric water vapour isotopologue remote sensing data ({H_2O,δD}-pairs) are generated for about 12 months and on quasi global scale using the thermal nadir spectra measured by the IASI satellite instruments, together with the retrieval algorithm as developed and validated in the context of the activities of MUSICA (Schneider et al. 2016). The model COSMOiso (Pfahl et al. 2012) is used to reveal the water sources and pathways that can be tagged by the MUSICA IASI {H_2O,δD}-pair observations. The project focuses on the three test areas: Central Europe, the subtropical North Atlantic, and the West African monsoon region.

The German-Japanese project TEDDY (TEsting isotopologues as Diabatic heating proxy for atmospheric Data analYses, https://gepris.dfg.de/gepris/projekt/416767181) is supported by German and Japanese national funds. The aim of this project is to use the global MUSICA IASI isotopologue data ({H_2O,δD}-pairs) as observational proxy for latent heat exchange in the framework of a LETKF (Local Ensemble Transform Kalman Filter) isotopologue assimilation approach (Yoshimura et al. 2014) and to assess its impact on the analyses fields of heating rates, temperature and wind. For this purpose, a comprehensive three-year database of quasi global MUSICA IASI {H_2O,δD}-pair remote sensing data is produced and assimilation studies using the two different water vapour isotopologue models IsoGSM (Yoshimura et al. 2008) and ICON-ART-Iso (Eckstein et al. 2018) are planned.

2.1.3 Retrievals of tropospheric water vapour isotopologues using current satellite data

Different institutions have currently (or have had very recently) retrievals in operation that generate tropospheric water vapour isotopologue data using satellite measurements made by instruments that are currently in orbit. The institutions and instruments for retrievals containing some information about the vertical distribution above the boundary layer are: (1) the Jet Propulsion Laboratory (https://www.jpl.nasa.gov/) using the instruments TES and AIRS, (2) the Université Libre de Bruxelles (https://www2.ulb.ac.be/cpm/atmosphere.html) using the instrument IASI, and (3) the Karlsruhe Institute of Technology (http://www.imk-asf.kit.edu/musica.php) using also the instrument IASI. The institutions and instruments for retrievals of total column abundances are: (1) the Netherlands Institute for Space Research (https://www.sron.nl/) using the instrument TROPOMI on Sentinel-5p, and (2) the University of Leicester (https://www2.le.ac.uk/departments/physics/research/eos/) using the instruments GOSAT and TROPOMI on Sentinel-5p.

2.1.4 Documenting and assuring quality of space-based remote sensing data products

The project FIDUCEO (Fidelity and uncertainty in climate data records from Earth Observations, http://www.fiduceo.eu/) will generate space-based remote sensing datasets using a rigorous treatment of uncertainty, in line with the recommendations from the discipline of metrology. The objectives are complete and traceable estimates of stability and uncertainty. For this purpose, a suite of software tools for reading/writing the data and for performing metrologically rigorous analysis - including tools for stability analyses and ensemble creation - will be developed. All data, software tools and methods will be freely and openly accessible under the Creative Commons licence, where possible. Information about the project and our methods will be available in a variety of forms, including workshops and e-learning modules. The aim is to have a broad and lasting impact on the field of climate data from space.

TUNER (Towards Unified Error Reporting, https://www.imk-asf.kit.edu/Projekte_2689.php) is a project aiming at providing consistent and inter-comparable error estimates for atmospheric temperature and composition measurements from space. Along with this, a consistent and inter-comparable characterization of spatial resolution and content of *a priori* information of the remotely sensed data shall be provided. This is important, because quantitative work with remotely sensed data -- data assimilation, data merging, time series analysis, testing of hypotheses etc. -- depend largely on the adequate characterization of the data. Currently, multiple retrieval methods are used by the different instrument groups, and along with these various approaches to error estimation are applied. Resulting errors are not always inter-comparable. Some kinds of uncertainties are sometimes not reported at all. The different altitude resolutions and the different content of prior information in the data products is a particular problem. TUNER shall identify data characterization methods currently in use, investigate completeness and inter-comparability of available error estimates, develop a recommendation how unified data characterization shall be performed and how data uncertainties shall be reported, provide unified error estimates for some selected data products, and instruct data users how to best utilize these.

2.2 Added value of this S5p+I H2O-ISO project

In this project a S5p water vapour isotopologue product (HDO/H_2O) will be developed, generated and evaluated (data quality and science impact). It is planned to generate data globally for all observations made over land for a 12 months period (July 2018 - June 2019). Furthermore, a roadmap for maximising the scientific impact of the data and for an operational data generation will be developed. These activities will contribute to the efforts of increasing the diversity and availability of reliable water isotopologue data and identify the future work needed for ensuring highest benefit of S5p for water cycle research.

2.2.1 Added value with respect to the other tropospheric satellite data

The measurements of the TROPOMI instrument on Sentinel-5p (in the following referred to as the S5p instrument) have important similarities to the measurements made by SCIAMACHY and GOSAT. For all three instruments the spectra cover a similar spectral region (the near infrared), have a similar spectral resolution, and use similar observation geometry (surface reflected sunlight). It has been already shown by Schneider et al. (2019) that the S5p water vapour isotopologue product has a similar sensitivity as the respective SCIAMACHY (Frankenberg et al, 2009) and GOSAT products (e.g. Boesch et al. 2013), i.e. it is sensitive to the total column abundances, which in the case of water is a good proxy for the tropospheric abundances. However, compared to SCIAMACHY and GOSAT the S5p measurements are available with a better horizontal resolution and/or coverage. Moreover, having a S5p isotopologue product in addition to the similar products from SCIAMACHY and GOSAT is very valuable, because of the long-term perspective of S5p (S5p-like measurements are guaranteed until the 2040s). Furthermore, we plan an improved validation for this new S5p data with respect to fiducial references, an uncertainty reporting in line with TUNER (https://www.imk-asf.kit.edu/Projekte_2689.php), and the generation and characterisation of the scientifically very useful $\{H_2O,\delta D\}$-pair data (in line with the MUSICA recommendations, Schneider et al. 2016).

IASI, TES and AIRS measure thermal nadir spectra. These offer sensitivities with respect to tropospheric water vapour isotopologues above the boundary layer. S5p data have a different vertical sensitivity (total column abundances), i.e. they add important value to IASI, TES, and AIRS data. The horizontal resolution and coverage of S5p measurements is similar to IASI measurements and better than for TES and AIRS.

2.2.2 Unique potential for continuous daily global profile observation

In particular interesting would be a combination of a thermal nadir sensor (like IASI) and a near infrared sensor (like S5p), because of the synergies concerning their vertical sensitivities. A combination of S5p with IASI is particularly interesting, because both instruments offer a similar horizontal coverage and resolution and the same long-term perspective. The Metop-SG A1, A2 and A3 satellites planned to be operative in the 2020s and 2030s will carry an IASI-NG (IASI Next Generation) as well as a Sentinel-5 instrument. Having IASI-NG and Sentinel-5 observing from the same satellite platform ensures that both instruments frequently observe the same atmospheric location and a combination of respective observations could allow us to distinguish the water vapour isotopologues in the boundary layer from the isotopologues in the free troposphere and these data product could be generated daily for all locations over land and for the next two decades. This project will develop a roadmap for such S5p+IASI combined product.

2.2.3 Benefit in the context of ongoing activities

In order to assure an optimal scientific impact of the new S5p data, within this project the new S5p data will be referenced to fiducial standards (in-situ aircraft data, MUSICA NDACC data, MUSICA IASI data). We expect most significant scientific impact of a S5p total column water vapour isotopologue abundances product if it is consistent to the already validated (fiducial referenced) MUSICA IASI free tropospheric water vapour isotopologue product, because then both products could be combined and a daily global (for observations over land) tropospheric water vapour isotopologue profile product could be generated.
ESA CCI+ Water Vapour and G-VAP community efforts: Documenting the consistency of the S5p water isotopologues to fiducial standards would be an important contribution to G-VAP and ideas for combining S5p and IASI products as well as a future combined product itself would be of particular interest for ESA CCI+ Water Vapour (as well as for G-VAP).
Research questions addressed by EUREC^{4}A, ISLAS, MOTIV, and TEDDY: Horizontally high resolved data with profile information (discrimination of boundary layer and free troposphere by combining S5p and IASI) would help to better investigate the interplay between shallow clouds and circulation (EUREC^{4}A), identify small-scale processes near the surface and in relation to topography (ISLAS), trace water sources and transport from the boundary layer (MOTIV), and add additional constraints for assessing the latent heating rates (TEDDY).
Mutual benefit with LEMON: The validation of the S5p and the future IASI+S5p combined product will strongly benefit from the aircraft measurements made in the context of the project LEMON, since the aircraft measurements will provide the needed verification profiles in a temperate climate zone. Vice versa, the LEMON data usage for our validation work will add a different perspective to the datasets produced during LEMON.

3 Assessment of Existing Items

In this section we give a review on the different existing atmospheric water vapour isotopologue measurements (in-situ as well as ground- and space-based remote sensing measurements) and on the different available model tools. We discuss the main characteristics of the observational data and the models and review existing cross-comparison studies. The focus is on the observational data and models that will be relevant for this S5p+I H2O-ISO project.

3.1 In-situ observations

The in-situ observations are generally well referenced to fiducial standards, because the measurement techniques involve a calibration with respect to known isotopologue standards. The calibrations are made in the laboratory by analysing the field samples or directly in the field using continuously operating calibration units.

3.1.1 In-situ observation made at the surface

Over the last two decades, the infrared laser spectroscopy technique has been used to measure the isotopic composition of water vapour near the Earth's surface. These data have now been assembled in a global database of high temporal resolution stable water isotopologue ratios (δ18O and δD), the SWVID (Wei et al. 2019). Currently, the database includes data collected at 35 sites in 15 Köppen climate zones from the years 2004 to 2017. The key variables in each dataset are hourly values of δ18O and δD in atmospheric water vapour. Additionally, to the isotopologue data, synchronized time series of standard meteorological variables from in situ observations and ERA5 re-analyses are also provided. The SWVID database is the first database to archive vapour isotopologue measurements for public use without any restriction.

Additionally, in-situ measurements of water vapour isotopologues have been made on campaign basis from ship. A summary of these campaigns that there performed between 2012 and 2015 can be found in Wei et al. (2019). Specific details on some of these campaigns and the respective measurements are given in Benetti et al. (2017).

3.1.2 In-situ observation made from aircraft

Limited observations of water isotopologues from aircraft were performed during the past 30 years. Most of them have their focus in the UTLS or the lower troposphere. Only a few measurements cover the middle troposphere (5-10 km).

Measurements in the UTLS:
During the CRYSTAL-FACE (Cirrus Regional Study of Tropical Anvils and Cirrus Layers Florida Area Cirrus Experiment) aircraft campaign water isotopologues were measured on the NASA WB-57 aircraft by the high-resolution tuneable laser absorption spectrometer ALIAS (Aircraft Laser Infrared Absorption Spectrometer). The goal of CRYSTAL-FACE measurement campaign was to investigate tropical cirrus cloud physical properties and formation processes in the subtropical and tropical UTLS. Water isotopologue mixing ratios were recorded on nine

flights from 7 through 29 July 2002 in the region around Florida (Webster and Heymsfield 2003). During another field campaign the ICOS (Integrated Cavity Output Spectroscopy) and Hoxotope (HOx total water isotopologues) instruments were flown on the NASA WB-57 during the AVE_WIIF (Aura Validation Isotope Intercomparison Flight) campaign during June/July 2005. Three five-hour flights sampled the UTLS with level legs between 10 and 19 km in the region near Ellington Field in Houston, Texas, USA (Hanisco et al. 2007). The ICOS and Hoxotope instruments were also flown on the WB-57 during the Costa Rica Aura Validation Experiment (CR-AVE) in January/February 2006 and during the Tropical Composition, Cloud and Climate Coupling (TC4) aircraft campaign in June/July 2007. Both campaigns were based in Alajuela, Costa Rica at 9.9°N (Sayres et al. 2010).

Tropospheric vertical profile measurements:
The first measurements of δD ratios were obtained from samples of tropospheric air collected during aircraft campaigns between 1965 and 1973 over various locations in the United States covering an altitude range from 0 to 9 km, later from 6 to 13 km, and is unique in the sense that it provides full annual climatologies (Ehhalt 1974). From February to June 1966, about three profiles were obtained each month. The samples were collected at eight altitudes: 1.52, 1.83, 2.29, 3.05, 4.47, 6.1, 7.62, and 9.15 km above sea level, with sampling times ranging from 15 min at the lowest altitudes to 1 hour at the four highest altitudes. From March 1971 to September 1973, the earlier flights were extended to higher altitudes with sampling altitudes and sampling times of 6.4 km (10 min), 7.6 km (15 min), 8.8 km (20 min), 10 km (20 min), 11.3 km (20 min), 11.9 km (30 min), and 13.1 km (30 min). An update of this data set applying a correction for the isotopic contamination by wall water in the sampling tube are presented in Ehhalt et al. (2005).

Vertical profile measurements of the stable isotopologue composition of vapour, including δD and $\delta^{18}O$, were made during the HyMeX SOP1 (Hydrological cycle in Mediterranean Experiment special observation period 1) campaign onboard the Dornier 128 D-IBUF aircraft (Sodemann et al. 2017). That campaign was performed in the western Mediterranean (Corsica, France) during September and October 2012. The measured profiles cover the altitude range from 0 to 4500 m. Measurements were made with a Picarro L2130i spectrometer customized with a triple-laser setup to allow fast measurements. Typical time resolutions of the measurements were about 15-30 s, resulting in an average horizontal resolution of about 1-2 km and vertical resolution of 150-300 m (Sodemann et al. 2017).

