Water Vapour Climate Change Initiative (WV_cci) - Phase One

Product Specification Document (PSD)

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1. INTRODUCTION

1.1 Purpose of the document

The purpose of this PSD is to provide detailed specifications on the different CDR products that will be delivered for the ECV Water Vapour within the WV_cci project. The specifications will aim at compliance with the user requirements from GCOS, CCI projects and established in consultation with the WV_cci user group and CRG that are summarised in the URD.

1.2 Definitions

Uncertainty definitions are accessible, among others, via:

- VIM, 2012: https://www.bipm.org/utils/common/documents/jcgm/JCGM_200_2012.pdf
  Comment: Strictly speaking not applicable as water vapour is not directly measured, based on 2008 version with minor corrections.
- ESA, 2010: http://cci.esa.int/sites/default/files/ESA_CCI_Project_Guidlines_V1.pdf
  Comment: based on VIM.
- ESA SST_cci: http://www.esa-sst-cci.org/PUG/pdf/SST_CCI-UCR-UOR-201-Issue-2-signed.pdf
- H2020 FIDUCEO: http://www.fiduceo.eu/vocabulary
- WMO, 2017: https://library.wmo.int/doc_num.php?explnum_id=4147
  Comment: based on VIM.

Here the terminology as defined in VIM (2012) is used as in URD:

- **Accuracy:** Here refers to the closeness between a measured value and the true value of the measurand, including the effects of systematic errors. JGCM (2012) also states that “the concept ‘measurement accuracy’ is not a quantity and is not given a numerical quantity value. A measurement is said to be more accurate when it offers a smaller measurement error.”

- **Bias**: An estimate of the systematic measurement error.

  The bias will typically be assessed as the systematic (mean) deviation to a consensus reference.

- **Precision:** Describes the random (unpredictable) variability of repeated measurements of the measurand.

- **Uncertainty:** Non-negative parameter, associated with the result of a measurement that characterizes the dispersion of the values that could reasonably be attributed to the measurand.

  This is the information on product quality which is included in the product.

- **Temporal resolution:** Frequency the observations are provided in.

- **Spatial resolution (horizontal and vertical):** Nominal resolution of an observation (taking into account the influence of the satellite's viewing geometry).

- **Stability:** Refers to the property of a measuring instrument, whereby its metrological properties remain constant in time. Alternatively, the maximum acceptable long-term change in the systematic error, usually per decade.

  The stability will typically be assessed as the change of the bias over time.

2. WATER DATA PRODUCT OVERVIEW

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

The primary datasets or CDRs that WV_cci will produce 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). In addition to the primary datasets, WV_cci will also make the input data (L2) that are used to generate the CDR-3 and CDR-4 available.

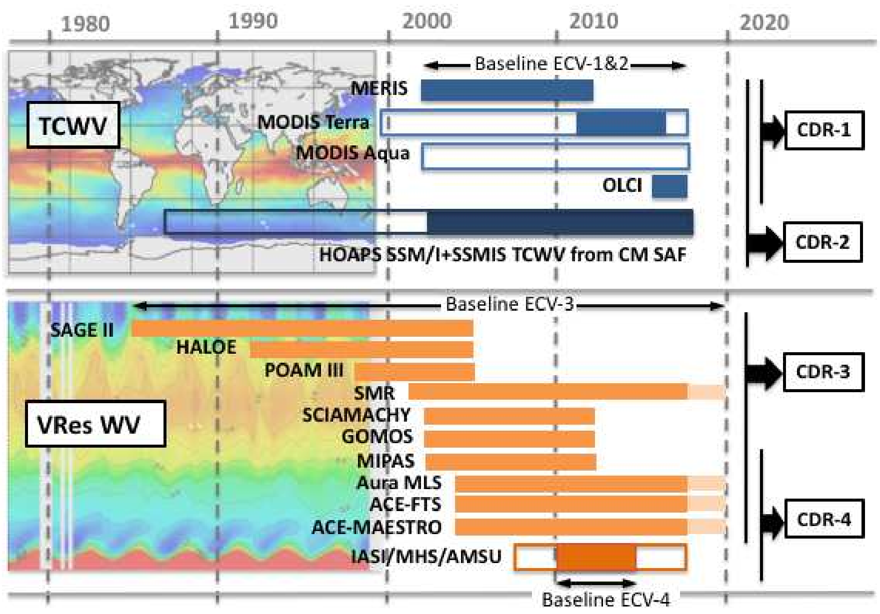

Figure 2-1: Instruments from which input observations (L2 data products) are obtained, and resulting climate data records (CDRs; L3 data products) for total column (TCWV; CDR-1 and CDR-2) and vertically resolved (VRes WV; CDR-3 and CDR-4) water vapour.

