

Water Vapour Climate Change Initiative (WV_cci) - CCI+ Phase 2



Product Specification Document (PSD)

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1. INTRODUCTION

1.1 Purpose of the document

The purpose of this Product Specification Document (PSD) is to provide detailed specifications on the different CDR products delivered for the ECV Water Vapour within the WV_cci project. The specifications aim at compliance with the user requirements from GCOS-200, other CCI projects as defined within the CCI Data Standards (v2.1) and established in consultation with the WV_cci user group and CRG that are summarised in the URD (v3.0).

1.2 Definitions

The terminology is given in the PVP (PVP, 2021).

2. WATER DATA PRODUCT OVERVIEW

This section provides an overview of the different water vapour data products that will be available from the WV_cci at the end of the project. Detailed specifications of these data products and their input data are provided in Section 3.

The primary datasets (or CDRs) that WV_cci produced are illustrated in Figure 2-1. These include gridded L3 total column water vapour over land (CDR-1) and merged over land and ocean (CDR-2), and also L3 vertically resolved water vapour with focus on the stratosphere (CDR-3) and with focus on the UTLS (CDR-4).

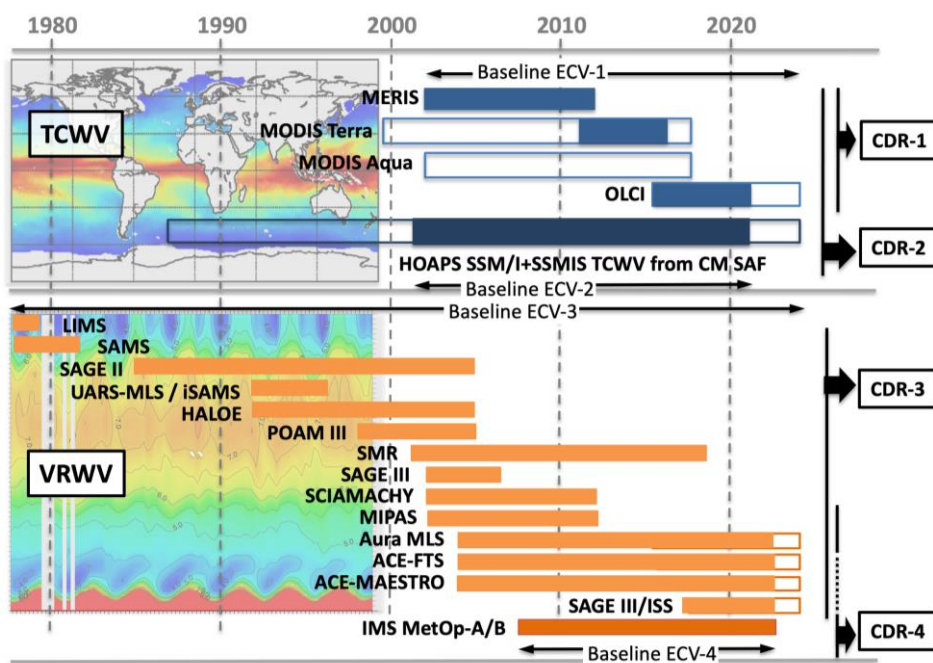


Figure 2-1: Instruments and considered time periods from which input observations (L2 data products) are obtained, and resulting climate data records (CDRs; L3 data products) for total column (TCWV; CDR-1 and CDR-2) and vertically resolved (VRes WV; CDR-3 and CDR-4) water vapour.

Table 2-1: Overview of final data products delivered by WV_cci

#	Product Name	Level	Notes	Time period
1	CDR-1	L3	TCWV gridded monthly and daily data (land)	2002–2023
2	CDR-2	L3	TCWV gridded monthly and daily data (land and ocean)	2002–2020

#	Product Name	Level	Notes	Time period
3	CDR-3	L3	Stratospheric vertically resolved zonal monthly mean WV CDR (2D-fields)	1978–2023
4	CDR-4	L3	UTLS vertically resolved monthly mean WV CDR (3D-fields)	2007–2023

2.1 CDR-1: TCWV (land)

This vertically integrated (total column) water vapour ECV, in units of kg/m^2 , is a gridded L3 data product over land based on ESA (MERIS, OLCI) and NASA instruments (MODIS). The final dataset covers the period July 2002 to December 2023.

2.2 CDR-2: TCWV (land and ocean)

The CDR-2 dataset is a global, i.e. land and ocean coverage, TCWV product in units of kg/m^2 . It contains the CDR-1 over land, coasts and sea-ice and the HOAPS microwave imager based TCWV data over ocean. The HOAPS data are generated by EUMETSAT CM SAF. It is planned that the CDR-2 will be released by the EUMETSAT CM SAF. The final dataset covers the period July 2002 to December 2020. Depending on developments within CM SAF an extension to December 2023 is envisaged.

2.3 CDR-3: Vertically resolved stratospheric water vapour climatologies

This vertically resolved water vapour ECV is a merged data product based on a range of ESA, third-party and NASA instruments including SAGE II, HALOE, UARS-MLS, POAM III, SAGE III, SMR, SCIAMACHY, MIPAS, Aura-MLS, ACE-FTS, ACE-MAESTRO, and SAGE III/ISS and spans the time period 1978 to the end of 2023. The extension backwards to 1978 of CDR-3 depends on the quality of the historical records from early satellite instruments NIMBUS-LIMS, NIMBUS-SAMS and UARS-iSAMS. The product is provided as zonal means and in units of ppmv (mixing ratios).

2.4 CDR-4: Vertically resolved water vapour profiles in the UTLS

This CDR consists of three-dimensional vertically resolved water vapour data, covering the troposphere and lower stratosphere from 2007 to 2023. The water vapour is based on RAL IMS, MIPAS and Aura-MLS. The global product includes mixing ratios in units of ppmv (mixing ratios).