Measurements with the Navion L17a aircraft were performed over the Alaskian interior boreal forest with a Picarro L1115-i isotopic water analyzer during three summers of 2011 to 2013 (Herman et al. 2014). Atmospheric profiles of in situ δD were obtained by changing altitude of the aircraft. Vertical profiles covering the altitude range from 0 to 4.5 km were obtained.

Vertical profiles of water vapor isotopologues covering the altitudes between 150 m and about 7000 m above sea level were obtained in the subtropical troposphere during the MUSICA project. The primary goal of the MUSICA airborne campaign was to perform validation measurements for two remote sensing instruments, the space-based IASI and a ground-based FTIR spectrometer. Measurements were made during 7 research flights in July and August 2013 over the Atlantic Ocean near the Canary Islands, Spain with the custom-designed tuneable diode laser spectrometer ISOWAT II (Dyroff et al. 2015). ISOWAT II was mounted with several other instruments in a CASA C212-200 aircraft, a medium sized transport aircraft powered by two turboprop engines. The vertical profiles were obtained with a high vertical resolution of around 3 m and a horizontal resolution of 75-95 m (Dyroff et al. 2015).

During the ObseRvations of Aerosols above Clouds and their intEractionS (ORACLES) field mission vertical profiles of δD were made with a WISPER system (Water Isotope Spectrometer for Precipitation and Entrainment), a modified Picarro L2120-i instrument, onboard the NASA P-3B Orion and ER-2 aircraft in the southeast Atlantic Ocean region. The ORACLES mission extended over a five-year period with three intensive observations periods in 2016, 2017 and 2018. ORACLE was designed to study key processes that determine climate impacts of African biomass burning aerosols. Vertical profiles were derived between 0 to 6 km (Herman et al. 2019).

In March 2018, during the run-up to the ISLAS project, in-situ profiles have been measured during 10 research flights around Iceland within the IGP campaign (Iceland and Greenland Seas Project, Renfrew et al. 2019) between surface and 3500 m a.s.l. with a vertical resolution of 150-300m. In June 2019 aircraft in-situ profiles have been measured during 10 days in the framework of the project LEMON in a limited area in the French Alps. These data are limited to the lowermost 3200 m above surface and have a vertical resolution of 50-150m.

Long-term measurements:
Long-term measurements in the upper troposphere are derived within the European research infrastructure IAGOS-CARIBIC (Brenninnkmeijer et al. 2007), a laboratory equipped with 15 instruments is deployed aboard a Lufthansa A340-600 for four intercontinental flights per month performing measurements mainly at ceiling altitude (9-11km). δD has been measured using the instrument ISOWAT (Dyroff et al. 2010). It is a tuneable diode-laser absorption spectrometer that simultaneously measures HDO and H_2O to derive δD in vapor. The instrument is mounted on CARIBIC since 2010 (https://www.caribic-atmospheric.com/).

3.2 Remote sensing datasets

3.2.1 Aircraft and balloon remote sensing datasets

Remote sensing measurements from balloon with focus on the stratosphere were made with the balloon-borne MIPAS-B (Michelsen Interferometer for Passive Atmospheric Sounding; Stowasser et al. 1999) and FIRS-2 (Far Infrared Spectrometer; Johnson et al. 2001) instruments.

Measurements of the high-resolution infrared absorption of sunlight by the atmosphere have been made with the NCAR aircraft-borne spectrometer, a Michelson type Fourier transform spectrometer that has been flown aboard a variety of National Science Foundation and NASA aircraft. Measurements have been made for more than 25 years (1978-2005) and flight altitudes have ranged mostly between 7 and 13 km. However, observations were usually made near the maximum altitude (10 – 12 km) of the specific aircraft, which include the NSF Sabreliner, NASA P3, NASA Electra and NASA DC-8 (Coffey et al. 2006).

3.2.2 Ground-based remote sensing datasets

The ground-based remote-sensing FTIR (Fourier-Transform InfraRed) instruments operated within the NDACC (Network for the Detection of Atmospheric Composition Change) and the TCCON (Total Carbon Column Observing Network) offer the possibility for measuring water vapour isotopologues (e.g. Schneider et al. 2006; 2010; 2012; 2016; Rokotyan 2014). For both networks solar absorption spectra are measured, often by the same instruments (mainly a Brucker IFS 125M) but in different spectral regions. Figure 1 depicts the global distributions of all FTIR instruments that are currently operative within the framework of NDACC and TCCON.

The NDACC FTIR measurements have a unique long-term characteristic (high quality spectra are available since the 1990s). In the meantime, there are about 20 globally distributed NDACC FTIR sites. The focus of NDACC is the long-term monitoring of stratospheric as well as tropospheric trace gases. The measurements are made in the middle infrared spectral region (750 - 4200 cm^{-1}). The very high resolution of the spectra (typically 0.005 cm^{-1}) and the relatively strong spectroscopic water vapour isotopologue signatures in the observed middle infrared spectral region ensure good sensitivity for the weak atmospheric variabilities (e.g. for the weak variabilities of water vapour isotopologue ratios). Barthlott et al. (2015) has proven good long-term, seasonal and latitudinal consistency of the NDACC FTIR data obtained at different sites and during different time periods. The NDACC FTIR spectral measurements were used within the project MUSICA for generating a {H_2O,δD}-pair reference product. The MUSICA NDACC FTIR analysis uses a unique retrieval strategy for all NDACC sites in order to create data of highest quality and consistency. The product is sensitive to tropospheric water vapour isotopologues (it is even possible to distinguish low tropospheric from middle free tropospheric signals with a degree of freedom of signal, DOFS, of 1.5-2). A method for documenting the complex nature of the MUSICA NDACC water vapour isotopologue data has been developed (Schneider et al. 2012) and the data have been calibrated with respect to aircraft- and ground-based in-situ measurements (for an overview see Schneider et al. 2016). The MUSICA NDACC data are available via the NDACC database (ftp://ftp.cpc.ncep.noaa.gov/ndacc/MUSICA/) for 12 different NDACC stations and for different time periods between 1996 and 2014 (for more details on data availability please refer to Barthlott et al. (2017)). NDACC FTIR spectra are continuously measured (also after 2014) and MUSICA NDACC data could be made available for time periods after 2014 as soon as dedicated funding becomes approved.

TCCON measurements have started at Park Falls (USA) and Lauder (New Zealand) in 2004. In the meantime, there are about 25 different sites contributing to the network. The focus of TCCON is the very precise measurement of column averaged mixing ratios of carbon species like CO_2 and CH_4. At all sites the retrievals are made with the same retrieval software, which is important for achieving a network wide data consistency. The measurements are typically made with a spectral resolution of 0.02 cm^{-1} and cover the near infrared spectral region (3800 - 9000 cm^{-1}) where O_2 signatures can be used for reducing important error sources (Yang et al. 2005). In this near infrared region, there are also spectroscopic signatures of H_2O and HDO (the latter are relatively weak) and column averaged mixing ratios of H_2O and HDO are automatically generated by the TCCON retrieval software. Retrieval products are generally

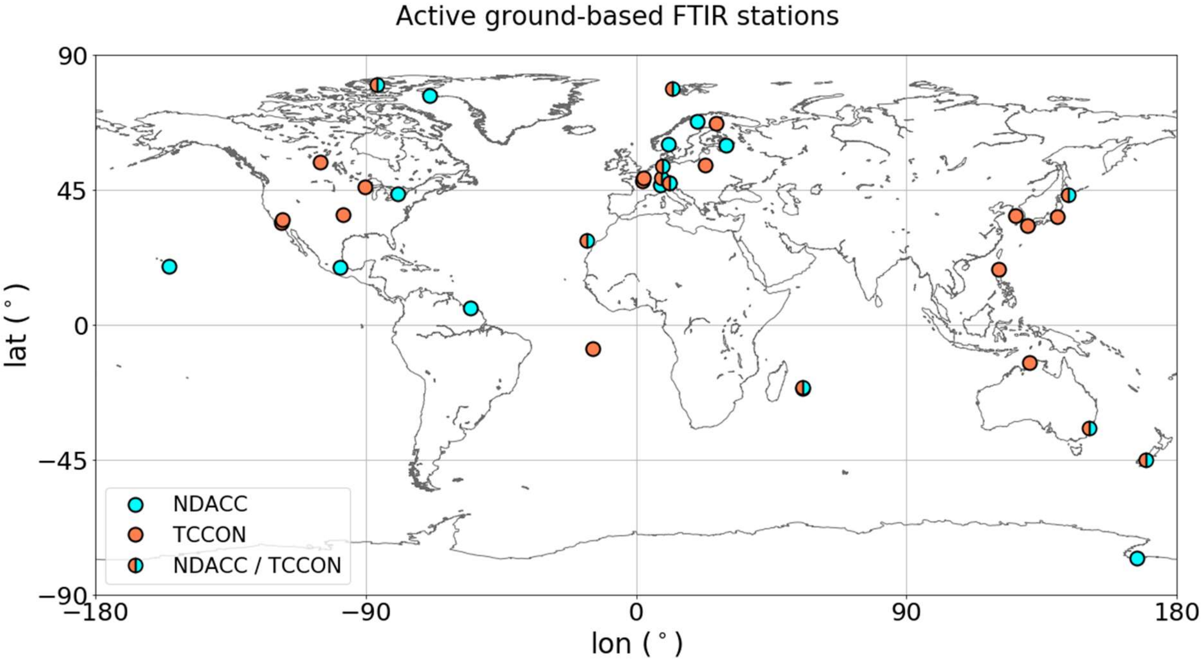

***Figure 1** Overview of the international ground-based measurement networks TCCON (orange) and NDACC (cyan). Only the stations with active FTIR spectrometers are shown.*

available with 12 months after the spectra measurement. The data can be downloaded at the TCCON database (https://tccondata.org/). TCOON data are generally well calibrated to in-situ aircraft references (Wunch et al. 2010). However, this is not the case for HDO. TCCON retrieves column averaged mixing ratios of H_2O and HDO and ratios between both can then be calculated after the retrieval process. This method can cause artefacts in the ratio data due to differences in the H_2O and HDO averaging kernels (see also discussion in Rokotyan et al., 2014).

3.2.3 Space-borne remote sensing datasets

The advantage of space-borne observations compared to ground-based observations is that space-borne observations can be obtained with a high temporal and spatial resolution on a global scale while ground-based observations are fixed to one certain location. In general, it is more difficult to measure the troposphere from space than the stratosphere, because scattering by cloud-and-aerosol and the height of the Earth surface have to be considered. Limb viewing methods such as limb emissions and solar occultation is not capable of lower troposphere measurements, which can be only achieved with a down-looking (nadir) measurement technique (https://www.eorc.jaxa.jp/GOSAT/instrument_1.html).

Space-borne observations with focus on the UTLS and above:
Space-based measurements of water isotopologues have been performed since the late 80s. The first measurements were performed in the upper troposphere and lower stratosphere during the ATMOS (Atmospheric Trace Molecule Spectroscopy) mission on the Space Shuttle over certain time periods in 1985 and 1992-1994 (April/May 1985, April 1992, April 1993 and

November 1994) and with limited spatial coverage (Moyer et al. 1996; Kuang et al. 2003). Measurements of HDO are obtained between 8 to 32 km with vertical resolution of ~2 km and a horizontal resolution of ~200 km.

In February 2001 the SMR (Sub-Millimetre Radiometer) on Odin was launched and measurements are still ongoing. SMR observes the thermal emission of trace gases from the Earth's limb in the 486-581 GHz spectral range (Urban et al. 2007). Observations by SMR were performed in a time-sharing mode with astronomical observations until 2007 and solely in aeronomy mode thereafter. Measurements of water isotopologues are derived between 20-70 km with a vertical resolution that is close to vertical sampling of ~3 km.

In March 2002 the Envisat (Environmental Satellite) was launched, carrying two instruments, making measurements of water isotopologues, namely MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) and SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography). The observations of these two instruments ceased on 8 April 2012, after the sudden loss of contact with the satellite. Nevertheless, 10 years of measurements were obtained with MIPAS and SCIAMACHY. MIPAS was a middle infrared Fourier transform spectrometer and measured the atmospheric emission spectrum in limb sounding geometry (Payne et al. 2007; Steinwagner et al. 2010). Measurements of water isotopologues are derived between 10-50 km. In the upper troposphere and lower stratosphere, the vertical resolution is typically about 5 km. Towards higher altitudes, the resolution degrades and in the upper stratosphere and lower mesosphere it is in the order of 8 to 10 km.

ACE-FTS (Atmospheric Chemistry Experiment – Fourier Transform Spectrometer) was launched aboard the Canadian SCISAT satellite on 12 August 2003 into a high inclination orbit with an altitude of 650 km. This orbit provides a latitudinal coverage from 85°S to 85°N, but is optimised for observations at high- and mid-latitudes. ACE-FTS performs observations in the infrared. The observations are based on the solar occultation technique and scans of the Earth's atmosphere are made 30 times a day (15 sunrise and 15 sunset). Measurements of water isotopologues are derived between 6.5 and 37.5 km (v2.2) and up to 46.9 km (v3.3), respectively (Nassar et al. 2007, Randel et al. 2012). The vertical sampling varies with altitude, ranging from about 1 km in the middle troposphere, to 3 to 4 km at around 20 km, and 6 km in the upper stratosphere and mesosphere.

