Product User Manual for Sentinel-5 Precursor: HDO/H2O Total Column Retrieval [L2__HDO___S]

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Prepared by	S. Mandal, T. Borsdorff, J. Landgraf (SRON)	

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1 Introduction

This is the Product User Manual (PUM) for the Sentinel-5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) HDO/H_2O total column level 2 data product, which covers the shortwave infrared (SWIR) spectral range between 2354 and 2374 nm. This data product is one of the deliverables of the ESA project 'Sentinel-5P Level-2 Processor Development' [RD01, RD02].

Product Identifier: **L2__HDO___S**

Example filename:

S5P_PAL__L2__HDO__S_20240105T145629_20240105T163759_32280_03_100300_20241118T204336.nc

The user manual describes the current processing baseline, product and quality information, and product availability status. The structure of the file follows the S5P-PAL: Sentinel 5P Product Algorithm Laboratory L2 Processor File Format Guidelines.

2 Purpose and Objectives

The purpose of this Product User Manual (PUM) is to provide users with detailed information about the Sentinel-5 Precursor (S5P) Tropospheric Monitoring Instrument (TROPOMI) HDO/H_2O total column level 2 data product. This manual outlines the data format, the structure of the product, and the content of the fields contained within the data files. It aims to assist users in understanding how to interpret the product and ensure correct usage for scientific analysis. Additionally, the PUM offers product and quality information, and includes details on product availability. This document will be updated as the data product evolves throughout the development and operational phases of the S5P mission.

3 Document Overview

This document begins with a brief description of Algorithm Description in Section 4, explaining the methodology and steps involved in processing the HDO/H_2O data product. This is followed by Section 5, which summarizes the product's key features and scientific relevance. In Section 6, the Product Description provides an in-depth breakdown of the data, including usage recommendations and a guide to the product's structure and fields. The document concludes with references, and abbreviations and acronyms, offering quick access to definitions of terms used throughout the manual.

4 Algorithm Description

The HDO/H_2O retrieval algorithm is adapted from the CO retrieval approach outlined in the Carbon Monoxide ATBD (Algorithm Theoretical Basis Document, [RD03]). It has been updated to account for an extended scientific HDO/H_2O total column data product from short-wave infrared (SWIR) measurements by the Tropospheric Monitoring Instrument (TROPOMI), including both clear-sky and cloudy scenes. The retrieval employs a forward model that incorporates scattering, and the algorithm simultaneously infers trace gas column information, surface properties, and effective cloud parameters from the observations. This approach significantly enhances coverage compared to the previous clear-sky-only data product, particularly by including scenes over low clouds, which enables data retrieval over oceans where the albedo in the SWIR spectral range is too low for cloud-free conditions.

Key retrieval configurations include:

- **Retrieval window:** 2354–2374 nm (SWIR band).
- **Fitted species:** H_2O, HDO, $H_2{}^{18}O$, and CH_4, using a profile scaling approach.
- **Spectral resolution:** 0.01 cm^{-1} to resolve absorption lines accurately.

The retrieval is implemented using the existing SICOR algorithm and processed in the offline reprocessing mode of the Sentinel-5 Precursor mission. In contrast to the earlier version, which focused on clear-sky observations using strict cloud filters from the SWIR pre-processor, the updated algorithm uses a scattering-aware retrieval approach to fit total columns of isotopes (H_2O, HDO, $H_2{}^{18}O$, CH_4, CO), surface albedo, spectral offsets, and wavelength-dependent reflectance. The retrieval window is optimized to capture strong HDO absorption lines, distinct from H_2O lines.

This comprehensive enhancement ensures improved data availability and accuracy, particularly over challenging surfaces like oceans. For further details, readers are referred to the ATBD for the HDO/H_2O data product [RD04].

5 Summary of the product HDO/H_2O

The hydrological cycle is a critical component in understanding climate change. Water vapor, as the strongest natural greenhouse gas, plays a key role in atmospheric feedback mechanisms and processes such as cloud formation. Accurate measurements of atmospheric humidity and its isotopic composition are essential for improving the projections of atmospheric general circulation models (GCMs), which are used to simulate climate-related processes.

Different water isotopologues, such as H_2O, $HD^{16}O$ (denoted as HDO), and $H_2{}^{18}O$, exhibit distinct isotopic signatures due to variations in equilibrium vapor pressures. These differences result in temperature-dependent isotope fractionation during phase changes, making the ratio of HDO to H_2O a valuable indicator of the source region’s temperature, location, and the transport history of air parcels. By capturing these isotopic ratios, measurements of HDO/H_2O offer a benchmark for evaluating and improving GCMs.