3. SPECIFICATIONS OF PRIMARY WATER VAPOUR DATA PRODUCTS

3.1 CDR-1

The NIR spectral range provides daytime, cloud-free retrieval of TCWV over land. Since most land surfaces are bright in the NIR, this spectral range is well suited for this purpose. The retrieval is based on the differential absorption technique (Fischer, 1988; Gao et al., 1993; Lindstrot et al., 2012). The basic principle of the method is the comparison of the measured radiance in an absorption band to a close by band with no or only few absorption features.

The specification of the TCWV product and the required input for the retrieval are described in the following.

3.1.1 Used input data

3.1.1.1 L1 Products

The input datasets for the generation of the CDR-1 water vapour data products are:

- MERIS L1b reduced resolution (2002–2012), 4th reprocessing
- MODIS TERRA MOD021KM (time period tbd)¹, collection 6.1
- MODIS AQUA MYD021KM ((time period tbd), collection 6.1
- OLCI L1b reduced resolution (2016–2023), 1st reprocessing.

The MERIS L1b data originates from the 4th reprocessing version. The L1b dataset from the OLCI 1st reprocessing is used as input. Both datasets are available at Brockmann Consult.

For MODIS, data from ERA5 are used as *a priori* input to the retrieval.

¹ The ingestion of MODIS data depends on the available processing resources (not yet clear at compilation time of this PSD version).

3.1.1.2 TCWV L2 Intermediate Products

The Level-2 TCWV product is the result of the TCWV L2 processing for any of the sensors MERIS, MODIS or OLCI. The TCWV L2 processing step uses the retrieval algorithm described in detail in the ATBD (ESA CCI Water Vapour, 2021). Making use of the land/water mask, TCWV is computed over both land and water, applying slightly different algorithms and lookup tables. The content of the Level-2 TCWV product is sensor-independent. Within WV_cci, the Level-2 TCWV products are not generally made publicly available.

3.1.2 Resolution and coverage in space and time

The final TCWV L3 land products delivered as the CDR-1 dataset are generated from the L2 products by:

- Temporal aggregation (daily averages and monthly averages)
- Spatial aggregation (global, WGS84, 0.5 and 0.05 degree resolution).

Table 3-1 provides an overview of the technical specifications.

Table 3-1: CDR-1 – Resolution and coverage in space and time

Dimension	Specification
Temporal resolution	Daily averages and monthly averages
Temporal coverage	July 2002 – December 2023
Spatial coverage	Global
Spatial resolution	0.5 or 0.05 deg

3.1.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of CDR-1 is summarised in Table 3-2.

Table 3-2: Expected quality of CDR-1

Quantity	Specification	Notes
Accuracy:	0.75 kg/m ²	Rounded-up mean bias relative to AIRS and GRUAN (PVIR, 2021).

Quantity	Specification	Notes
Systematic component	(initial estimate)	
Accuracy: Random component	2.75 kg/m ² (initial estimate)	Rounded-up cRMSD relative to AIRS and GRUAN (PVIR, 2021).
Stability	0.5 (kg/m ²)/decade (initial estimate)	Rounded-up mean stability relative to AIRS and ERA5 based on 2002–2017 period (PVIR, 2021). The evaluation of stability on a global scale is challenging.

3.1.4 Product layers, auxiliary output, format and metadata

Table 3-3 gives an overview of the product layers in CDR-1. For clarity, the definition of *tcwv_ran* (i.e. propagated retrieval uncertainty) and *tcwv_err* (i.e., averaged retrieval uncertainty) recalled here (see E3UB v2.1 for details):

$$tcwv_{ran} = \sqrt{\frac{1}{N} \sum_{i=1}^N \sigma_i^2}$$

$$tcwv_{err} = \frac{1}{N} \sum_{i=1}^N \sigma_i$$

with N =number of valid values and σ_i = estimated retrieval uncertainty per L2 pixel. Unphysical values are declared as an undefined or missing value. The uncertainty describes the reliability of the TCWV data. The quality flag can take four values: 0 – no known issues; 1 – cost function above a value of 1; 2 – cost function above 2; 3 – invalid (see Table 3-3).

Table 3-3: Product layers in TCWV L3 product (CDR-1)

NIR: near infrared, MW: microwave

Name in product	Unit	Type	Description
tcwv	kg/m ²	float32	Total Column Water Vapour
stdv	kg/m ²	float32	Standard deviation of Total Column Water Vapour
tcwv_err	kg/m ²	float32	Average retrieval uncertainty
tcwv_ran	kg/m ²	float32	Propagated retrieval uncertainty
tcwv_quality_flag ^{*,**}	n/a	int8	Quality flag of Total Column Water Vapour

Name in product	Unit	Type	Description
			0: no known issues, 1: cost function above 1, 2: cost function above 2, 3: invalid
surface_type_flag	n/a	int8	Surface mask 0: land, 1: ocean, 2: clouds_NIR, 3: heavy_precipitation_MW, 4: sea_ice, 5: coast, 6: partly_cloudy over land, 7: partly_sea_ice
num_obs	n/a	int16	Number of TCWV L2 retrievals contributing to L3 grid cell
num_days_tcwv***	n/a	int16	Number of valid days in monthly CDR (over land without clouds)

* Monthly TCWV data files do not contain the "tcwv_quality_flag".

**Implementation for CDR-2: 0 = no known issues, 1 = cost function above 2, 2 = "invalid",

***Daily TCWV data files do not contain the "num_days_tcwv".

An estimate of the file sizes is given in Table 3-4.

Table 3-4: Estimate of final product output data volume (CDR-1)

	Month	Year	Full period
Size	1.2 GB	14 GB	225 GB

The file format used for storing the data is NetCDF-4 classic. All (NetCDF) files follow the NetCDF Climate and Forecast (CF) Metadata Conventions version 1.7. CF standard names are used for the main variables and global attributes required to ensure compliance with CCI Data Standards have been added. Compliance with the CCI Data Standards was cross-checked and confirmed as the products were being generated. The metadata information, that will be provided with the data files, is explained in Table 3-5 and Table 3-6.