Space-borne observations with focus on the troposphere:
In Table 1 an overview is given on the tropospheric isotopologue measurements from satellites that will be described in the following paragraphs and which are the once that are most relevant for this project. Listed are the instrument name, the measurement technique, the total measurement period of the instrument, the pixel size of the instrument and the vertical range where isotopologue measurements are available, and the references for the isotopologue products of the respective satellite instruments.

***Table 1** Overview of space-borne remote sensing sensors that provide the capability for tropospheric water isotopologue retrievals.*

Instrument	Technique	Measurement Period	Pixel size/ Altitude range	References
ADEOS-I/IMG	nadir	08/1996-06/1997	8 x 8 km 0 - 8 km	Zhakarov et al. 2004 Herbin et al. 2007
Envisat/ SCIAMACHY	nadir	03/2002-04/2012	120 x 30 km entire column	Scheepmaker et al. 2013 Schneider et al. 2018
Aqua/AIRS	nadir	Since 2002	13.5 km entire column	Worden et al. 2019
Aura/TES	nadir, limb	2004-2018	5.3 x 8.5 km 850-500 hPa (v4) 900-350 hPa (v5)	Worden et al. 2006 Worden et al. 2012
Metop/IASI	nadir	Since 2006	12 km 2 - 7 km	Herbin et al. 2009 Schneider and Hase 2011
GOSAT/ TANSO-FTS	nadir	Since 2009	10.5 km entire column	Frankenberg et al. 2013 Boesch et al, 2013
S5p/TROPOMI	nadir	Since 10/2017	7 x 7 km entire column	Veefkind et al. 2012 Scheepmaker et al. 2016 Schneider et al. 2019

First measurements in the troposphere were performed with the IMG (Interferometric Monitor for Greenhouse gases) instrument on board ADEOS-I from August 1996 until June 1997 when operations ceased. ADEOS-I was a sun-synchronous ground-track repeat polar orbiting satellite at about 800 km altitude that provided global coverage in 4 days. The IMG instrument was a nadir-viewing Fourier transform interferometer that recorded the thermal infrared emission of the Earth-atmosphere system (Zhakarov et al. 2004, Herbin et al. 2007). The IMG HDO data have a vertical resolution of 4-5 km and vertical profiles from 0 - 8 km can be derived and vertical columns from 0 - 16 km (Herbin et al. 2007).

SCIAMACHY launched in 2002 on board Envisat observed electromagnetic radiation upwelling from the Earth's atmosphere in three measurement modes: occultation, nadir, and limb geometry. Due to the usage of these different measurement modes, trace gas observations by SCIAMACHY are made in both the troposphere and stratosphere, however column abundances of water isotopologues can only be derived in the troposphere with highest sensitivity between 0-2 km. The SCIAMACHY instrument was the first instrument to provide global retrievals of water isotopologues with high sensitivity near the ground (Frankenberg et al. 2009). Schneider et al. (2018) present re-processed of SCIAMACHY water isotopologue data for the whole time period between 2002 and 2012.

The AIRS (Atmospheric Infrared Sounder) instrument is a nadir-viewing, scanning infrared spectrometer on board the NASA Aqua satellite that had been launched in 2002. AIRS measures the thermal radiance between approximately 3 and 12 μm with a resolving power of approximately 1200. A single footprint has a diameter of ~15 km in the nadir; with the ~1650 km swath, the AIRS instrument can measure nearly the whole globe in a single day. The Aqua satellite is part of the "A-Train" that consists of multiple satellites in a sun-synchronous orbit at 705 km with an approximately 13:30 equator crossing time. Measurements of total column are derived with AIRS. So far, HDO/H_2O has been retrieved for 5 days between 2006 and 2010 in the latitude range -40° to 80° to evaluate the retrieval approach and for error characterization of the AIRS data. Retrieval of HDO and H_2O data from the start of the mission to the present is planned in the near future (Worden et al. 2019).

The TES (Tropospheric Emission Spectrometer) instrument was launched in 2004 on board Aura and is also part of the "A-train". TES is a Fourier transform spectrometer that originally was designed to measure the thermal infrared (IR) radiances in both the limb and nadir viewing geometry (Worden et al. 2006, Worden et al. 2012). TES provides global vertically resolved tropospheric measurements every 2 days (Herman et al. 2014). Operations ceased in 2018. Also with TES long-term spectra were obtained, spanning 14 years. HDO/H_2O estimates can be derived between 925 hPa and 450 hPa in the tropics and during summertime at high latitudes (version 5 retrieval data, Worden et al. 2012). Aura/TES retrievals of tropical HDO and H_2O for the time period 2005-2011 have been used for model evaluation (Field et al. 2014).

In 2006 IASI (Infrared Atmospheric Sounding Interferometer) was launched onboard the Metop-A (Meteorological Operational Satellite Program of Europe) satellite. Metop-A is Europe's first polar-orbiting (LEO) satellite dedicated to operational meteorology. The Metop program is planned as a series of three satellites to be launched sequentially over an observational period of 14 years, starting in 2006 with Metop-A (launched on 19 October 2006). Metop-B (launched on 17 September 2012) has started being operational on 24 April 2013. The third satellite, Metop-C, has been launched on 7 November 2018. IASI is the main payload instrument for the purpose of supporting Numerical Weather prediction. As TES, IASI is a Fourier transform spectrometer and operates in the nadir viewing geometry. IASI measures in the infrared part of the electromagnetic spectrum at a horizontal resolution of 12 km over a swath width of about 2,200 km. With 14 orbits in a sun-synchronous mid-morning orbit (9:30 LT, descending node) global observations can be provided twice a day. Water isotopologue measurements are presented between 2-8 km (with a degree of freedom of signal, DOFS up to 2.0) by two different research groups: (1) a group from ULB (the ULB IASI product, Herbin et al. 2009; Lacour et al. 2012) and (2) a group from the KIT (Karlsruhe Institute of Technology, the MUSICA IASI product, Schneider and Hase 2011; Schneider et al. 2016). Measurements with IASI are still ongoing and will be continued in the future.

The ULB IASI retrieval uses two small spectral microwindows (1193–1223 and 1251–1253 cm−1) and fits humidity, δD and CH4 below 10 km altitude as well as surface skin temperature (Lacour et al. 2012). This retrieval is similar to the TES version 4 (Worden et al. 2006). ULB IASI data are available for cloud free scenes for a varying number of years (up to 5 years) between 2009 and 2013 and for certain latitudinal and longitudinal bands (Lacour et al. 2015, Lacour et al. 2017).

The MUSICA IASI retrieval works with a single broad spectral window (1190 - 1400 cm^{-1}) and simultaneously fits humidity, δD, CH_4, N_2O, HNO_3, temperature throughout the whole atmosphere as well as surface skin temperature (Schneider and Hase 2011; Schneider et al. 2016). This retrieval is similar to the TES version 5 retrieval (Worden et al. 2012). MUSICA IASI data are continuously available for cloud free scenes for some small areas between 2007 and 2017 (García et al. 2018), for February and August 2014 on global scale (e.g. Schneider et al. 2016). Very recently and in the context of the projects MOTIV and TEDDY global data have been generated for July and August 2013 and for the whole 2016-2018 time period. Further global scale retrievals for 2015 and 2019 are planned within the next 12 months.

The TANSO Fourier Transform Spectrometer (FTS) onboard GOSAT (Japanese Greenhouse Observing Satellite) was launched on 23 January 2009 into a sun-synchronous orbit with a local overpass time of 13:00 LT. Around 10.000 soundings with 82 km^2 circular spatial footprints are recorded daily, repeating a regularly spaced global footprint grid every 3 days. From the TANSO-FTS measurements total column abundances of H_2O and HDO have been retrieved globally using the SCIAMACHY retrieval (Frankenberg et al. 2013, Boesch et al. 2013). GOSAT-2, the successor of GOSAT has been launched on 29 October 2018 and the first Level 1 measurements from TANSO-FTS-2 were released in April 2019. Further measurements from TANSO-FTS-2 will be available in the near future. More information is available on the GOSAT-2 webpage (http://www.gosat-2.nies.go.jp/).

The Tropospheric Monitoring Instrument (TROPOMI) was launched on 13 October 2017 aboard the Copernicus Sentinel-5 Precursor (S5p) satellite. The Sentinel-5 Precursor (S5p) is the first of the atmospheric composition Sentinels with a planned mission lifetime of seven years. The TROPOMI instrument is a nadir-viewing, imaging spectrometer covering wavelength bands between the ultraviolet and the shortwave infrared. The instrument operates with a swath width of ~2600 km on the Earth's surface. TROPOMI allows water isotopologue total column retrievals on a daily global coverage with a spatial resolution of up to 7 km × 7 km (Veefkind et al. 2012, Scheepmaker et al. 2016, Schneider et al. 2019). The first data set of HDO/H_2O derived from cloud free retrievals for 2018-2019 were presented by Schneider et al. (2019). Further retrievals of HDO/H_2O over low clouds will be considered in future work.

Figure 2 gives an overview on currently available tropospheric water isotopologue data retrieved from space-borne measurements. Here, we consider data that has been obtained since 2002 and for time periods longer than 1 year, therefore the measurements from IMG are not included in this figure. Shown is the total measurement time period of the respective instruments. Time periods for which retrieved δD data are available are marked by green and blue colour (for total column data and vertical profile data, respectively). Quasi global datasets are additionally marked by a black frame. From most of these space-borne instruments long-term radiance measurements are available, covering 10 or more years, however the number of processed water vapour isotopologue data is comparably low, despite the increased community request. More data retrievals are often restricted due to the high demand of computational resources required for processing such large data volumes.

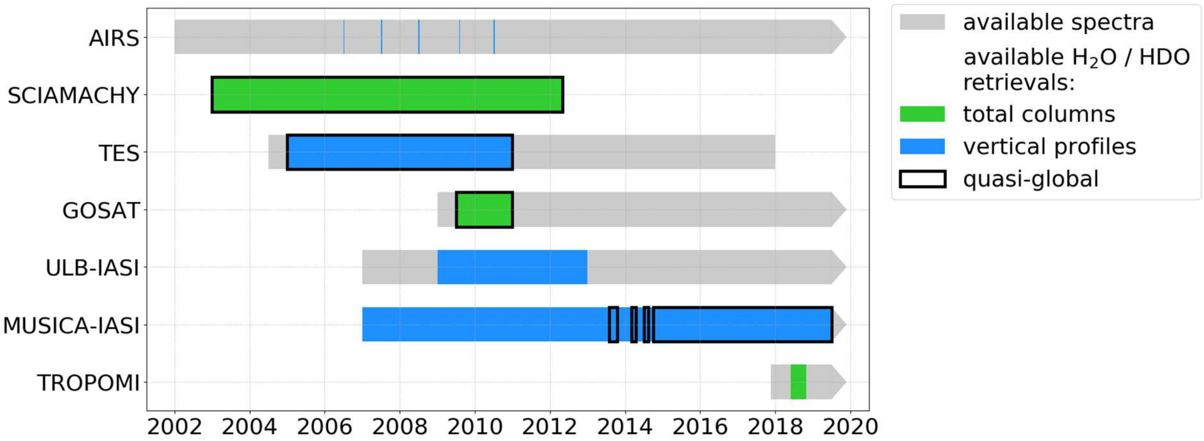

Figure 2 *Overview of tropospheric water isotopologue retrievals from satellite sensors. The grey bars indicate the time periods with available radiance measurements for each sensor (see Table 1). The periods for which water isotopic information has already been retrieved are shown in green for total column products and in blue for vertically resolved profiles. In case of quasi-global retrievals, the bars are framed in black.*

3.3 Modeling techniques

During the last decades various techniques of modeling water isotopologues have been developed and established as a powerful tool for studying atmospheric moisture transport and processes. The formalisms describing equilibrium and kinetic fractionation processes of different water isotopologues are well-known and can be used to extend an existing hydrological cycle in a model by the additional simulation of stable water isotopologues like $H_2{}^{16}O$, HDO and $H_2{}^{18}O$. Originating in paleoclimatic applications, the isotopologue-enabled atmospheric modeling has evolved along many different atmospheric scales, ranging from large-scale and long-term climate studies to cloud-resolving large-eddy-simulations (see, for instance, the overviews given in Yoshimura 2015 and Galewsky et al. 2016).
In the following general circulation models (GCM), regional climate models (RCM) and large eddy simulations (LES, i.e. cloud-resolving models) will be discussed. A comprehensive list of atmospheric isotopologue-enabled models is given to the best of our knowledge in Table 2.