HDO/H_2O Level-2 Requirements: To enhance the understanding of HDO/H_2O on a global scale, satellite-based measurements of the total HDO/H_2O column are essential. These measurements should achieve an accuracy better than 20% and a precision of 10%, even under challenging conditions such as low surface reflection in the shortwave infrared spectral range. The error budget is designed to ensure that both instrument and forward model errors contribute equally, with individual error contributions not exceeding 8%. These requirements establish the thresholds for the HDO/H_2O Level-2 product.

Advances with TROPOMI: The TROPOMI instrument significantly extends the global HDO/H_2O datasets by offering high spatial resolution and wide swath coverage. Similar to earlier instruments like SCIAMACHY, TROPOMI's shortwave infrared (SWIR) measurements are highly sensitive to HDO/H_2O near the surface. However, TROPOMI's improved resolution and shorter revisit times provide an increased volume of near-surface cloud-free data, enabling detailed analysis of spatial and temporal gradients of HDO/H_2O.

The HDO/H_2O retrieval algorithm adapts the TROPOMI CO retrieval algorithm to suit the isotopologue ratio measurement requirements. The algorithm is optimized to handle challenges such as elevated scattering layers and cloud conditions by utilizing a non-scattering mode and pre-filtering for heavily cloudy pixels. It provides column averaging kernels for both HDO and H_2O, facilitating proper comparisons with isotope-enabled GCMs and supporting the study of the hydrological cycle at higher resolution.

6 Product Description

6.1.1 Recommendations for data usage

It is recommended to use TROPOMI HDO/H2O data associated with a quality assurance value `qa_value` > 0.4. The `qa_value` is provided as part of the HDO/H2O data product, and the overall definition used in the current data release is summarized in Table . A more detailed discussion on the `qa_value` parameter can be found in the validation papers [RD05, RD06].

qa_value	Condition	Remark
1.0	• Aerosol optical thickness < 0.3 • Aerosol height < 500 • Surface albedo > 0.02 • Solar zenith angle < 80° • Iterations ≤ 10 • Reduced chi-squared ≤ 150 • Reduced chi-squared prefit ≤ 150	Clear-sky and clear-sky-like observations
0.7	• Aerosol optical thickness ≥ 0.3 • Aerosol height < 5000 • Solar zenith angle < 80° • Iterations ≤ 10 • Reduced chi-squared ≤ 150 • Reduced chi-squared prefit ≤ 150	Mid-level clouds
0.4	Either: • Aerosol optical thickness ≥ 0.3 AND aerosol height > 5000 • OR aerosol optical thickness ≤ 0.3 AND aerosol height ≥ 500 • Solar zenith angle < 80° • Iterations ≤ 10 • Reduced chi-squared ≤ 150 • Reduced chi-squared prefit ≤ 150	High-clouds, experimental dataset
0.0	• Solar zenith angle ≥ 80° • OR iterations > 10 • OR reduced chi-squared > 150 • OR reduced chi-squared prefit > 150	Corrupted or defective data

Table 1: `qa_value` definition

In this section, we describe the data product and its contents within the various groups in the NetCDF file. The file is structured with the **/PRODUCT** group as the main container for the target products. Within the **/PRODUCT** group, there is a **/SUPPORT_DATA** group, which is further divided into the following subgroups: **DETAILED_RESULTS**, **GEOLOCATIONS**, and **INPUT_DATA**. Below, we provide a detailed description of the contents of each group and subgroup

6.1.2 /PRODUCT

Variable Name	Description	Units	Dimensions
corner	Dimension for geolocation bounds	-	corner
delta_time	Offset of start time of measurement	Milliseconds since 2024-12-31 02:18:03	time, scanline
deltad	Delta expression of HDO to H_2O ratio	1	time, scanline, ground_pixel
deltad_precision	Standard error of delta expression of HDO to H_2O ratio	1	time, scanline, ground_pixel
glintflag	Glint flag	1	time, scanline, ground_pixel
ground_pixel	Across-track dimension index	1	ground_pixel
h2o_column	Vertically integrated column of water	Molec. cm^{-2}	time, scanline, ground_pixel
h2o_column_precision	Standard error of vertically integrated column of water	Molec. cm^{-2}	time, scanline, ground_pixel
h2o_profile_apriori	A-priori vertically integrated partial column of water in layers	Molec. cm^{-2}	time, scanline, ground_pixel, layer
hdo_column	Vertically integrated column of heavy water	Molec. cm^{-2}	time, scanline, ground_pixel
hdo_column_precision	Standard error of vertically integrated column of heavy water	Molec. cm^{-2}	time, scanline, ground_pixel
hdo_profile_apriori	A-priori vertically integrated partial column of heavy water in layers	Molec. cm^{-2}	time, scanline, ground_pixel, layer
latitude	Pixel center latitude	Degrees north	time, scanline, ground_pixel
layer	Number of layers	-	layer
level	Number of levels	-	level
longitude	Pixel center longitude	Degrees east	time, scanline, ground_pixel
nwin	Number of windows	-	nwin
qa_value	Data quality value	1	time, scanline, ground_pixel
scanline	Along-track dimension index	1	scanline
time	Reference time for the measurements	Seconds since 2010-01-01 00:00:00	time