Table 3-5: Metadata in TCWV over land (CDR-1): Global attributes

Metadata name	Comment
title	
institution	
source	Source description of the datasets in the final products.
history	History of sequential processing steps.
references	

Metadata name	Comment
tracking_id	A unique ID per data product in UUID format (128 bit), generated by the processing code, e.g., "e24e9f56-4fb5-11eb-8b65-00259056ae12".
Conventions	CF conventions (version number)
product_version	
format_version	Version of CCI data standards
summary	Summary of what is included in given data product.
keywords	
id	ID of product category within the project, e.g., 10.5676/EUM_SAF_CM/COMBI/V001
naming-authority	
keywords-vocabulary	
cdm_data_type	Common Data Model data type, e.g., 'grid' (explained in more detail e.g., in Nativi et al., 2008)
comment	
date_created	
creator_name	Institution(s) involved in the creation of the data product.
creator_url	
creator_email	
project	
geospatial_lat_min	
geospatial_lat_max	
geospatial_lon_min	
geospatial_lon_max	
geospatial_vertical_min	
geospatial_vertical_max	
time_coverage_duration	Temporal duration given in CF format (e.g., 'P1D' for a daily product)
time_coverage_resolution	Temporal duration of a sequence of products given in CF format (e.g., 'P1M' for a sequence of monthly products)
time_coverage_start	
time_coverage_end	
standard_name_vocabulary	Vocabulary containing the standard metadata names used in the attributes (here: NetCDF Climate and Forecast (CF) Metadata Convention version 67)

Metadata name	Comment
license	
platform	Platform(s) carrying the sensor(s) which the input data was obtained from.
sensor	Sensor(s) which the input data was obtained from.
spatial_resolution	
geospatial_lat_units	
geospatial_lon_units	
geospatial_lat_resolution	
geospatial_lon_resolution	
key_variables	

Table 3-6: Metadata in TCWV over land (CDR-1): Variable attributes
Not all variables must contain the full set of metadata as listed here

Metadata name	Comment
long_name	
standard_name	
units	
calendar	Calendar for 'time' variable (here: 'gregorian')
axis	Axis referring to coordinate variables ('Y' for latitude, 'X' for longitude)
bounds	Reference to time/coordinate bounds variables (time_bnds, lat_bnds, lon_bnds)
comment	
valid_range	
reference_datum	Reference datum for latitude and longitude variables (here: geographical coordinates, WGS84 projection)
_FillValue	
coordinates	Reference to coordinates variables (lat, lon)
ancillary_variables	Ancillary variables related to given variable (e.g., stdv and num_obs for tcwv)
actual_range	Variable data range in given product.
valid_range	Valid data range for given variable.
wkt	wkt string for 'crs' variable (Coordinate Reference System)
i2m	Coordinates bounding box in 'crs' variable (Coordinate Reference System)

Metadata name	Comment
flag_values	
flag_meanings	

3.2 CDR-2

The CDR-2 TCWV product combines the land-based CDR-1 product and the ocean-based microwave imager HOAPS product from EUMETSAT CM SAF. Coastal areas and sea-ice regions are filled with NIR-based products. This way, sensor specific advantages have been utilised to produce a global product without changing the characteristics of the individual sensor products. The approach was first proposed for the ESA GlobVapour project and the resulting product is described in Lindstrot et al. (2014).

3.2.1 Used input data

CDR-1 is used to cover land areas. Additionally, NIR based TCWV data using the CDR-1 retrieval as baseline is used to cover sea-ice and coastal areas. Input data specifications for CDR-1 are described in Section 3.1.

Over ocean TCWV from the CM SAF HOAPS product is used only. The HOAPS product suite is a purely microwave imager-based satellite product (except SST from microwave imagers and a static profile data base from ERA-Interim). HOAPS was originally developed at the MPI-M and the University of Hamburg and has been successfully transferred into the operational environment of EUMETSAT CM SAF. Since version 3.1 CM SAF is generating all HOAPS products which includes among others a TCWV product. This product is defined over the global ice-free ocean with a 50 km distance to nearest coasts. TCWV is retrieved with a 1D-Var scheme under clear-sky and cloudy-sky conditions and can not be reliably applied in presence of strong scattering events such as in strong precipitation cases. CM SAF will generate the TCWV data by applying the HOAPS version 4 software using SSM/I, SSMIS, AMSR-E, TMI and potentially GMI and AMSR-2 data as input. The SSM/I and SSMIS are elements of a FCDR from CM SAF (Fennig et al., 2022) while the remaining sensors were/will be intercalibrated to the CM SAF FCDR. TCWV from HOAPS will have very similar specifications as the HOAPS data used during phase 1. In particular, the same approaches to compute daily averages and uncertainty estimates will be used again. CM SAF will generate input to CDR-2 with the following specifications: 0.5° /

0.05° (oversampled) spatial resolution, daily and monthly resolution, global ice-free coverage over the period July 2002 – December 2020.

3.2.2 Resolution and coverage in space and time

The technical specifications for CDR-2 are the same as described in Section 3.1.2. However, in addition to the application of the NIR retrieval over clear-sky land areas, the retrieval is also applied to sea-ice and coastal areas, both in clear-sky conditions.

3.2.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of CDR-2 is summarised in Table 3-7.

Table 3-7: Expected quality of CDR-2

The evaluation of the quality will strongly depend on the reference / data record used for comparison

Quantity	Specification	Notes
Accuracy: Systematic component	0.75 kg/m ² (initial estimate)	Rounded-up mean bias relative to AIRS (PVIR, 2021).
Accuracy: Random component	2 kg/m ² (initial estimate)	Rounded-up mean cRMSD relative to AIRS (PVIR, 2021).
Stability	0.2 (kg/m ²)/decade (initial estimate)	Generously rounded-up mean stability relative to AIRS (PVIR, 2021). The evaluation of stability on a global scale is challenging.

3.2.4 Product layers, auxiliary output, format and metadata

The product layers are the same as for CDR-1 and are recalled for convenience in Table 3-8.