3.3.1 General circulation models

General circulation models (GCM) are targeted on creating reliable climate predictions on a global and long-term scale. One of the main challenges hereby is to build a realistic representation of the atmospheric water cycle, since H_2O is the strongest greenhouse gas (Schmidt et al. 2010) and an important contributor to the atmospheric energy budget by inducing latent heat fluxes (Holton and Hakim, 2013) and forming clouds (Shine and Sinha, 1991). An isotopic equipment of such a GCM requires to extend the whole prognostic water cycle with the processes affecting the isotopic composition (Werner et al. 2011, Noone and Sturm 2010). During the last decades this technique has been realized for several general circulation models, e.g. LMDZ4 (Risi et al. 2010b), ECHAM5 (Werner et al. 2011) and GISS (Schmidt et al. 2007) and validated against in-situ and remote sensing measurements (see Section 3.4). For starting a joint venture between the different isotope-enabled GCMs the

project SWING was created with the aim to create unified intercomparisons, merged products and evaluations against precipitation measurements from GNIP stations (see Section 2.1, Risi et al. 2012a).
A very recent isotopically equipped GCM is ICON-ART-Iso that builds on the NWP packages of the nonhydrostatic global forecast model ICON of the German Weather Service (DWD). In combination with the 2-way-nested grid refinement technique for chosen areas it enables high-

Table 2 *Isotope-enabled General Circulation Models (GCM), Regional Climate Models (RCM) and Large Eddy Simulations (LES). The models that have already been cross-compared with remote-sensing products are printed in black font colour.*

Model	Type	Key features	Reference
ICON-ART-Iso	GCM	nonhydrostatic NWP model, 2-way-nested grid refinement	Eckstein et al. 2018
COSMOiso	RCM	nonhydrostatic model fractionation coupled with surface model (TERRAiso)	Pfahl et al. 2012
REMOiso	RCM	first regional model with stable water isotopologues	Sturm et al. 2005
RSM	RCM	spectral model	Yoshimura et al. 2010
SAM	RCM	nonhydrostatic model	Blossey et al. 2010
LMDZiso	GCM	nested grid refinement, fractionation coupled with surface model (ORCHIDEE)	Risi et al. 2010c
IsoGSM	GCM	spectral model	Yoshimura et al. 2008
ECHAM6-wiso	GCM	spectral model, fractionation coupled with surface model (JSBACH) and ocean model (MPIOM)	Werner et al. 2011
GISS	GCM	fractionation coupled with ocean model	Schmidt et al. 2007
HadCM3	GCM	fractionation coupled with ocean model	Tindall et al. 2009
NCAR iCAM	GCM	first comparison with space-based water isotopologue products	Lee et al. 2009
MUGCM	GCM	spectral primitive equation model	Noone and Simmons 2002
MIROC	GCM	spectral model	Kurita et al. 2011
GENESIS	GCM	spectral model,	Matthieu et al. 2002
iCESM	GCM	fully-coupled climate model	Brady et al. 2019
SPEEDY	GCM	primitive equation dynamics	Dee et al. 2015
DHARMA	LES	based on large eddy simulation model	Smith et al. 2006
SAM	LES	based on large eddy simulation model	Khairoutdinov and Randall 2003
CLIMBER	GCM	intermediate-complexity model	Roche et al. 2004
iLOVECLIM	GCM	intermediate-complexity model	Roche et al. 2013
ISOLESC	LES	based on NCAR LES	Wei et al. 2018

resolution simulations in space and time. This allows for simultaneously representing large dynamical circulations and resolving fine-scaled processes and moreover combines these different scales with mutual feedback. ICON-ART-Iso benefits from the tracer framework implemented into the model by Schröter et al. (2018), as it facilitates a flexible set up of artificial tracers tagging chosen air masses and moisture sources within a single model run (e.g. Joussaume et al. 1984). Also, it provides the option of flexibly controlling the different fractionation processes and determine their impacts (Eckstein et al. 2018).

3.3.2 Regional climate models

Additionally, stable water isotopologues were incorporated into regional climate models (RCM, see Table 2). Every regional model requires data provided by a global model to set the lateral boundary conditions for the atmospheric state, including isotopic information for isotope-enabled RCMs. Due to the smaller spatial domains very high grid resolutions can be achieved, reaching the limits of the classical hydrostatic convection parameterizations, so that convection becomes implicitly resolvable (Sturm et al. 2010, Blossey et al. 2010).

COSMO-iso is an isotope-enabled nonhydrostatic RCM and can be used for both event-based and climatological isotopologue studies. It has been shown that the simulated isotopologue ratios reflect microphysical cloud processes as well as the large-scale circulation (Pfahl et al. 2012, Christner et al. 2018). Moreover, ongoing studies investigate the ability of implicitly representing convective processes by reducing the horizontal resolution down to 7 km and switching off the explicit parameterizations for deep convection (A. De Vries, personal communication, 2019).

3.3.3 Large eddy simulations (cloud-resolving models)

A new approach was developed in the recent work of Wei et al. (2018), where they simulate atmospheric water isotopologue profiles based on the NCAR large eddy simulation (LES) model. This provides the ability to analyse the isotopic composition of the atmospheric boundary layer and to study very local hydrological processes, since horizontal and vertical resolutions down to 25 and 20m can be considered.

3.4 Cross-comparisons

In this Section we give a review on cross-comparisons between different observational data and discuss studies performing cross-comparisons between remote sensing observations and models. The focus are studies using space-based remote sensing observations of the troposphere, because they are most relevant for this project. An overview of the satellite instruments whose tropospheric water vapour isotopologue products have been compared to different observational data and models is given in Table 3.

3.4.1 Cross-comparisons between observations

Comparisons between different observational data is an important aspect of data validation. By performing comparisons to data that are calibrated to fiducial references, the fiducial reference can be transferred to other datasets. If no comparison to fiducially referenced data

is possible the intercomparisons can prove the consistency between the different datasets and thus serve as an indicator for the reliability of the different datasets.
The most common approach are comparisons on the basis of coincident measurements that are found by well-defined criteria (e.g. Lossow et al. 2011; Schneider et al. 2016). Another approach is the comparison of latitudinal cross sections for different altitudes and seasons (e.g. Risi et al. 2012a). Dependent on the length of the data set also climatological comparisons can be performed. Differences are generally quantified by calculating the absolute and relative differences between the respective data sets, the absolute and relative bias, the correlation coefficient and the standard deviation. Additionally, comparisons of the {H_2O,δD}-pair

***Table 3** Cross-comparisons of tropospheric water vapour isotopologue data from satellite with other data sets and/or model simulations.*

Sensor for comparison	vs. space-based	vs. ground-based / aircraft	vs. model	References
TES	-	-	NCAR CAM2	Lee et al. 2009
	SCIAMACHY	GNIP	LMDZ	Lee et al. 2012
	-	-	MIROC	Kurita et al. 2009
	-	Picarro/LGR	-	Worden et al. 2011
	-	Picarro (0-4km)	-	Herman et al. 2014
	SCIAMACHY	-	ECHAM	Sutanto et al. 2015
	-	-	GISS ModelE	Field et al. 2012
	-	-	GISS ModelE	Field et al. 2014
SCIAMACHY	-	TCCON, NDACC	-	Sheepmaker et al. 2015
	-	GNIP	IsoGSM	Frankenberg et al. 2009
	-	GNIP	ECHAM5-wiso	Werner et al. 2011
	TES, ACE, MIPAS	NDACC, TCCON	LMDZ, SWING2	Risi et al. 2012
	TES	-	IsoGSM	Yoshimura et al. 2011
	TES	GNIP	LMDZ	Risi et al. 2010a
GOSAT	-	TCCON	-	Boesch et al. 2013
	SCIAMACHY	NDACC	LMDZ	Frankenberg et al. 2013
	TES	GNIP, SNIP	LMDZ, SWING2	Gryazin et al. 2014
	TES	-	LMDZ	Risi et al. 2013
AIRS	TES	-	-	Worden et al. 2019
	-	Picarro (0-6km)	-	Herman et al. 2019
IASI	TES	-	-	Lacour et al. 2018
	TES	NDACC, TCCON	-	Lacour et al. 2015
	-	ISOWAT II (0-7km), Picarro	-	Schneider et al. 2015; Schneider et al. 2016
	-	-	ECHAM5-wiso	Schneider et al. 2017
	-	Picarro, ICOS	ECHAM5-wiso, LMDZiso	Bonne et al. 2015
	-	NDACC	-	Wiegele et al. 2014
	-	GNIP, CARIBIC	ICON-ART-iso	Eckstein et al. 2018
	-	-	LMDZ	Tuinenburg et al. 2015
	-	-	LMDZ	Lacour et al. 2012
	-	-	LMDZ	Pommier et al. 2014
S5p	-	TCCON, NDACC	-	Schneider et al. 2019

distribution are made, because this distribution is closely related to different tropospheric water cycle processes (Noone 2012). When comparing to remote sensing data the different vertical sensitivities of the remote sensing data products have to be considered. This information is provided by the averaging kernels and most comparison studies are made in line with the recommendations as given by Rodgers (2000) and Rodgers and Conners (2003).

Observations with focus on the UTLS and above:
Due to the lack of other observational datasets cross-comparisons between space-based observations are essential for empirically evaluating the quality of stratospheric datasets since balloon or aircraft reference observations especially of water isotopologues are quite rare and their availability is limited in space and time. Stratospheric HDO measurements from Envisat/MIPAS were compared with observations from SMR and ACE-FTS by Lossow et al. (2011). Further comparison of stratospheric HDO, H_2O and δD followed then within the SPARC WAVAS-II project (Högberg et al. 2019).

Observations with focus on the troposphere:
The MUSICA NDACC and MUSICA IASI water vapour isotopologue data (H_2O and δD) have been compared and calibrated with respect to aircraft-based in-situ profiles data measured in July/August 2013 between 0 and 7 km over the subtropical Northern Atlantic in the surroundings of Tenerife Island using the ISOWAT-II instrument (Dyroff et al. 2015; Schneider et al. 2015; 2016). Furthermore, the MUSICA NDACC and MUSICA IASI {H_2O,δD}-pair distribution have shown to identify different water cycle transport pathways in analogy to mountain-based in-situ measurements that are representative for broad vertical layers (Schneider et al. 2016; González et al. 2016). Through these efforts the MUSICA NDACC and MUSICA IASI data are well referenced to fiducial standards.
The reliability of the MUSICA NDACC and MUSICA IASI water isotopologue data has also been demonstrated by their intercomparison at different sites and several years, which revealed a good consistency between both datasets (e.g. Wiegele et al. 2014).
The TES δD data have been compared to aircraft profiles measured in July 2013 between 0 and 4.5 km a.s.l. over the Alaskan interior boreal forest (Herman et al. 2014) using a Picarro in-situ analyzer.
The MUSICA NDACC and TCCON data have been set in context to many other water isotopologue data products (Risi et al. 2012a). Because the MUSICA NDACC dataset offers validated, long-term, highly-resolved, and globally spread vertical water tropospheric isotopologue data, it has also been used outside of MUSICA as validation reference for different satellite measurements (e.g. SCIAMACHY, Scheepmaker et al. 2015; ULB IASI, Lacour et al. 2015; GOSAT, Boesch et al. 2013; TROPOMI S5p, Schneider et al. 2019) and model simulations (e.g. Schneider et al. 2010; Risi et al. 2012a). In some of these studies additional comparisons to TCCON data have been performed. Comparisons between MUSICA NDACC and TCCON are reported in Schneider et al. (2019).
Pure space-based cross comparisons for tropospheric isotopologue data sets were performed by Worden et al. (2019), comparing TES with AIRS, and Lacour et al. (2018), comparing TES with IASI.

3.4.2 Cross-comparisons between remote sensing observations and models

Isotope-enable models are capable of linking different water cycle processes with isotopologue signals and therefore are essential for a scientifically robust interpretation of isotopologue observations. At the same time comparisons between isotopologue model data and reliable observational data are important for improving and evaluating the model simulations by facilitating the detection of model biases and shortcomings (e.g. Risi et al. 2012b, Steen-Larsen et al. 2013) and the tuning of dynamical and physical parameter (Mauritsen et al. 2012, Hourdin et al. 2013).

Models have been extensively compared to in-situ measurements from e.g. GNIP stations, field campaigns and aircraft data (e.g. Jouzel et al. 1987, Hoffman et al. 1998, Schmidt et al. 2005, Lee et al. 2007, Yoshimura et al. 2008, Risi et al. 2012a, Pfahl et al. 2012, Gryazin et al. 2014, Steen-Larsen et al. 2016, Eckstein et al. 2018). During the last decade models have also been increasingly compared to remote sensing products obtained from ground-based FTIR stations within TCCON and NDACC (e.g. Schneider et al. 2010, Risi et al. 2012a, Christner et al. 2018) as well as from space-borne sensors (e.g. Risi et al. 2010a, Werner et al. 2011, Yoshimura et al. 2011, Schneider et al. 2017, Eckstein et al. 2018).

We will focus on studies using space-based remote sensing observations of tropospheric isotopologues. In this context it is important to state that measurements of tropospheric δD or {H_2O,δD}-pairs from space are feasible; however, measurements of d-excess or not feasible (d-excess has been identified as a very useful tracer for moisture transport pathways). In the following, we firstly, introduce the basic techniques for considering the different vertical sensitivities of the remote sensing products for the comparison with the models, secondly, discuss comparisons against vertically resolved satellite products and thirdly, we describe comparisons against total column-averaged satellite products.

Model adjustments according to the remote sensing data characteristics:
The averaging kernel matrix (*A*) describes how variabilities of the atmospheric state (x) propagate into the remote sensing retrieval product (state vector x_{ret}). The relation between the real atmosphere and the observed atmosphere (i.e. the retrieval output) is in a first approximation given by (e.g. Rodgers 2000):

$$x_{ret} = \boldsymbol{A} * (x - x_a) + x_a,$$

where x_a is the assumed a priori state. For reliable cross-comparisons these characteristic of the remote sensing data product has to be considered. For model comparisons this is generally ensured by applying the equation above to the model data (i.e. substitute *x* by x_{model}). However, for highly variable trace gases like water vapour the averaging the kernel matrix is also often variable (at least for products retrieved from thermal nadir spectra) and *A* depends, for instance, on the atmospheric water vapour and temperature profiles. Therefore, it is recommendable to consider averaging kernels that are specific for every single observation event. A further problem is that the modeled atmospheric state (e.g. temperature and humidity profiles) does generally not perfectly match with the real atmospheric state (the state that is observed the remote sensing instrument). For this reason, the averaging kernels obtained from the remote sensing retrieval can generally not be used for the model atmosphere. Instead, the kernels need to be specifically determined for the meteorological conditions as present in the model (e.g. discussion in Schneider et al. 2017). Figure 3 demonstrates the importance of considering the remote sensing data characteristics (i.e. applying the averaging kernels) for model comparisons. Shown are contour lines for normalized probability distributions of {H_2O,δD}-pairs. The left panel depicts the distributions obtained from the model ECHAM5-wiso. The middle panel depicts the same, but after applying the averaging kernels. The difference between the left and the middle panel is very significant, demonstrating that a comparison to the observed distribution (right panel) only makes sense, if the averaging model data are accordingly adjusted.