6.1.3 /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS

Variable Name	Description	Units	Dimensions
aerosol_geometric_thickness	Geometric thickness of aerosol layer	km	time, scanline, ground_pixel
aerosol_geometric_thickness_precision	Precision of aerosol geometric thickness	km	time, scanline, ground_pixel
aerosol_height	Height of aerosol layer	km	time, scanline, ground_pixel
aerosol_height_apriori	A priori height of aerosol layer	km	time, scanline, ground_pixel
aerosol_height_precision	Precision of aerosol height	km	time, scanline, ground_pixel
aerosol_optical_thickness	Optical thickness of aerosol layer	1	time, scanline, ground_pixel
aerosol_optical_thickness_apriori	A priori optical thickness of aerosol layer	1	time, scanline, ground_pixel
aerosol_optical_thickness_precision	Precision of aerosol optical thickness	1	time, scanline, ground_pixel
ch4_column	Vertically integrated column of methane	Molec. cm^{-2}	time, scanline, ground_pixel
ch4_column_apriori	A priori vertically integrated column of methane	Molec. cm^{-2}	time, scanline, ground_pixel
ch4_column_prefit	Prefit vertically integrated column of methane	Molec. cm^{-2}	time, scanline, ground_pixel
ch4_profile_apriori	A priori profile of methane	Molec. cm^{-2}	time, scanline, ground_pixel, layer
chi_square	Chi-squared value	1	time, scanline, ground_pixel
chi_square_band	Chi-squared value for band	1	time, scanline, ground_pixel
chi_square_prefit	Chi-squared value prefit	1	time, scanline, ground_pixel
co_column	Vertically integrated column of carbon monoxide	Molec. cm^{-2}	time, scanline, ground_pixel
co_column_precision	Precision of carbon monoxide column	Molec. cm^{-2}	time, scanline, ground_pixel
co_profile_apriori	A priori profile of carbon monoxide	Molec. cm^{-2}	time, scanline, ground_pixel, layer
convergence	Convergence status	1	time, scanline, ground_pixel
degrees_of_freedom_total	Total degrees of freedom	1	time, scanline, ground_pixel

Variable Name	Description	Units	Dimensions
degrees_of_freedom_total_prefit	Total degrees of freedom prefit	1	time, scanline, ground_pixel
h2o_column_averaging_kernel	Column averaging kernel for water vapor column	1	time, scanline, ground_pixel, layer
hdo_column_averaging_kernel	Column averaging kernel for heavy water column	1	time, scanline, ground_pixel, layer
iterations	Number of iterations	1	time, scanline, ground_pixel
multiplicative_offset	Multiplicative offset	1	time, scanline, ground_pixel, nwin
number_of_spectral_points_in_prefit	Number of spectral points in prefit	1	time, scanline, ground_pixel, nwin
number_of_spectral_points_in_retrieval	Number of spectral points in retrieval	1	time, scanline, ground_pixel, nwin
Rms	Root mean square of residuals	1	time, scanline, ground_pixel
spectral_shift	Spectral shift	nm	time, scanline, ground_pixel, nwin
surface_albedo	Surface albedo	1	time, scanline, ground_pixel, nwin
surface_albedo_apriori	A priori surface albedo	1	time, scanline, ground_pixel, nwin
surface_albedo_precision	Precision of surface albedo	1	time, scanline, ground_pixel, nwin
surface_albedo_prefit	Prefit surface albedo	1	time, scanline, ground_pixel, nwin
surface_albedo_prefit_apriori	Prefit a priori surface albedo	1	time, scanline, ground_pixel, nwin