Table 3-8: Product layers in TCWV L3 product (CDR-2)

NIR: near infrared, MW: microwave

Name in product	Unit	Type	Description
tcwv	kg/m ²	float32	Total Column Water Vapour
stdv	kg/m ²	float32	Standard deviation of Total Column Water Vapour
tcwv_err	kg/m ²	float32	Average retrieval uncertainty
tcwv_ran	kg/m ²	float32	Propagated retrieval uncertainty

Name in product	Unit	Type	Description
tcwv_quality_flag**	n/a	int8	Quality flag of Total Column Water Vapour 0: no known issues, 1: cost function above 1, 2: cost function above 2, 3: invalid
surface_type_flag	n/a	int8	Surface mask 0: land, 1: ocean, 2: clouds over land_NIR, 3: heavy_precipitation_MW, 34: sea_ice, 45: coast, 56: partly_cloudy over land, 67: partly_sea_ice
num_obs	n/a	int16	Number of TCWV L2 retrievals contributing to L3 grid cell
num_days_tcwv***	n/a	int16	Number of valid days in monthly CDR (over land without clouds)
num_hours****	n/a	int16	Number of valid hours in daily CDR (over land without clouds)

* Monthly TCWV estimates do not include the "tcwv_quality_flag".

**Implementation for CDR-2: 0 = no known issues, 1 = cost function above 2, 3 = "invalid",

***Daily TCWV data files do not contain the "num_days_tcwv".

**** Not available over land, sea-ice and coasts.

An estimate of the file sizes is given in Table 3-9.

Table 3-9: Estimate of final product output data volume (CDR-2)

	Month	Year	Full period
Size	1.2 GB	14 GB	225 GB

The file format used for storing the data is NetCDF-4 classic. All (NetCDF) files follow the NetCDF Climate and Forecast (CF) Metadata Conventions version 1.7. CF standard names used for the main variables and global attributes required to ensure compliance with CCI Data Standards were added. Compliance with the CCI Data Standards was cross-checked and confirmed while the products were being generated. The metadata information, that will be provided with the data files, is basically the same as for CDR-1 and was explained in Table 3-5 and Table 3-6.

3.3 Regional, high resolution TCWV

Current WV_cci TCWV products have resolutions of 0.05 x 0.05 and 0.5 x 0.5 degrees, depending on the sensors used. However, NIR satellite data input into the CDR-1 and CDR-2 products have pixel resolutions between 300 and 1000 m. Therefore, the generation of a high-resolution TCWV product allows investigations at sub-model-grid scales, relating inhomogeneity in water vapour fields to other processes.

3.3.1 Used input data

The input datasets for the generation of the regional, high-resolution water vapour data products are the same as for the standard-resolution global land products (see section 3.1.1). However, only a subperiod will be considered here.

3.3.2 Resolution and coverage in space and time

As target region for the high-resolution datasets, North Africa has been identified and selected as most appropriate. These high-resolution datasets are generated in the same way from the L2 products as CDR-1 by:

- Temporal aggregation (daily averages and monthly averages)
- Spatial aggregation (WGS84, regional, 0.01 degrees (~1 km) resolution).

Table 3-10 provides an overview of the technical specifications.

Table 3-10: Regional products – Resolution and coverage in space and time

Dimension	Specification
Temporal resolution	Daily averages and monthly averages
Temporal coverage	Sufficient sub-period of the global dataset (not yet finally specified at compilation time of this PSD)
Spatial coverage	Regional (North Africa), boundary coordinates not yet finally specified at compilation time of this PSD
Spatial resolution	0.01 deg (approx. 1 km)

3.3.3 Uncertainty estimates, quality indicators, and expected accuracy

With the high-resolution product using the same input data and retrievals as CDR-1, we make the assumption that the uncertainty estimates, quality indicators, and expected accuracy will be equivalent (see section 3.1). It might occur that cRMSD and uncertainty estimates are slightly larger given the higher spatial resolution.

3.3.4 Product layers, auxiliary output, format and metadata

The regional, high-resolution products will basically contain the same product layers, auxiliary output, format and metadata as the global land product (see Table 3-1). Specific deviations which might be regarded as necessary during product generation will be described in a later version of this PSD. This will likely include variables that describe the surface heterogeneity.

3.4 CDR-3

3.4.1 Used input data

CDR-3 used as input data observations from international satellite limb sounders as obtained directly from the different data providers as both single profile data (see Section 3.4.1.1) and zonal monthly mean climatologies processed for the SPARC Data Initiative (see Section 3.4.1.2). The usage of historical data reuse of earlier satellite data records from NIMBUS-LIMS, NIMBUS-SAMS and UARS-iSAMS for the extension back to 1978 depends on the results of the assessment of the data availability and data quality.

3.4.1.1 L2 (HARMOZ-like) satellite limb sounder profiles

The original profile data have been assembled by the SPARC WAVAS activity for the following satellite limb sounders: ACE-FTS, ACE-MAESTRO, Aura-MLS, HALOE, MIPAS, POAM III, SAGE II, SCIAMACHY, and SMR.

These observations have been converted into a harmonised format, following the conventions of the HARMOZ dataset of Ozone profiles, HARMOZ (Sofieva et al., 2013). The harmonised dataset consists of original retrieved water vapour profiles (Level 2) from each instrument, which are screened for invalid data according to the recommendations of the instrument teams. The harmonised dataset was processed into two versions: on a common fixed pressure grid and on a common fixed altitude

grid, both in NetCDF-4 format. The pressure grid corresponds to vertical sampling of ~1 km below 20 km and 2–3 km above 20 km. The fixed altitude grid has 1-km steps between 10 and 70 km. The vertical range of the water vapour profiles is specific for each instrument, thus all information contained in the original data is preserved. Geolocation, uncertainty estimates, and vertical resolution are provided for each profile. For each instrument, optional parameters, which are related to the data quality and the profile position, are also included. These water vapour datasets are published by KIT under the name WAVAS_SAHAR (Laeng, 2019).