Comparisons against vertically resolved products:
First model comparisons with the sensor TES were performed by creating monthly mean maps for the TES averaging kernels and applying them to model data after collocating the modeled atmosphere with the actual meteorology from the observations (Risi et al. 2010a, Risi et al. 2012a). Yoshimura et al. (2011) applied a very similar technique for IsoGSM results, but instead of monthly mean values they used the actual TES kernels.
Schneider et al. (2016) presented an a posteriori processing for combined {H_2O,δD}-pair products to allow for simultaneous investigations of H_2O and δD. This method reduces the complexity and effects of the kernels and thus enables reasonable comparisons of {H_2O,δD}-pair distributions even without applying the averaging kernels to the model output.
A first attempt to explicitly using kernels in line with the modeled atmosphere is realized in Field et al. (2012), where they created statistical relationships between remote sensing characteristics of TES and some selected categorical parameters. Based on these relations the averaging kernels can then be predicted for a limited amount of combinations of surface and atmospheric conditions.
A further approach for simulating the averaging kernels is presented in Schneider et al. (2017). They introduce a forward operator for simulating the averaging kernels for a modeled atmosphere based on physical principles of radiative transfer. It is designed according the IASI retrieval characteristics from Schneider et al. (2016) and provides simulated kernels with uncertainties laying within the uncertainty of the a posteriori processed MUSICA IASI {H_2O,δD}-pair product. The model adjustment as discussed in the context of Figure 3 has been made using this approach.

Comparisons against vertical integrated total column products:
For total column products of H_2O and HDO that are based on SCIAMACHY retrievals the full averaging kernels are not provided, as they do not vary in space and time. However, the potential occurrences of differences in the sensitivities of H_2O and δD and non-vanishing cross-dependencies between H_2O and δD might be additional uncertainty factors for the interpretation of the comparisons to model data (Yoshimura et al. 2011, Sutanto et al. 2015). As the according kernels for GOSAT total column products are provided, Risi et al. (2013) and Gryazin et al. (2014) used a method similar to TES comparisons (e.g. Risi et al. 2012a) for collocating and applying the averaging kernels from GOSAT retrievals to model data.

Scientific outcome from cross-comparisons between model and space-borne observations:
Risi et al. (2012b) suggested that middle/upper tropospheric δD if provided together with H_2O can be very useful for diagnosing the pathways that determine upper tropospheric humidity. Field et al. (2014) showed that middle/upper tropospheric δD is very sensitive to model parameters that affect the vertical moisture transport in the model. These outcomes are in line with Schneider et al. (2017) where the differences between modelled and observed free

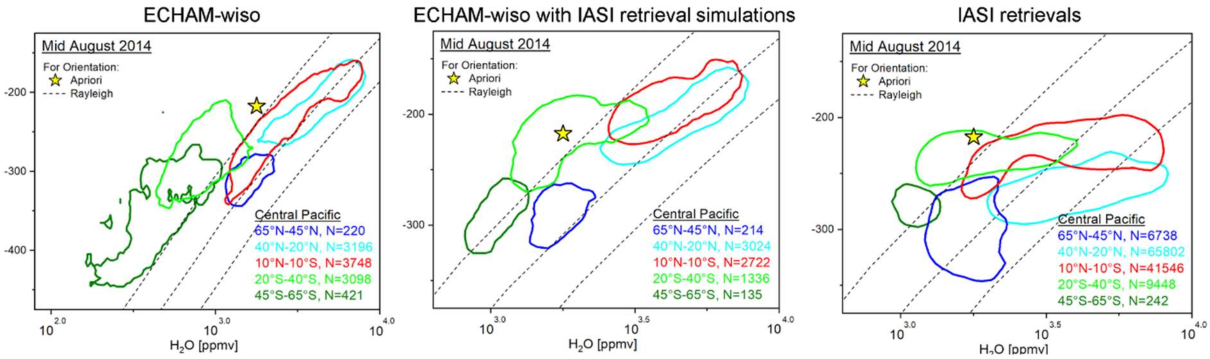

Figure 3 *{H2O,dD} - pair distributions obtained from ECHAM5-wiso simulations as original model output sampled for IASI overpasses at 5 km (left), as processed according to the IASI sensitivities (middle) and from IASI retrievals (right). The coloured contour lines mark the areas that contain 66% of all {H2O,δD} - pairs. The black dashed lines represent Rayleigh curves corresponding to different initialisation conditions and atmospheres (Figure adapted from Schneider et al., 2017).*

tropospheric {H_2O,δD}-pair distribution could be explained by an excess of vertical mixing in the model.

The theoretical study of Yoshimura et al. (2014) suggests that free tropospheric δD allows conclusions on horizontal transport. This is also confirmed by Schneider et al. (2015,2016) where a distinct {H_2O,δD}-pair distributions can be clearly observed over the subtropical Atlantic for air masses that have been advected from the African continent.

The possibilities of using space-based tropospheric water vapour isotopologue data in combination with models for moisture pathway studies is a state-of-the-art research topic and addressed, for instance, within the current projects MOTIV and TEDDY.

4 Associated Datasets

This project S5p+I H2O-ISO will work with S5p measurements made between July 2018 and June 2019. For the observations over land a total column averaged water vapour isotopologue retrieval will be developed and validated. For this development and validation reference datasets with the following characteristics are needed: (1) the reference data should cover the period between July 2018 and June 2019, (2) they should be representative for different climate zones over land, (3) they should be sensitive to water throughout the troposphere, and (4) they should be traceable to fiducial references. There is no single dataset that fulfils all these requirements. Nevertheless, the requirements can be achieved by an integrated usage of the different datasets as listed in Table 4. Each of the dataset fulfils one or several of the requirements. Figure 4 gives an overview on the vertical representativeness of the different datasets.

4.1 MUSICA NDACC

NDACC FTIR spectra have been recorded during the July 2018 - June 2019 period on cloud-free days at about 20 globally distributed NDACC stations. The spectra measured at three stations will be processed with the MUSICA NDACC processor. This will generate a water isotopologue product ({H_2O,δD} pairs) sensitive to tropospheric water vapour (it is even possible to distinguish low tropospheric amounts from middle free tropospheric amounts, DOFS is between 1.5 and 2) and referenced to fiducial standards (the MUSICA NDACC data are calibrated to aircraft measurements). We select the three stations where the spectra measurements are coordinated at KIT, which ensures a time efficient data processing. These stations are representative for different climate zones: the subtropical station at Tenerife Island (close to the west coast of Northern Africa, i.e. close to the Sahara desert), the mid-latitudinal station at Karlsruhe (Central Europe), and the arctic station in Kiruna (Northern Scandinavia). The MUSICA NDACC data will be the reference for validating the S5p tropospheric column-averaged data δD product. Furthermore, the profile information of the MUSICA NDACC data could be very useful for the future development and validation of a combined product (S5p+IASI combined product, see Section 2.2.2).

4.2 TCCON

TCCON spectra have been recorded during the July 2018 - June 2019 period on cloud-free days at about 25 globally distributed stations. The measured spectra are processed by the different principle investigators with a common software tool and the TCCON retrieval products are made available at the TCCON database website within 12 months after the measurements. The TCCON H_2O and HDO products are sensitive to the total column averaged mixing ratios, i.e. they are well representative for tropospheric column averaged mixing ratios. The TCCON H_2O product is calibrated to fiducial standard, but the TCCON HDO product is not calibrated. The TCCON δD values are calculated a posteriori from the retrieved H_2O and HDO data. In order to achieve some calibration of the TCCON δD data we will perform comparisons between TCCON and MUSICA NDACC data at Tenerife and Karlsruhe (where NDACC and TCCON use the same FTIR instrument) as well as in Northern Scandinavia (where NDACC and TCCON spectra are measured at two nearby stations Kiruna and Sodankylä, respectively).

Similar to Schneider et al. (2019), we will determine a TCCON calibration factor with respect to MUSICA NDACC, in order to transfer the fiducial reference to the TCCON data. TCCON data will be used as reference for tropospheric column-averaged δD values for the development and validation for the tropics and the southern hemisphere. For this reason, we

***Table 4** Observational isotopologue data to be used for the development and validation.*

Observational Dataset	Temporal Coverage	Horizontal Resolution/Coverage	Vertical Resolution/Coverage
MUSICA NDACC: {H_2O,δD} pairs	July 2018 – June 2019	- Point measurement - Three sites: Kiruna: 420m a.s.l.; 67.9°N; 20.4°E Karlsruhe: 110m a.s.l.; 49.1°N; 8.4°E Tenerife: 2370m a.s.l.; 28.3°N; 16.5°W	- sensitivity between surface and tropopause - Weak profiling capability (DOFS: 1.5-2)
TCCON: column averaged mixing ratios of H_2O and HDO	July 2018 – June 2019	- Point measurement - Six sites: Sodankylä: 190m a.s.l.; 67.4°N; 26.6°E Karlsruhe: 110m a.s.l.; 49.1°N; 8.4°E Tenerife: 2370m a.s.l.; 28.3°N; 16.5°W Bourgos: 40m a.s.l.; 18.5°N; 120.7°E Darwin: 30m a.s.l.; 12.4°S; 130.9°E Wollongong: 30m a.s.l.; 34.4°S; 150.9°E	- sensitivity between surface and tropopause - Vertically integrated data (DOFS=1)
GOSAT: column averaged mixing ratios of H_2O and HDO	July 2018 – June 2019	- individual pixels separated by about 250 km with ground pixels with a diameter of approx. 10.5 km - global cover over land and sunglint over the oceans within ± 40 of the sub-solar latitude	- sensitivity between surface and tropopause - Vertically integrated data (DOFS=1)
MUSICA IASI {H_2O,δD} pairs	July 2018 – June 2019	- 12km diameter of nadir pixels - quasi global	- sensitivity between 800 and 350 hPa (2 to 7km a.s.l.) - Weak profiling capability (DOFS: 1-2)
LEMON aircraft profiles: {H_2O,δD} pairs	June 2019	Limited area in the French Alps near Annecy (45.7-45.9N,6.1-6.2E)	- Vertical resolution: 50-150m - 0 to 3200 m a.s.l.
IGP aircraft profiles: {H_2O,δD} pairs	March 2018	Iceland-Greenland seas and western Iceland (65.7-70.7N, 16.8-21.0W)	- Vertical resolution: 150-300m - 0 to 3500 m a.s.l.

will use TCCON data from the two tropical stations Bourgos on the Phillipines and Darwin in Northern Australia as well as from Wollongong (south-east Australia).
Similar to Schneider et al. (2019), we will determine a TCCON calibration factor with respect to MUSICA NDACC, in order to transfer the fiducial reference to the TCCON data. TCCON data will be used as reference for tropospheric column-averaged δD values for the development and validation for the tropics and the southern hemisphere. For this reason we will use TCCON data from the two tropical stations Bourgos on the Phillipines and Darwin in Northern Australia as well as from Wollongong (south-east Australia).

4.3 GOSAT

For the July 2018 - June 2019 period total column averaged mixing ratios of H_2O and HDO will be retrieved from GOSAT measurements using the algorithm as presented by Boesch et al. (2013). The δD values are calculated a posteriori from the retrieved H_2O and HDO data. These GOSAT δD data have already been referenced to the MUSICA NDACC data (Boesch et al. 2013). In general the GOSAT data are expected to have vertical representativeness similar to S5p (i.e. for the tropospheric column), but with a coarser horizontal resolution. The GOSAT data will be useful for documenting the consistency of the S5p column-averaged δD data product on a global scale.