6.1.4 /PRODUCT/SUPPORT_DATA/GEOLOCATIONS

Variable Name	Description	Units	Dimensions
latitude_bounds	Latitude bounds of the pixel corners	None	time, scanline, ground_pixel, corner
longitude_bounds	Longitude bounds of the pixel corners	None	time, scanline, ground_pixel, corner
solar_azimuth_angle	Solar azimuth angle	Degrees	time, scanline, ground_pixel
solar_zenith_angle	Solar zenith angle	Degrees	time, scanline, ground_pixel

Variable Name	Description	Units	Dimensions
viewing_azimuth_angle	Viewing azimuth angle	Degrees	time, scanline, ground_pixel
viewing_zenith_angle	Viewing zenith angle	Degrees	time, scanline, ground_pixel

6.1.5 /PRODUCT/SUPPORT_DATA/INPUT_DATA

Variable Name	Description	Units	Dimensions
altitude_levels	Altitude at layer interfaces above sea level	m	time, scanline, ground_pixel, level
dry_air_subcolumns	Vertically integrated partial column of dry air in layers	Molec. cm^{-2}	time, scanline, ground_pixel, layer
landflag	Most frequent land classification of ground pixel	None	time, scanline, ground_pixel
pressure_levels	Air pressure at layer interfaces	Pa	time,scanline, ground_pixel
skin_temperature	Skin temperature	K	time, scanline, ground_pixel
surface_altitude	Surface altitude above sea level	m	time, scanline, ground_pixel
surface_altitude_stdv	Standard deviation of sub-pixel variations of surface altitude	m	time, scanline, ground_pixel
surface_pressure	Surface air pressure	Pa	time, scanline, ground_pixel
Temperature	Air temperature in layers	K	time, scanline, ground_pixel, layer
u10	Ten meter U wind component	m/s	time, scanline, ground_pixel
v10	Ten meter V wind component	m/s	time, scanline, ground_pixel

6.1.6 List of known issues

The 'long_name' attribute of /PRODUCT/SUPPORT_DATA/INPUT_DATA/surface_pressure is incorrectly named 'long_namce'. This is a typographical error. While it does not impact product functionality, it should be noted for clarity. This issue will be addressed in a future product update.

References

[RD01] Sentinel-5P Level 2 Processor Development – Statement of Work. source: ESA; ref: S5P-SWESA-GS-053; date: 2012.

[RD02] Sentinel-5 Precursor Calibration and Validation Plan for the Operational Phase **source**: ESA; ref: ESA-EOPG-CSCOP-PL-0073; issue: 1.0 date 2017-06-11 **url**:https://sentinels.copernicus.eu/documents/247904/2474724/Sentinel-5P-Calibration-and-Validation-Plan.pdf

[RD03] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor: Carbon Monoxide Total Column Retrieval, **source**: SRON ref: SRON-S5P-LEV2-RP-002 **url**: https://sentinel.esa.int/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-Carbon-Monoxide-Total-Column-Retrieval.pdf/fe176d58-1e9f-4d26-af83-3ee6b0265ee5

[RD04] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor: HDO/H2O Total Column Retrieval, **source**: SRON ref: SRON-ESG-RP-2024-020 **url**:

[RD05] Schneider, A. and Borsdorff, T. and aan de Brugh, J. and Aemisegger, F. and Feist, D. G. and Kivi, R. and Hase, F. and Schneider, M. and Landgraf, J: First data set of H2O/HDO columns from the Tropospheric Monitoring Instrument (TROPOMI); DOI: 10.5194/amt-13-85-2020
url: https://amt.copernicus.org/articles/13/85/2020/

[RD06] Schneider, A. and Borsdorff, T. and aan de Brugh, J. and Lorente, A. and Aemisegger, F. and Noone, D. and Henze, D. and Kivi, R. and Landgraf, J: Retrieving H2O/HDO columns over cloudy and clear-sky scenes from the Tropospheric Monitoring Instrument (TROPOMI)
DOI: 10.5194/amt-15-2251-2022
url: https://amt.copernicus.org/articles/15/2251/2022

Abbreviations and acronyms

ATBD	Algorithm Theoretical Basis Document
CH_4	Methane
ESA	European Space Agency
ESL	Expert Support Laboratory
NDACC	Network for the Detection of Atmospheric Composition Change
OFFL	Offline
PUM	Product User Manual
S5P	Sentinel-5 Precursor
SZA	Solar Zenith Angle
TCCON	Total Carbon Column Observing Network
TROPOMI	TROPOspheric Monitoring Instrument
VZA	Viewing Zenith Angle