3.4.1.2 L3 satellite limb sounder zonal mean climatologies

Intermediate instrument time series of L3 zonal monthly mean water vapour fields, which are based on L2 observations that are used for generating the harmonised L2 limb vertical profile WAVAS_SAHAR dataset and which are described in Section 3.4.1.1 were used to produce the final CDR-3. These were provided to WV_cci via the SPARC Data Initiative (SPARC, 2017; Hegglin et al, 2013) and updated to include the latest data versions, now also including climatologies from ACE-MAESTRO and SAGE III/ISS (Hegglin et al., 2020).

The zonal monthly mean time series of water vapour (in volume mixing ratio, VMR) have been calculated for each instrument on the SPARC Data Initiative climatology grid, using 5 degree latitude bins (with midpoints at 87.5°S, 82.5°S, 77.5°S, . . . , 87.5°N) and 28 pressure levels (300, 250, 200, 170, 150, 130, 115, 100, 90, 80, 70, 50, 30, 20, 15, 10, 7, 5, 3, 2, 1.5, 1, 0.7, 0.5, 0.3, 0.2, 0.15, and 0.1 hPa). To this end, profile data have been carefully screened before binning and a hybrid log–linear interpolation in the vertical has been performed. For instruments that provide data on an altitude grid, a conversion from altitude to pressure levels was performed using retrieved temperature/pressure profiles or meteorological analyses (ECMWF, GEOS-5, or NCEP). Similarly, this information was used to convert retrieved number densities into VMR, where needed. Along with the monthly zonal mean value, the standard deviation and the number of averaged data values are given for each grid point.

Note, considered were a sub-selection of the available instrument retrieval versions in WAVAS_SAHAR that have achieved specified quality targets in the L2 limb vertical profile data Round Robin evaluation and some that are additionally assessed within the SPARC Data Initiative (Hegglin et al., 2013). The final instruments chosen included: SAGE II, SAGE III, HALOE, UARS-MLS, POAM III, SMR, MIPAS (IMK), SCIAMACHY, ACE-FTS, ACE-MAESTRO, Aura-MLS and SAGE III/ISS.

3.4.2 Resolution and coverage in space and time

The spatial, vertical and temporal resolution and coverage of CDR-3 follows the SPARC Data Initiative convention using a latitude-pressure grid. Table 3-11 lists the associated technical specifications.

Table 3-11: CDR-3 (L3) – Resolution and coverage in space and time

Dimension	Specification	Notes
Temporal resolution	Monthly mean	
Temporal coverage	1978-2023	
Spatial coverage	Zonal mean	Latitude-pressure coordinates
Latitudinal resolution	SPARC Data Initiative latitude grid	The 5° latitude bins are centered around: 87.5°S, 82.5°S, 77.5°S, ... , 87.5°N
Vertical resolution	SPARC Data Initiative pressure grid	Levels: 300, 250, 200, 170, 150, 130, 115, 100, 90, 80, 70, 50, 30, 20, 15, 10, 7, 5, 3, 2, 1.5, 1, 0.7, 0.5, 0.3, 0.2, 0.15, and 0.1 hPa

3.4.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of CDR-3 is summarised in Table 3-12.

Table 3-12: Expected quality of CDR-3 (L3)

Quantity	Specification	Notes
Accuracy: Systematic component	10–20% (initial estimate)	Bias or systematic difference to other data records such as SWOOSH and GOZCARDs and also a multi-model mean from chemistry climate models
Accuracy: Random component	5–10% (initial estimate)	The cRMSD in the monthly mean values to above data records
Stability	2% per decade	Stability cannot be quantified satisfactorily over the full 1978–2023 time period due to a lack of high-quality reference observations. However, this estimate is given under the assumption that the merged product will be produced out of datasets having small drifts (estimated to be 0.3% dec ⁻¹) with respect to each other.

3.4.4 Product layers, auxiliary output, format and metadata

Table 3-13 and Table 3-14 compile the product layers, shown here separately for main and additional variables.

Table 3-13: CDR-3 (L3) – Main variable list and description

Variable shortname	unit	Dimensions	Longname/description/comment
lat	degrees_north	N_{lat}	Latitude / predefined latitude bands
plev	hPa	$N_{pressure}$	Pressure / predefined atmospheric pressure grid
time	months since 15 January 1980-01-01	N_{time}	Time
zmh2o	mole mole-1	$N_{time} \times N_{lat} \times N_{pressure}$	Zonal Mean Water Vapour Volume Mixing Ratio

Table 3-14: CDR-3 (L3) – Additional variable list and description

Variable shortname	unit	Dimensions	Longname/description/comment
zmh2o_uncertainty	%	$N_{lat} \times N_{pressure} \times N_{time}$	Uncertainty of Zonal Mean Water Vapour Volume Mixing Ratio
zmh2o_stdv	mole mole-1	$N_{lat} \times N_{pressure} \times N_{time}$	Standard Deviation of Zonal Mean Water Vapour Volume Mixing Ratio
quality_flag	N/A	$N_{lat} \times N_{pressure} \times N_{time}$	Quality Flag of Zonal Mean Water Vapour Volume Mixing Ratio

An estimate of the file sizes is given in Table 3-15.

Table 3-15: Estimate of final product output data volume (CDR-3)

	Month	Year	Full period
Size	40 kB	500 kB	23 MB

The file format used for storing the data is NetCDF-4 classic. All (NetCDF) files follow the NetCDF Climate and Forecast (CF) Metadata Conventions version 1.7. CF standard names used for the main variables and global attributes required to ensure compliance with CCI Data Standards were added. Compliance with the CCI Data Standards was cross-checked and confirmed as the products were being generated.

The metadata information, that will be provided with the data files, is explained in Table 3-16.