4.4 MUSICA IASI

For the July 2018 - June 2019 period IASI spectra are available from IASI-A and IASI-B (aboard Metop-A and -B, respectively). The spectra for cloud free scenes will be processed with the MUSICA IASI processing algorithm. This will generate a water vapour isotopologue product

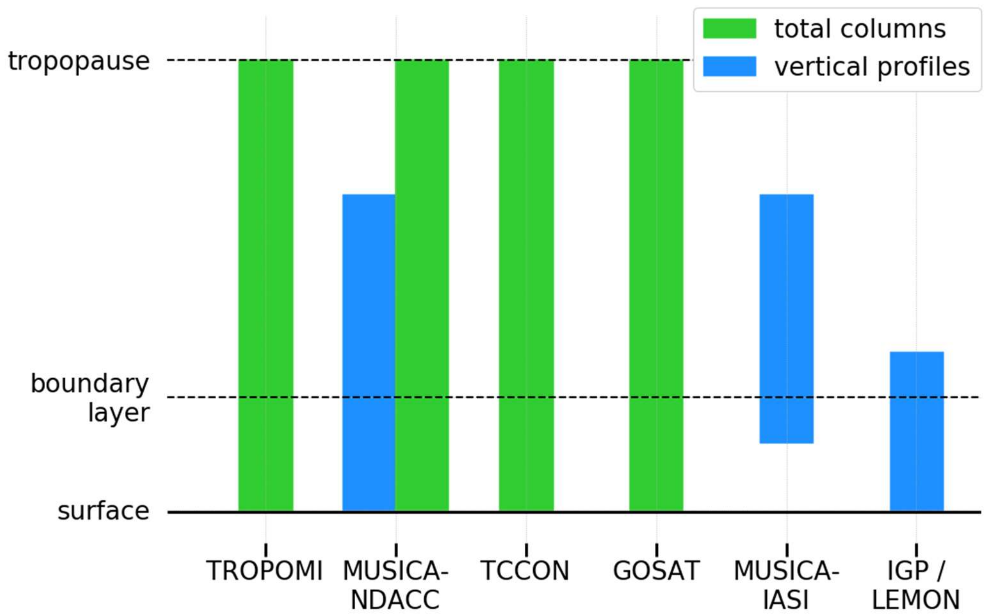

***Figure 4** Vertical representativeness of TROPOMI data and of the associated data. Green colour means column integrated data and blue means data containing some information about the vertical distribution. Note: generally, more than 50% of the water vapour total column is allocated in the boundary layer.*

({H_2O,δD} pairs) that is referenced to fiducial standards (the MUSICA IASI data are calibrated to aircraft measurements) and representative for the middle free troposphere with some profile information at lower latitudes (DOFS up to 2.0). The weak sensitivity with respect to boundary layer water vapour (where most of the tropospheric water vapour resides), significantly compromises the usage of MUSICA IASI data as reference for the S5p tropospheric column averaged δD data product.

As outlined in Section 2.2, a vertically resolved tropospheric water vapour isotopologue product with good horizontal coverage and resolution will be of great benefit for the research community and in this context the MUSICA IASI data are decisive. A tropospheric water vapour isotopologue profile product can be developed by combining the information about tropospheric columns (obtained from S5p) with the information about the free troposphere (obtained from IASI). Within this project we will briefly discuss the formalism for generating such S5p+IASI combined product.

4.5 LEMON and IGP aircraft profiles

During the period July 2018 - June 2019 the aircraft campaign of the project LEMON took place and measured water vapour isotopologue profiles ({H_2O,δD} pairs). The calibration of the in-situ instruments with respect to well known isotopologue standards ensures the fiducial reference of these data. However, these aircraft data are limited to the lowermost 3200 m above surface, to 10 days in June 2019, and to a limited area in the French Alps, which reduces its comparability to the total column abundances measured by S5p and for validations during different seasons and for different climate zones. Nevertheless, the LEMON profile data will be very useful for the future development and evaluation of a S5p+IASI combined product.
Water vapour isotopologue profiles have also been measured in-situ from aircraft during the IGP campaign in March 2018 over Iceland and the Iceland-Greenland Sea (Renfrew et al. 2019). The data have a similar characteristic as the LEMON data (referenced to fiducial standards, but with a wider horizontal and vertical coverage than the LEMON data). They cannot be used for S5p validation activities because S5p Level-1 data availability starts in June/July 2018. Nevertheless, these profile observations can make contributions to the impact study by investigating how much of the vertical structure detected from the aircraft can be seen in a typical S5p data product.

5 Test Areas

This project S5p+I H2O-ISO shall prove the validity of the S5p water vapour isotopologue data for different global climate zones and assess the impact of the new data in the context of currently ongoing activities (see review in Section 2). This goal can be achieved by a focus on the four test areas as depicted in Figure 5: (1) Central Europe, (2) West Africa, (3) Iceland/Scandinavia, and (4) the Western Pacific Tropics and the Southern Hemisphere.

5.1 Central Europe

This area is well-suited due to the availability of most of the associated datasets from Table 4: MUSICA NDACC, TCCON, GOSAT, MUSICA IASI, and LEMON in-situ profiles. This will allow a comprehensive comparison in the context of the development and validation activities of the S5p product (the column-averaged δD) as well as of the future development and evaluation of a S5p+IASI combined product.
Furthermore, this area is also considered in the MOTIV project (see Section 2.1.2). For MOTIV COSMO-iso and ICON-ART-Iso water vapour isotopologue model sensitivity test studies are performed for the year 2016. Using these model calculations together with the characteristic sensitivity of the S5p product and of a future S5p+IASI combined product will allow impact studies for central Europe.

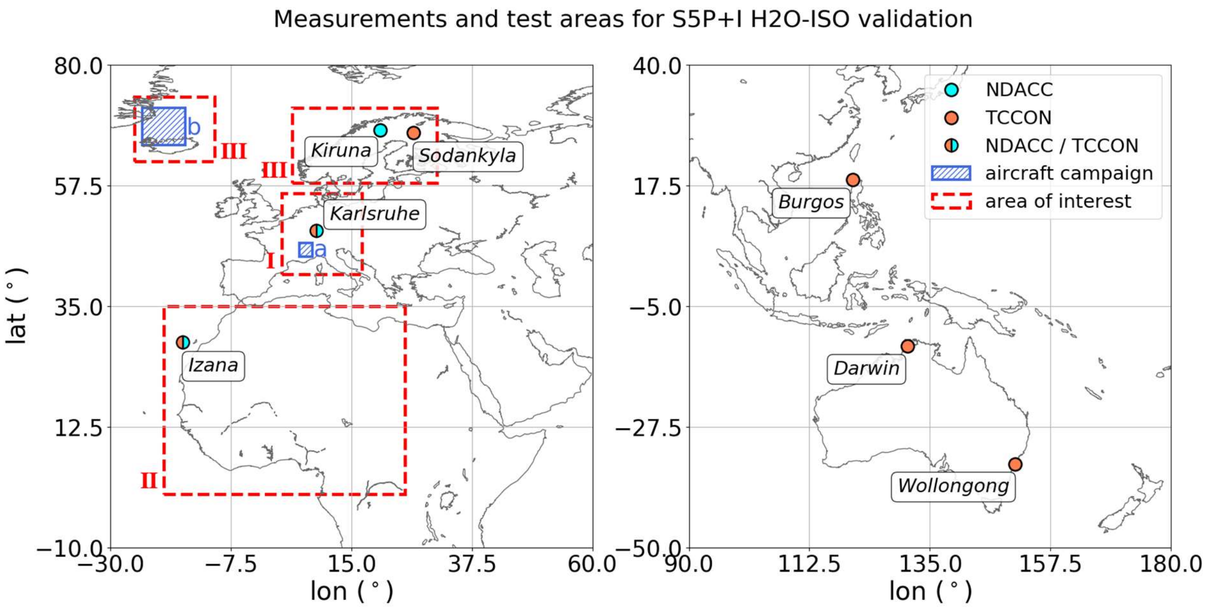

Figure 5 *Collection of the test areas and observations defined for the TROPOMI validation and impact assessment. The cyan and orange dots indicate the chosen NDACC and TCCON stations, respectively. The regions over Central Europe (red, I), West Africa (red, II) and Iceland/Scandinavia (red, III) serve as areas of interest and will be provided with model data. Additionally, the observations from the aircraft campaigns LEMON (blue, a) and IGP (blue, b) might be useful for validation.*

5.2 West Africa

For this area the associated datasets of MUSICA NDACC, GOSAT and MUSICA IASI will be available for the whole July 2018 - June 2019 period. In this area the GOSAT data will be the most important dataset for validating tropospheric column averaged data. The MUSICA NDACC data are from the high altitude station (2370 m a.s.l.) on Tenerife Island and are thus not representative for the whole troposphere and not fully collocated to the S5p observations over the African continent. Nevertheless, the high altitude MUSICA NDACC data will be useful in the future for proving the validity of an upcoming S5p+IASI combined product.
This area is also considered in the MOTIV project (see Section 2.1.2), i.e. COSMO-iso and ICON-ART-Iso simulations will be available for the year 2016, which can be used for impact studies over West Africa. This area is also of interest for the project TEDDY (see Section 2.1.2), because the heating rates within the Hadley cell are one focus of TEDDY. In this context the S5p product could be additionally considered within TEDDY's assimilation experiments in order to investigate if the S5p data have an impact on the diabatic heating rates over West Africa (in particularly interesting would be to investigate whether they put additional constraints if used together with MUSICA IASI data).
The interplay of lower tropospheric uplifting (diurnal extension of the boundary layer) and upper tropospheric downwelling (Hadley Cell) over northern West Africa causes strong vertical gradients in the isotopologue ratios. A comparison of the gradients as typically simulated in 2016 and the gradients as observed in a combined product offers promising possibilities for the development and evaluation of an S5p+IASI combined product.

5.3 Iceland/Scandinavia

For this area associated datasets of MUSICA NDACC, TCCON, GOSAT, and MUSICA IASI will be available for large parts of the July 2018 - June 2019 period. MUSICA NDACC and the TCCON data will not be available during polar night and very high quality data can only be produced from spectra measured with a solar elevation above about 20° (Schneider et al. 2016), which limits the data availability at high latitudes typically to between March and September. MUSICA IASI data have typically also weak sensitivities for a dry and cold troposphere, i.e. high quality MUSICA IASI data are also very rare for a high latitudinal winter atmosphere. For GOSAT and S5p there will be limitations due to low SNR caused by either low solar zenith angles or snow cover for high latitudinal winter. Data could potentially be available from March to September; however, for high-latitude spring and winter season retrievals would be considered experimental due to lower precision. For these reasons the comparisons needed for the development and validation activities have to focus on the summer season. For parts of that area, IGP in-situ profiles are available for March 2018, but unfortunately no S5p Level-1 data is available.
The area coincides with parts of the research area of the project ISLAS (see Section 2.1.2). The work with sophisticated model tools for identifying the isotopologue signals from small-scale processes is expected to provide opportunities to document the impact of the new S5p product, in particular the impact of the data that allow a discrimination of boundary layer and free troposphere (as in a future S5p+IASI combined product), and regarding the spatial representativeness of in-situ measurements with limited spatial coverage.

5.4 Western Pacific tropics and the southern hemisphere

For this area associated datasets of TCCON, GOSAT, and MUSICA IASI will be available. This area is important for documenting the validity of the S5p column-averaged for the tropics and the southern hemisphere. A successful usage of the TCCON data for this validation activity requires a correct referencing of the TCCON data to the MUSICA NDACC data at the stations where NDACC and TCCON measurements are made in parallel (see Section 4.2)
The Pacific Tropics are of great interest for the TEDDY project (see Section 2.1.2) using the S5p product in addition to the MUSICA IASI data within TEDDY's assimilation experiments would help to assess the additional impact of S5p for analysing the heating rates in the context of the Walker circulation.

6 Risk Analysis

In this section we draw up a consolidated risk analysis discussing components of the project that have risk potential for the project outcome.

6.1 S5p water vapour isotopologue retrieval development and operation

The UoL retrieval algorithm is extensively used to retrieve a range of trace gases from different space-based spectrometers. The retrieval software is robust and mature and has been used to retrieved HDO from GOSAT (Boesch et al. 2013) and has already been applied to S5p L1b data (Figure 6). Furthermore, the usefulness of S5p data for retrievals of HDO has been shown by Schneider et al. (2019). Therefore, we consider algorithmic risks to be small. The most significant risk to the retrieval performance is the performance of the S5p instrument itself and risk of potential instrumental artefacts. For example, a stripping pattern has been identified in CO S5p retrievals (Borsdorff et al. 2019), but potential solutions have already been presented and applied by Borsdorff et al. (2019).

6.2 Associated datasets

NDACC FTIR spectra have been continuously measured and the MUSICA NDACC water isotopologue retrievals have been performed very successfully in the past. There is very low risk in producing the MUSICA NDACC dataset for the July 2018 – June 2019 period and for the three stations Kiruna, Karlsruhe, and Izana.
TCCON spectra have been continuously measured and the TCCON standard products become routinely available typically 12 months after measurement. So there is very low risk in

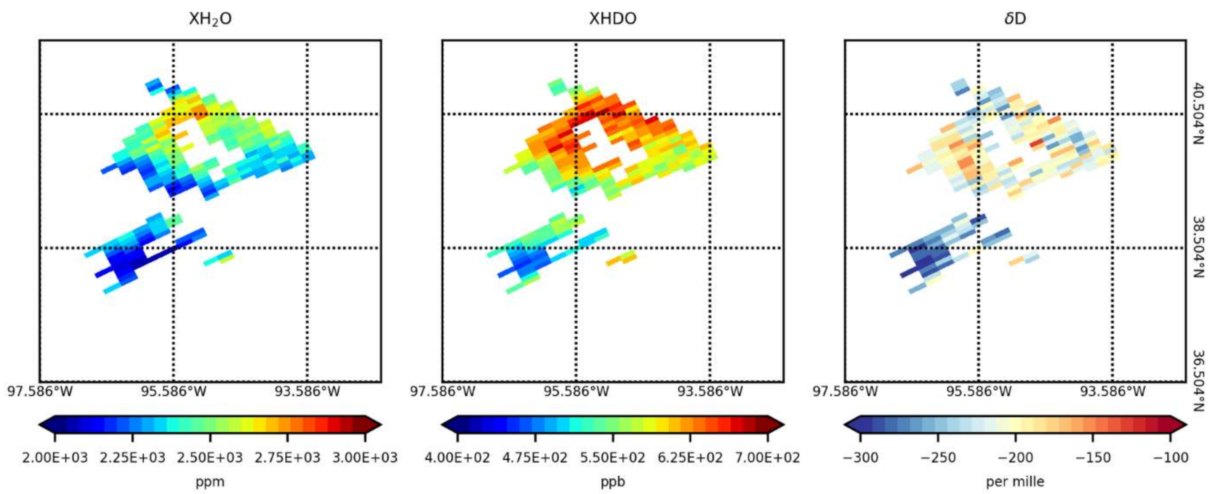

Figure 6 *XH_2O and XHDO columns retrieved from S5p with University of Leicester Full Physics (UoL-FP) algorithm for an overpass over Lamont on 4th May 2018. The left and centre panel show the XH_2O and XHDO retrievals respectively, while the right panel shows the inferred values for δD.*

having TCCON data for the July 2018 – June 2019 period. However, there is some risk concerning the reliable transfer of fiducial references to the TCCON data.
The UoL retrieval is setup to generate GOSAT HDO/H2O and has been used to generate HDO/H_2O from GOSAT for 2009 and 2010 globally. This same retrieval will be used to generate GOSAT HDO/H_2O data for July 2018 – June 2019 time period for this project. There is very low risk in the availability of this datasets, especially considering our expertise in generating global long-term CO_2 and CH_4 datasets from GOSAT for the Copernicus Climate Change Service C3S and the availability of the GOSAT level-1 data.
Currently there are three IASI instruments aboard three different satellites in orbit and all three are measuring continuously. The MUSICA IASI retrieval is continuously applied within several international research projects and there is very low risk in producing the MUSICA IASI dataset on a global scale for the June 2018 – July 2019 time period.
Two aircraft campaigns in Iceland (March 2018) and Southern France (June 2019) have successfully measured vertically highly resolved water vapour isotopologue profiles in the first three kilometres above ground. These data are already available, i.e. there is no risk.