Table 3-16: Metadata in stratospheric VRWV (CDR-3)

Metadata name	Comment
Title	
Institution	
Source	Source description of the datasets included in the final product.
References	
History	History of sequential processing steps.
Tracking_id	A universally unique identifier for the data product in UUID format (128 bit), generated by the processing code (e.g., ee307c3a-9d50-4140-b66e-9de5f818f4db).
Conventions	CF conventions version number.
Product_version	
Format_version	Version of CCI data standards.
Summary	Summary of what is included in given data product.
Keywords	
Id	Identifier of product category as given in the file name.
Naming authority	Organization or entity responsible for assigning the unique identifier.
Comment	
Date created	
Creator-name	Institution involved in the generation of the data product.
Creator-url	
Creator-email	
Project	Project within which dataset was produced.
Geospatial lat_min	
Geospatial lat_max	
Geospatial lat_units	
Geospatial lat_resolution	
Geospatial vertical_min	
Geospatial vertical_max	
Geospatial vertical_units	

Metadata name	Comment
Time coverage_start	
Time coverage_end	
Time coverage_duration	Temporal duration given in CF format (e.g., 'P1M' for a monthly product)
Standard_name_vocabulary	Standard used to define the standard names of the physical quantity within the data (e.g., CF Standard name table)
Licence	
Platform	Names of satellite instrument platforms
Sensor	Names of satellite instruments
Key_variables	Primary variable stored in file

3.5 CDR-4

CDR-4 input data consist of L2 vertical profile data from RAL IMS satellite profiles (see product specification in DARD v3.1) and limb sounders (MIPAS and Aura-MLS, see product specification in Section 3.4.1.1).

3.5.1 Used input data

CDR-4 used as input data for the stratosphere observations from international satellite limb sounders as obtained directly from the different data providers (see information in Section 3.4.1.1). However, for this version we focussed only on MIPAS and Aura-MLS. For the troposphere below 300 hPa, we used water vapour retrievals as derived using the RAL IMS scheme, which provides profiles of water vapour from combining measurements of Metop IASI, AMSU and MHS. In the UTLS region between 100 hPa and 300 hPa, a bias-correction, which is based on the climatological VRWV field from balloon-borne hygrometer profiles, is applied to the L2 VRWV profiles from Aura-MLS, MIPAS, and RAL IMS. The final CDR-4 product comprises merged VRWV profiles from 1000 hPa up to 10 hPa (1000, 950, 900, 850, 800, 750, 700, 650, 600, 550, 500, 450, 400, 350, 300, 250, 225, 200, 175, 150, 125, 100, 70, 50, 30, 10 hPa) with a horizontal resolution of 5 degrees and 5 degrees in latitude and longitude.

3.5.2 Resolution and coverage in space and time

The spatial, vertical and temporal resolution and coverage of CDR-4 is similar to the SPARC Data Initiative convention (see Section 3.4.2) but using a latitude–longitude–pressure grid. Table 3-17 lists the associated technical specifications.

Table 3-17: CDR-4 – Resolution and coverage in space and time

Dimension	Specification	Notes
Temporal resolution	Monthly mean	
Temporal extent	2007–2023	
Spatial domain	Global	Latitude–longitude–pressure coordinates
Vertical resolution	Pressure grid	26 levels: 1000, 950, 900, 850, 800, 750, 700, 650, 600, 550, 500, 450, 400, 350, 300, 250, 225, 200, 175, 150, 125, 100, 70, 50, 30, 10 hPa
Vertical extent	1000–10 hPa	From the troposphere to the stratosphere, with special focus on the UTLS
Latitudinal resolution	5 degrees	90°S to 90°N
Longitudinal resolution	5 degrees	180°W to 180°E

3.5.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of CDR-4 is summarised in Table 3-18.

Table 3-18: Expected quality of CDR-4

Quantity	Specification	Notes
Accuracy: Systematic component	20–40% (initial estimate)	Bias against other datasets such as reanalyses, FPH sondes. Value is highly uncertain, since information is currently not available. Initial estimate is based on Hegglin et al. (2013)
Accuracy: Random component	10–20% (initial estimate)	cRMSD based on monthly means against other datasets. Value highly uncertain, since information is currently not available. Initial estimate is based on Hegglin et al. (2013)
Stability	2% dec ⁻¹ (initial estimate)	Value highly uncertain, since information is currently not available.

Quantity	Specification	Notes
		Same assumption used as for CDR-3, see Table 3-12

3.5.4 Product layers, auxiliary output, format and metadata

Table 3-19 and Table 3-20 compile the product layers, shown here separately for main and additional variables.

Table 3-19: CDR-4 (L3) – Main variable list and description

Variable shortname	unit	Dimensions	Longname/description/comment
lat	degrees_north	N _{lat}	Latitude / predefined latitude bands
lon	degrees_east	N _{lon}	Longitude / predefined longitude bands
plev	hPa	N _{pressure}	Pressure / predefined atmospheric pressure grid
time	months since 15 January 1980-01-01	N _{time}	time
vmrh2o	ppmv	N _{lon} X N _{lat} X N _{pressure} X N _{time}	Water Vapour Volume Mixing Ratio

Table 3-20: CDR-4 (L3) – Additional variable list and description

Variable shortname	unit	Dimensions	Longname/description/comment
vmrh2o_stdv	ppmv	N _{lon} X N _{lat} X N _{pressure} X N _{time}	Standard Deviation of Water Vapour Volume Mixing Ratio
vmrh2o_uncertainty	%	N _{lon} X N _{lat} X N _{pressure} X N _{time}	Uncertainty of Water Vapor Volume Mixing Ratio
quality_flag	N/A	N _{lon} X N _{lat} X N _{pressure} X N _{time}	Quality Flag of Water Vapor Volume Mixing Ratio

An estimate of the file sizes is given in Table 3-21.

Table 3-21: Estimate of final product output data volume (CDR-4)

	Month	Year	Full period
Size	1 MB	10 MB	170 MB

The file format used for storing the data is NetCDF-4 classic. All (NetCDF) files follow the NetCDF Climate and Forecast (CF) Metadata Conventions version 1.7. CF standard names used for the main variables and global attributes required to ensure compliance with CCI Data Standards were added. Compliance with the CCI Data Standards was cross-checked and confirmed as the products were being generated. The metadata information, that will be provided with the data files, is explained in Table 3-22.