6.3 Model simulations

Partners at the ETH Zurich perform COSMO-iso simulations for the year 2013 and 2016 in context of the project MOTIV for test area 1 and 2 (see Section 5.1 and 5.2, respectively). Different simulation runs have already been made and the data are available for this project. There is some risk that the MOTIV specific model sensitivity test runs are not optimal for the purposes of this S5p project.
COSMO-iso is also operated at the computational infrastructures of UoB. Simulations for Iceland and the surrounding areas of the North Atlantic (test area 3, see Section 5.3) are available for the period of the IGP campaign (March 2018). There is some risk of these IGP specific model simulations are not optimal for the purposes of this S5p project.
The proposed global ICON-ART-Iso simulations for covering the test areas 1 and 2 (see Section 5.1 and 5.2, respectively) will be performed on the high-performance facilities of KIT, where the model has been developed and successfully tested. However, it is a recently developed model, still including some minor issues. Eckstein et al. (2018) show comparisons against stationary GNIP data revealing a too large variability in the delta excess of model precipitation that is supposed to emerge from the simulation of $H_2{}^{18}O$. Ongoing studies were already able to reduce this effect, still there might be a small risk concerning the precision of the modeled isotopic information.

6.4 Dependence on international research projects

The COSMO-iso simulations of the project MOTIV are made for 2013 and 2016 for the test areas 1 and 2 (see Section 5.1 and 5.2, respectively). It may be brought in discussion with the project partners whether further simulations can be performed for the time period 2018/2019. As this is an extension for MOTIV in the sense of the proposed work and targets, the carrying out of these additional simulations bears certain risks.
The realization of further simulations for the Scandinavian component of test area 3 (see Section 5.3), covering the NDACC and TCCON stations will also be useful for the impact assessment. The exact time and location of the simulation domain will depend on the

requirements of the ISLAS project during the next two years but will be harmonized with S5p requirements.

Another optional and promising application of the S5p data is provided by the project TEDDY (see Section 2.1.2). Depending on the development progress of the S5p product (e.g. its generation on a global scale and for longer time periods) the products can be used for data assimilation using the model IsoGSM. However, there is important risk concerning the progress of the relevant TEDDY work packages until the second half of the S5p+I H2O-ISO project period.

This S5p+I H2O-ISO project would clearly benefit from extensions of work packages addressed within different international research projects. However, not realizing these additional activities within these research projects will not significantly affect the overall outcome of the S5p+I H2O-ISO project.

7 Scientific and Operational Requirements

The aim of this project is the development and validation of a new S5p water vapour isotopologue product with simultaneous consideration of the needs of the scientific community and of the potential future application within operational processing chains. For achieving this aim a successful elaboration of the following scientific and operational issues is required.

7.1 Scientific requirements

7.1.1 Software development

A software generating a H_2O/HDO column-averaged dataset from the S5p TROPOMI spectra has to be developed. It should be fully traceable what kind of constraints are applied in the retrieval process. The software should generate the retrieved atmospheric state vector as well as the auxiliary data needed for a comprehensive characterisation of the product: the used a priori, the averaging kernel, the a posteriori uncertainty matrix, and the uncertainty covariance matrices for the dominating error sources.

7.1.2 Theoretical characterisation and uncertainty assessment

The product should be well characterised by providing the following data for each individual observation (see also Section 7.1.1): the retrieved state vector, the used a priori state vector, the averaging kernel, the a priori uncertainty matrix, the a posteriori uncertainty matrix, and the uncertainty covariance matrices for the dominating uncertainty sources. For this purpose the leading uncertainties should be assessed in line with Rodgers (2000) and the TUNER (Towards Unified Error Reporting, https://www.imk-asf.kit.edu/Projekte_2689.php) recommendations.
The characterisation of remote sensing ratio products needs special care. Firstly, for demonstrating the feasibility of deriving a scientifically valuable ratio product HDO/H_2O (or δD). It will be important to document that the ratio product is not significantly affected by differences in the H_2O and HDO averaging kernels. This can be done by using the method as developed during MUSICA (Schneider et al. 2016). Secondly, it should be traceable how the uncertainties in H_2O and HDO propagate into the HDO/H_2O ratio product (e.g. using the method as proposed by Schneider et al. 2012, for a full consideration of correlated errors).
From our experiences with using water vapour isotopologue data for scientific applications (e.g. within the projects MUSICA, MOTIV, and TEDDY), we conclude that the S5p column integrated HDO/H_2O (or δD) product should have a systematic and random uncertainty of less than 50‰. This is the threshold for being able to identify different water cycle processes (see for instance figures in Noone, 2012). Our target will be an uncertainty of 10-20‰, which is be similar to the uncertainty of the MUSICA IASI and MUSICA NDACC δD remote sensing products and has shown to be sufficient for investigating a variety of atmospheric water cycle processes. We estimate the uncertainty needed for a very detailed detection of fluxes between the surface and the atmosphere to be below 5‰, whereby at the same time a horizontal resolution of a few hundred meters would be required. However, it is rather unrealistic to achieve such low uncertainty levels together with the required high horizontal resolution from space-based remote sensing techniques.

7.1.3 Calibration with respect to fiducial standards

The products have to be compared to fiducial standards HDO/H_2O (by using the associated datasets and test areas as described in Sections 4 and 5). If possible, biases should be explained and for the choice of the used spectroscopic database these comparisons should be taken into account. The final objective should be HDO/H_2O data that are calibrated to the fiducial references.

7.1.4 Impact documentation

The scientific impact of the S5p product should be documented in the context of ongoing scientific projects. A focus on the projects coordinated by UoB and KIT (ISLAS, MOTIV, TEDDY) and on the test areas as described in Section 5 will best ensure successful impact studies and is thus strongly recommended.
ISLAS: S5p offers a much better temporal and horizontal coverage than GOSAT and it should be documented to what extent diurnal cycle signals or small-scale horizontal variances can be detected in the S5p data but not in the GOSAT data. An improved detection of these signals and variances would positively impact on the science questions addressed by ISLAS.
MOTIV: The S5p tropospheric column-averaged product is affected by isotopologue signals of the boundary layer. It should be investigated if these signals are sufficiently strong for being detected. Their detection would offer possibilities for investigating boundary layer processes (e.g. continental recycling or transport from the boundary layer to the free troposphere) and thus have an important impact in the science questions addressed by MOTIV.
TEDDY: The S5p HDO/H_2O product (available over land only) has a different sensitivity as the IASI HDO/H_2O product. Using the S5p data in addition to the MUSICA IASI data within TEDDY's assimilation experiments could demonstrate the added value of the S5p data.

7.1.5 Support for upcoming developments

For addressing scientific questions in the field of the tropospheric water cycle the HDO/H_2O ratio (or δD) are particularly promising if provided together with high quality H_2O data (e.g. Noone, 2012). In this context an S5p {H_2O,δD}-pair product would be highly desirable. This is something that goes beyond this S5p+I H2O-ISO project; however, it should be kept in mind for all the activities of this project and a roadmap towards such S5p {H_2O,δD}-pair product should be elaborated.
Very promising for scientific applications would be a boundary layer isotopologue product that is independent from isotopologue composition of the free troposphere (see Section 2.1.2). By an a posteriori combination of the MUSICA IASI retrieval output and the S5p retrieval output such product could be generated (see theory as described in Rodgers, 2000, and Rodgers and Connor, 2003). Again, this is something that is beyond this S5p+I H2O-ISO project. Nevertheless, it must be considered in the context of a roadmap with the purpose of supporting the development and validation of a future S5p+IASI combined product.

7.2 Operational requirements

7.2.1 HDO/H_2O column-averaged data

An outline of an operational scheme for the production of water isotopologues in near real time is given below (Figure 7). A requirement for such a scheme the provision of calibrated L1B datasets, meteorological data sampled for S5p soundings, and the availability of cloud mask or flags in near real time. The processing scheme itself will need to be sufficiently fast to allow near real time data processing. The scheme needs to produce well documented and characterised datasets in netCDF CF compliant data format. A validation module is needed to ensure the data fidelity before it is made available to end users and data archiving. Monitoring of the data quality against ground-based validation data will be required for the whole processing cycle.

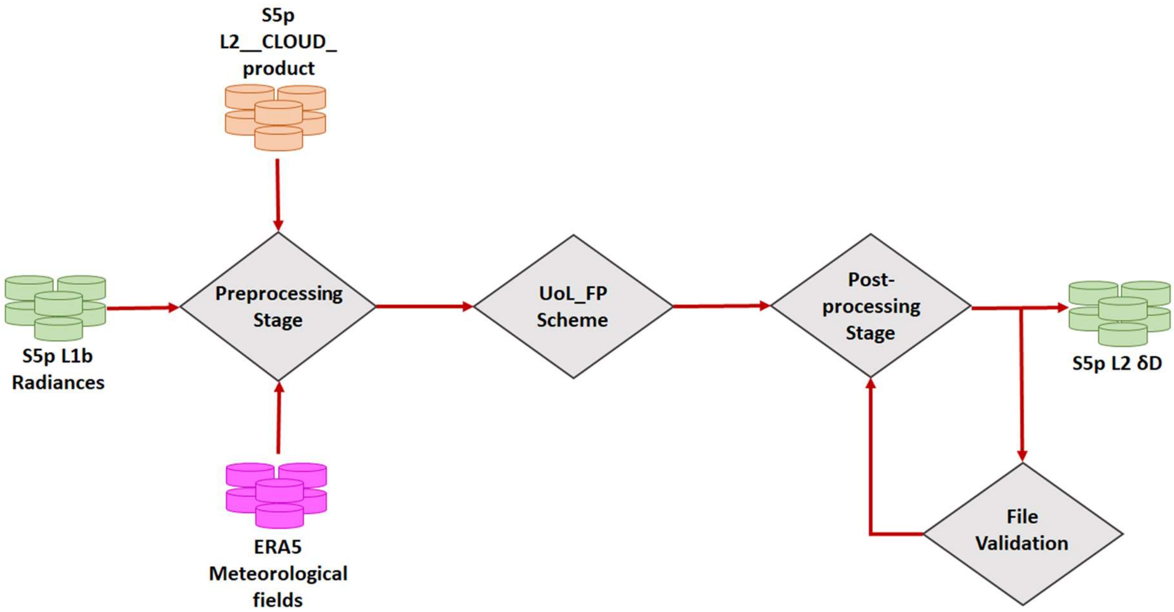

Figure 7 *Outline of an operational S5p processing scheme.*

7.2.2 Data volume and processing time

Spectral radiances from the TROMPOMI instrument on-board S5p represent a real step change in volume relative to its predecessors (SCIAMACHY, GOME/GOME-2, GOSAT, OCO-2 and OMI). For the SWIR bands, a single orbit L1b file contains on average over 670,000 ground pixels.Based on the current set-up of the UoL-FP processor (optimised for GOSAT), if all these were to be clear-sky and observed over land 116 CPU days are required. However, with these spread across 200 nodes processing would take around 14 hours. The key caveat to note here is that this is based on a full physics setup where the XH_2O and XHDO are retrieved separately. For operational requirements this becomes impractical, therefore, we will use of a faster scaler retrieval similar to implementation used by Boesch et al. 2013 for GOSAT.

This implementation (especially when scattering is turned off) will reduce the CPU time needed from 121 days to (potentially) under 24 hours. The performance increase in the retrieval would allow for near-real time (NRT) applications to be considered.

For this project, we will focus on retrievals for the period between July 2018 and June 2019 and on the areas of interest (I-III from Fig. 5, left panel). Estimates take into account the removal of ocean and cloud covered pixels. The expected monthly volume of S5p pixels within the West Africa region of interest would take approximately 65 CPU days, which would account to 8-16 CPU hours when spread across a HPC system (based on access to 100-200 nodes). An overview of the monthly data volume for all the different regions of interest is given in Table 5.