Table 3-22: Metadata in UTLS VRWV (CDR-4)

Metadata name	Comment
Title	
Institution	
Source	Source description of the datasets included in the final product.
References	
Tracking_id	A universally unique identifier for the data product in UUID format (128 bit), generated by the processing code (e.g., ee307c3a-9d50-4140-b66e-9de5f818f4db).
Conventions	CF conventions version number.
Product_version	
Format_version	Version of CCI data standards.
Summary	Summary of what is included in given data product.
Keywords	
Id	Identifier of product category as given in the file name.
Keywords_vocabulary	Standard used to define the keywords associated with the data (e.g., CF Standard name table)
Cdm_data_type	Common Data Model data type, e.g., 'grid' (explained in more detail e.g., in Nativi et al., 2008)
Comment	
Creator-name	Institution involved in the generation of the data product.
Creator-url	
Creator-email	
Project	

Metadata name	Comment
Geospatial lat_min	
Geospatial lat_max	
Geospatial lat_units	
Geospatial lat_resolution	
Geospatial lon_min	
Geospatial lon_max	
Geospatial lon_units	
Geospatial lon_resolution	
Geospatial vertical_min	
Geospatial vertical_max	
Spatial_resolution	
Time coverage_start	
Time coverage_end	
Time coverage_duration	Temporal duration given in CF format (e.g., 'P1M' for a monthly product)
Time coverage_resolution	
Standard_name_vocabulary	Standard used to define the standard names of the physical quantity within the data (e.g., CF Standard name table)
Licence	
Platform	Names of satellite instrument platforms
Sensor	Names of satellite instruments
Key_variables	Primary variable stored in file

4. COMPLIANCE WITH USER REQUIREMENTS

We here discuss the compliance of the different envisaged WV_cci CDRs with the user requirements as derived in the URD (v3.0).

It is noted that the URD v3.0 does not (yet) include the new requirements defined in GCOS-245.

4.1 Level 3 CDR-1 and CDR-2

For the Level 3 CDR-1 and CDR-2 TCWV product, compliance with the user requirements as defined in the URD are judged to be as follows.

Resolution:

These products (with a resolution of 0.05°/0.5° and daily and monthly estimates) aims at fulfilling breakthrough requirements on spatial and temporal resolution. Note that the over ocean TCWV data relies on microwave observations and thus is oversampled for the 0.05° spatial grid. It is further noted that the daily estimates over land rely on one estimate per day at maximum at the equator. This might be uncritical in view of the small diurnal cycle of TCWV which was analysed on basis of GNSS data.

Accuracy:

The maximum systematic (random) component of the uncertainty is estimated to be 0.75 kg/m² (2.75 kg/m²) and based on the precursor, MERIS and SSM/I only product. This transforms into approximately 3.5% (13%) when using an average global TCWV value of 22 kg/m² as observed by the ESA GlobVapour product in July 2006. Thus, it is expected that the threshold requirement for the random component is within reach and that the breakthrough requirement on the systematic component will likely be achieved. Note that the provided initial estimates are based on intercomparisons using monthly means. Thus, the cRMSD contains differences in sampling and not necessarily the clear-sky sampling bias which is however contributing to the total uncertainty. Further note that the cRMSD of daily data will likely be larger due to larger natural variability.

Stability:

CDR-2 version 3.1 from WV_cci phase 1 exhibits a stability of 0.09 kg/m²/decade relative to AIRS. This would be slightly below optimum requirement. A value of 0.2 kg/m²/decade, as given in Table 3-7, is close to the breakthrough requirement. The stability depends on the considered region and the data record used for comparison:

during phase 1 values between -0.39 and $+0.18$ $\text{kg/m}^2/\text{decade}$ were observed when looking at results for land, ocean and global data. For climate change analysis, it was recommended to analyse clear-sky data over only when focusing on land areas and to disregard data over land from April 2016 onwards (PVIR, 2021). The clear-sky nature of CDR-2 over land cannot be changed. The recalibration, harmonisation and homogenisation of NIR data is not carried out within WV_cci. In particular, to our knowledge, the harmonisation and homogenisation of MERIS and OLCI with MODIS is not addressed at all in Level 1 space. Thus, stability issues might still be present even after phase 2.

4.2 Level 3 CDR-3

For Level 3 zonal mean stratospheric profiles, compliance with the user requirements as defined in the URD (v3.0) are judged to be as follows.

Resolution:

As follows from the compliance assessment of the L2 data, the expected horizontal and vertical resolution of the L3 CDR-3 (since they are limited to the characteristics of the L2 input data) are compliant with the threshold requirements, but do not achieve breakthrough requirements as defined in the URD. Note that WV_cci will deliver CDR-3 as zonal monthly means and not as three-dimensional fields in order to optimise data quality and to avoid too many data gaps, which while not ideal, still 20% of the stratospheric data users find useful (Level 2 CDR-3 will also be available). The monthly temporal resolution also achieves the threshold requirements.

Accuracy:

The uncertainty in the systematic component is expected to be constrained to between 10 and 20% and hence lies halfway between threshold and breakthrough requirements. The same is true for the uncertainty in the random component, with the expected 5–10%.

Stability:

The expected stability of $2\% \text{ dec}^{-1}$ is better than the threshold ($2.5\% \text{ dec}^{-1}$), but is not quite compliant with the breakthrough requirement ($<1\% \text{ dec}^{-1}$).

4.3 Level 3 CDR-4

For the Level 3 CDR-4 vertically resolved UTLS product, compliance with the user requirements as defined in the URD (v3.0) are judged to be as follows.

Resolution:

The L3 CDR-4 product (monthly averages with a resolution of 5°) aims at providing high vertical resolution within the UTLS regions. As follows the compliance assessment on the vertical resolution for I2 input data, the vertical resolution of the L3 CDR-4 (1–2 km) is compliant with the threshold requirement. The horizontal resolution of CDR-4 is set as 5 degrees in order to optimise data quality from limb sounders in stratosphere and UTLS, which still fulfils threshold requirements. The monthly data also meets the threshold requirements for temporal resolution.

Accuracy:

The uncertainty in the systematic component is estimated to be between 20 and 40%, which would not meet the threshold requirement. For the uncertainty in the random component, an expected 10–20% may just about achieve the threshold requirement.

Stability:

The expected stability of 2% dec⁻¹ is expected to be larger than the threshold (1% dec⁻¹).

5. SUMMARY AND CONCLUSIONS

The presented PSD lays out the product specifications for the WV_cci products. The compliance analysis with respect to accuracy was based on initial estimates of the expected product uncertainties. Demonstrating the stability of all WV_cci products has turned out to be a challenge. Overall, it is anticipated that the CDRs envisaged within WV_cci will be compliant with the new threshold and partly with the new target user requirements as defined by the URD.

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APPENDIX 2: GLOSSARY

This appendix explains all utilised abbreviations of this document.

Term	Definition
ABC(t)	Atmosphere Biosphere Climat (teledetection)
ACE-FTS	Atmospheric Chemistry Experiment Fourier Transform Spectrometer
ACE-MAESTRO	Atmospheric Chemistry Experiment Measurements of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation
AMSR-E	Advanced Microwave Scanning Radiometer for EOS
AMSU	Advanced Microwave Sounding Unit
ARA	Atmospheric Radiation Analysis
ARSA	Analyzed RadioSoundings Archive
AVHRR	Advanced Very High Resolution Radiometer
BC	Brockmann Consult
CARIBIC	Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container
CCI	Climate Change Initiative
CDO	Climate Data Operators
CDR	Climate Data Record
CDS	Copernicus Climate Data Store
CEDA	Centre for Environmental Data Analysis
CF	Conventions for Climate and Forecast
CM SAF	EUMETSAT Satellite Application Facility on Climate Monitoring
CMAM	Canadian Middle Atmosphere Model
CMIP	Coupled Model intercomparison Project
CMUG	Climate Modelling User Group
CRG	Climate Research Group
DLR	Deutschen Zentrums für Luft- und Raumfahrt
DWD	Deutscher Wetterdienst (German MetService)
ECCE	Environment and Climate Change Canada
ECMWF	European Centre for Medium-Range Weather Forecasts
ECV	Essential Climate Variable
EDA	ERA5 - reduced resolution ten member ensemble
EMiR	ERS/Envisat MWR Recalibration and Water Vapour Thematic Data Record Generation

Term	Definition
Envisat	Environmental Satellite
ERA5	ECMWF Re-Analysis 5
ERA-Interim	ECMWF Re-Analysis Interim
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GCOS	Global Climate Observing System
GEOS-5	Goddard Earth Observing System Model, Version 5
GMI	Global Precipitation Microwave Imager
GNSS	Global Navigation Satellite System
GOMOS	Global Ozone Monitoring by Occultation of Stars
GOZCARDS	Global Ozone Chemistry And Related trace gas Data records for the Stratosphere
GPS	Global Positioning System
GRUAN	GCOS Reference Upper-Air Network
HARMOZ	HARMonized dataset of Ozone profiles
HALOE	Halogen Occultation Experiment
HIRDLS	High Resolution Dynamics Limb Sounder
HOAPS	Hamburg Ocean Atmosphere Parameters and Fluxes from Satellite Data
IAGOS	In-service Aircraft for a Global Observing System
IASI	Infrared Atmospheric Sounder Interferometer
ILAS-II	Improved Limb Atmospheric Spectrometer-II
IMS	Infrared Microwave Sounding
IPSL-CM	Institut Pierre Simon Laplace Climate Model
IR	Infrared
LMD	Laboratoire Météorologie Dynamique
LMS	Lowermost stratosphere
LST	Land Surface Temperature
LWP	Vertically integrated liquid water
MERIS	Medium Resolution Imaging Spectrometer Instrument
MERRA-2	Modern-Era Retrospective analysis for Research and Applications, Version 2
MHS	Microwave Humidity Sounder
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder

Term	Definition
MODIS	Moderate Resolution Imaging Spectrometer
MOZAIC	Measurement of OZone by Airbus In-service airCraft
MPI-M	Max-Planck Institute for Meteorology
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCEO	National Centre for Earth Observation
NCEP	National Centers for Atmospheric Prediction
NDVI	Normalized Difference Vegetation Index
NIR	Near IR
NOAA	National Oceanic & Atmospheric Administration
NWP	Numerical Weather Prediction
OLCI	Ocean and Land Colour Instrument
PCs	Principle components
POAM	Polar Ozone and Aerosol Measurement
PSD	Product Specification Document
RAL	Rutherford Appleton Laboratory
RMS	Root mean square
RR	Reduced resolution
RTTOV	Radiative Transfer for TOVS
SAGE	Stratospheric Aerosol and Gas Experiment
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
SCISAT	Scientific Satellite
SE	Spectral Earth
SMILES	Solar wind Magnetosphere Ionosphere Link Explorer
SMR	Software Modification Report
SNR	Signal-to-noise ratio
SOFIE	Solar Occultation For Ice Experiment
SPARC	Stratosphere-troposphere Processes And their Role in Climate
SPURT	Spurenstofftransport in der Tropopausenregion, trace gas transport in the tropopause region
SSM/I	Special Sensor Microwave Imager
SSMIS	Special Sensor Microwave Imager Sounder
SST	Sea Surface Temperature

Term	Definition
SuomiNet	Global ground based GPS network (named after Verner Suomi)
SWOOSH	Stratospheric Water and OzOne Satellite Homogenized data set
TBD	To be determined
TCWV	Total Column Water Vapour
TMI	Tropical Rainfall Measuring Mission's Microwave Imager
TOA	Top Of Atmosphere
UKMO	United Kingdom Meteorological Office
UoL	University of Leicester
UoR	University of Reading
URD	User Requirements Document
UT	Upper troposphere
UTLS	Upper Troposphere and Lower Stratosphere
UV	Ultraviolet
vis	Visible
VMR	Volume mixing ratio
VRes	Vertically resolved
WACCM	Whole Atmosphere Community Climate Model
WAVAS-I	Water Vapour Assessment
WAVAS-II	Water Vapour Assessment 2
WCRP	World Climate Research Programme
WGS	World Geodetic System 1984
WMO	World Meteorological Organization
WV	Water Vapour
WV_cci	Water Vapour climate change initiative

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