Table 5 *Data volume estimates per month for the different areas of interest (AOI).*

AOI	L1b data volume (Gb)	Original number of S5P pixels (N)	Fraction removed ocean pixels (P)	Fraction of pixels removed due to Cloud (C)	Final estimate for number of S5p pixels N*(1-P)*(1-C)
Europe (I)	107	892,934	0.23	0.4	412,535
West Africa (II)	135	6,152,320	0.24	0.4	2,805,457
Iceland (IIIa)	348	1,267,313	0.75	0.4	190,096
Scandinavia (IIIb)	357	2,218,124	0.34	0.4	878,377

7.2.3 Upcoming developments

An S5p+IASI combined product will offer the water isotopologue information in the boundary layer independently from the free troposphere. The development of such product is a logical next step. It can be generated a posteriori from IASI and S5p retrieval outputs according to the theory as described in as Rodgers (2000) and Rodgers and Connor (2003). For an operational generation of the S5p+IASI combined product an operational output of the retrieved state vector together with the a priori state vector, the averaging kernel matrix, the a priori covariance matrix, the a posteriori covariance matrix and the measurement noise uncertainty matrix is required.

8 Harmonisation Across S5p+I Themes

Harmonization across the S5p+I themes can be of mutual benefit for the different themes. In this section we discuss the S5p+I H2O-ISO particularities for the different components for which harmonisation could be considered.

8.1 L1 input files

The prototype demonstration of the HDO TROPOMI retrieval will be for mid-2018 to mid-2019 for areas of interest (Western Africa, Central Europe and Northern Europe). The HDO retrieval will only use the SWIR band and TROPOMI L1B SWIR data will be required for this time and space. The SWIR region has a lower spatial resolution compared to the UV/Vis bands. This will introduce dependencies on the other themes if L2 output is used within workflow.

8.2 Met/Model data

The harmonisation of reanalysis or model data fields need to be considered across themes. The use of ERA5 profiles is currently planned for HDO retrievals.

Table 6 *Convention for output filenames. All components use an underscore to separate them with the exception of the file extension, which uses a period. Indices for characters begin at 0. This convention is adapted from Table 2 in the Sentinel-5 precursor/TROPOMI Level 2 product user manual for cloud properties showing the components of an S5P product file name.*

Start	End	Length	Meaning/Value
0	3	3	Mission name **S5P**
4	8	4	Processing stream **OFFL**
9	19	10	Product identifier **L2__H2O_IS**
20	35	15	Start of granule in UTC as “**YYYYMMDDTHHMMSS**”. The “T” is a fixed character
36	51	15	End of the granule in UTC as “**YYYYMMDDTHHMMSS**”. The “T” is a fixed character
52	57	5	Orbit number
58	60	2	Collection number
61	67	6	Processor version number as “**MMmmpp**”, with “MM” the major version number, “mm”the minor version number, and “pp” the patch level.
68	83	15	The time of processing for this granule in UTC as “**YYYYMMDDTHHMMSS**”. The “T” is a fixed character.
84	86	2	The file name extension **nc**

8.3 Cloud masking

Three cloud detection algorithms are available: from VIIRS data, from the KNMI TROPOMI-FRESCO algorithm (Wang et al. 2008), or from the DLR TROPOMI-CLOUD algorithm (Loyola et al. 2018). The L1b S5p data used for the retrieval will need to be screened for cloud but the δD dataset is relatively insensitive to small cloud perturbation. It is expected that either of the three cloud algorithms will provide the dataset for required cloud screening.

8.4 Radiative transfer

The UoL FP retrieval algorithm employs a full multiple-scattering radiative transfer solver as part of the forward model. The main radiative transfer model is LIDORT which is used in combination with a fast 2-orders-of-scattering vector radiative transfer code to approximate polarisation. In addition, the code can use the Principal Component Analysis method (PCA) of or the low-streams interpolation functionality (LSI) to accelerate the radiative transfer component of the retrieval algorithm.
As part of an algorithm trade-off, we will use a non-scattering forward model to increase the computational efficiency and which is expected to be sufficient for the δD retrieval (as it used the HDO/H_2O ratio). The radiative transfer will make use of spectroscopic tables (HITRAN, DLR) and there is scope for harmonisation across themes.
Therefore, analysis/description of radiative transfer codes used in the project (pros and cons) along with spectroscopy used should be considered as part of the harmonisation activities.

8.5 Output files

The data output will be netCDF CF compliant and use CCI format where possible. The current proposed structure is based on the file structure used in existing C3S and CCI projects.. We propose an output filename, format and structure in terms of naming conventions and units (SI) in compliance with existing TROPOMI products. Table 6 provides details on the output data filename format that we plan to use, while Table 7 gives an overview of the initial variables to be included in the output data files. Additionally, the adoption of TUNER (Towards Unified Error Reporting, https://www.imk-asf.kit.edu/Projekte_2689.php) or FIDUCEO (Fidelity and uncertainty in climate data records from Earth Observations, http://www.fiduceo.eu/) standards/terminology for provided variables/parameters will be used.

***Table 7** Initial variables to be included in the output data files based on current C3S and CCI data production. Inclusion of SI units are also shown as these will be the units used for the prototype data products.*

Name	Type	Dimensions	Units	Description
solar_zenith_angle	float	n	degree	Angle between line of sight to the sun and local vertical
sensor_zenith_angle	float	n	degree	Angle between the line of sight to the sensor and the local vertical

time	double	n	seconds since 1970-01-01 00:00:00	Measurement time
longitude	float	n	degrees_east	Centre longitude
latitude	float	n	degrees_north	Centre latitude
pressure_levels	float	n, m	hPa	Vertical altitude coordinate in pressure units as used for averaging kernels
pressure_weight	float	n, m		Pressure weights as used for averaging kernels
xh2o	float	n	1e-6 (SI unit: kg/kg)	Retrieved column-averaged dry-air mole fraction of atmospheric water vapour (XH_2O) in ppm.
xhdo	float	n	1e-6 (SI unit: kg/kg)	Retrieved column-averaged dry-air mole fraction of atmospheric deuterium hydrogen monoxide (XHDO) in ppm.
x_delta_D	float	n	‰ (Per Mille) (SI unit: 1)	Retrieved column-averaged dry-air mole fraction of Deuterium ratio to VSMOW
xh2o_uncertainty	float	n	1e-6 (SI unit: kg/kg)	Statistical uncertainty of XH_2O in ppm (1σ)
xhdo_uncertainty	float	n	1e-6 (SI unit: kg/kg)	Statistical uncertainty of XHDO in ppm (1σ)
x_delta_D_uncertainty	float	n	‰ (Per Mille) (SI unit: 1)	Statistical uncertainty of Deuterium ratio (1σ)
retrieved_h2o_scaler	float	n	SI unit: 1	Retrieved H_2O scaler for h2o_profile_apriori
retrieved_h2o_scaler_uncertainty	float	n	%	Uncertainty of retrieved H_2O scaler for h2o_profile_apriori
retrieved_hdo_scaler	float	n	SI unit: 1	Retrieved HDO scaler for h2o_profile_apriori
retrieved_h2o_scaler_uncertainty	float	n	%	Uncertainty of retrieved HDO scaler for h2o_profile_apriori

xh2o_scaler_averaging_kernel	float	n, m	SI unit: 1	XH_2O averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XH_2O retrieval
xhdo_scaler_averaging_kernel	float	n, m	SI unit: 1	XHDO averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XH_2O retrieval
exposure_id	char	n, 22	n/a	Exposure identification number of the sounding
surface_altitude	float	n	metres	Altitude is the (geometric) height above the geoid, which is the reference geopotential surface
surface_altitude_stdev	float	n	metres	Standard deviation of the surface elevation within the area of the GOSAT sounding, as derived from the SRTM database
surface_air_pressure_apriori	float	n	hPa	A-priori surface pressure value
surface_air_pressure_apriori_std	float	n	hPa	A-priori surface pressure standard deviation
air_temperature_apriori	float	n, m	K	Air temperature is the bulk temperature of the air, not the surface (skin) temperature
h2o_profile_apriori	float	n, m	1e-6 (SI unit: kg/kg)	A-priori mole fraction profile of atmospheric H_2O in ppm
r_outcome	int	n	SI unit: 1	Retrieval outcome flag
r_chi2	float	n	SI unit: 1	Retrieval $\chi 2$ value
r_num_div	int	n	SI unit: 1	Number of divergent steps in the retrieval
retr_flag	int	n	SI unit: 1	Retrieval type flag (0 = land, 1 = glint)

9 Acronyms and Abbreviations

Acronym	Meaning
ABL	Algorithm Baseline
ACE	Atmospheric Chemistry Experiment
ACT	Across Track
ADEOS-I	Advanced Earth Observing Satellite
AIRS	Atmospheric Infrared Sounder
ALIAS	Aircraft Laser Infrared Absorption Spectrometer
ALT	Along Track
AOI	Area Of Interest
AVE_WIIF	Aura Validation Isotope Intercomparison Flight
CCI	Climate Change Initiative
CF	Climate and Forecast Metadata Convention
CMUG	Climate Modelling User Group
COSMO	Consortium for Small-scale Modelling
CR-AVE	Costa Rica Aura Validation Experiment
CRYSTAL-FACE	Cirrus Regional Study of Tropical Anvils and Cirrus Layers Florida Area Cirrus Experiment
DLR	German AerospaceCenter
DWD	German Weather Service
DOFS	Degree of Freedom for Signal
ECHAM	ECMWF and Hamburg
ENVISAT	Environmental Satellite
ERA	European Reanalysis
EUREC^{4}A	Elucidating the Role of Clouds-Circulation Coupling in Climate
FTIR	Fourier-Transform InfraRed
FTS	Fourier Transform Spectrometer
GCM	Global Circulation Model
GCOS	Global Climate Observing System
GEWEX	Global Energy and Water Exchanges
GNIP	Global Network of Isotopes in Precipitation
GNIR	Global Network of Isotopes in Rivers
GOME	Global Ozone Monitoring Experiment
GOSAT	Greenhouse Gases Observing Satellite
G-VAP	GEWEX Water Vapor Assessment
HITRAN	High-resolution transmission molecular absorption database

Hoxotope	HOx total water isotopologues
HyMeX SOP1	Hydrological cycle in Mediterranean Experiment special observation period 1
IAEA	International Atomic Energy Agency
IASI	Infrared Atmospheric Sounding Interferometer
IASI-NG	IASI Next Generation
ICON-ART	Icosahedral Nonhydrostatic - Aerosols and Reactive Trace Gases
ICOS	Integrated Cavity Output Spectroscopy
IGP	Iceland Greenland Seas Project
IMG	Interferometric Monitor for Greenhouse gases
IR	Infrared
ISLAS	Isotopes Links to Atmospheric water's Sources
ISS	International Space Station
IsoGSM	Isotope-incorporated Global Spectral Model
ISOWAT II	Version 2 of a tuneable diode-laser absorption spectrometer for detecting isotopologues of water vapour
KIT	Karlsruhe Institute of Technology
KNMI	The Royal Netherlands Meteorological Institute
LEMON	Lidar Emitter and Multi-species greenhouse gases Observation instrument
LEO	Low Earth Orbit
LES	Large Eddy Simulation
LETKF	Local Ensemble Transform Kalman Filter
Lidar	Light Detection And Ranging
LIDORT	Linearized Discrete Ordinate Radiative Transfer
LMDz	Laboratoire de Météorologie Dynamique
LSI	Low-streams interpolation functionality
LT	Local Time
Metop-SG	Meteorological Operational Satellite - Second Generation
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MOTIV	Moisture Transport pathways and Isotopologues in water Vapour
MUSICA	Multi-platform remote Sensing of Isotopologues for investigating the Cycle of Atmospheric water
NetCDF	Network Common Data Form
NCAR	National Centre of Atmospheric Research
NDACC	Network for the Detection of Atmospheric Composition Change

NRT	Near Real Time
NWP	Numerical Weather Prediction
OCO-2	Orbiting Carbon Observatory
ORACLES	Aerosols above Clouds and their intEractionS
OMI	Ozone Monitoring Instrument
PAGES	Past Global Changes
PCA	Principal Component Analysis
RB	Requirement Baseline Document
RCM	Regional Climate Model
S5p+I	Sentinel-5p+Innovation
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SMILES	Superconducting Submillimetre-Wave Limb-Emission Sounder
SMOS	Soil Moisture and Ocean Salinity
SMR	Sub-Millimetre Radiometer
SNOWISO	Signals from the surface snow: post-depositional processes controlling the ice core isotopic fingerprint
SPARC	Stratosphere-troposphere Processes And their Role in Climate
SWVID	Stable Water Isotope Database
SWING	Stable Water Isotope Intercomparison Group
TANSO	Thermal And Near infrared Sensor for carbon Observations
TC4	Tropical Composition, Cloud and Climate Coupling
TCCON	Total Carbon Column Observing Network
TEDDY	Testing isotopologues as Diabatic heating proxy for atmospheric Data analyses
TES	Tropospheric Emission Spectrometer
TROPOMI	Tropospheric Monitoring Instrument
UoB	University of Bergen
UoL	University of Leicester
UTLS	Upper Troposphere / Lower Stratosphere
WAVAS	Water Vapor Assessment
WCRP	World Climate Research Programme
WMO	World Meteorological Organization
WISPER	Water Isotope Spectrometer for Precipitation and Entrainment

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