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)	2002-2017
2	CRD-2	L3	TCWV gridded monthly and daily data (land and ocean)	2002-2017

#	Product Name	Level	Notes	Time period
3	CDR-3	L2 & L3	Stratospheric vertically resolved zonal monthly mean WV CDR (2D)	1985-2019
4	CDR-4	L2 & L3	UTLS vertically resolved monthly mean WV CDR (3D)	2010-2014

2.1 CDR-1: TCWV (land)

This vertically integrated (total column) water vapour ECV, in units of kg/m^2, will be a gridded L3 data product over land based on ESA (MERIS, OLCI) and NASA instruments (MODIS). The final dataset will cover the period July 2002 to December 2017.

2.2 CDR-2: TCWV (land and ocean)

The CDR-2 dataset will be a global, i.e., land and ocean coverage, TCWV product in units of kg/m^2. It will contain the CDR-1 over land, coasts and sea-ice and the HOAPS microwave imager based TCWV data over ocean. The HOAPS data will be provided by EUMETSAT CM SAF. The final dataset will cover the period July 2002 to December 2017.

2.3 CDR-3: Vertically resolved stratospheric water vapour climatologies

This vertically resolved water vapour ECV will be a merged data product based on a range of ESA, third-party and NASA instruments including SAGE II, HALOE, POAM III, Odin SMR, MIPAS, SCIAMACHY, GOMOS, ACE-MAESTRO, ACE-FTS and Aura-MLS and spanning the time period 1985 to the end of 2019. The product will be 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 will consist of three-dimensional vertically resolved water vapour data, covering the troposphere and lower stratosphere from 2010 to 2014. The water vapour based on IMS, MIPAS, ACE-FTS, ACE-MAESTRO, and Aura-MLS. The global product will include mixing ratios in units of ppmv.

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

The input data sets for the generation of the CDR-1 water vapour data products will be:

- MERIS L1b reduced resolution (2002-2012), 4th reprocessing,
- MODIS TERRA MOD021KM (2011-2017), collection 6,
- OLCI L1b reduced resolution (2016-2017), 1st reprocessing,

For additional processing proposed as an option for this project, the extended input data sets would be:

- MODIS TERRA MOD021KM (2000-2017), collection 6,
- MODIS AQUA MYD021KM (2002-2017), collection 6.

The MERIS L1b data will originate from the latest available data reprocessing version. It is envisaged to use the 4th reprocessing for the final production run, however, at compilation time of this document this data set is still under ESA review and not yet available. In the meantime, the 3rd reprocessing version of L1b reduced resolution data set will be used as fallback. The same applies for the OLCI 1st reprocessing, here, OLCI NRT/NTC products could be used as fallback. Both fallback data sets are available at BC.

Data from ERA5 will be used as a priori input to the retrieval.

3.1.2 Resolution and coverage in space and time

3.1.2.1 TCWV L2 Products

For each L1b input product, a corresponding TCWV L2 product will be generated on the same grid. The TCWV retrieval will be applied on pixels classified as **land and cloud-free**. The collection of the generated L2 products will in return serve as input for the TCWV L3 product generation.

Table 3-1 gives an overview of the product layers in these products. In addition, the TCWV L2 product will contain a copy of the tie point grids of the L1b input product.

Table 3-1: Product layers in TCWV L2 products.

Name in product	Unit	Type	Description
tcwv	kg/m^2	int16	Total Column Water Vapour
tcwv_uncertainty (TBD – BC/SE)	kg/m^2	int16	Uncertainty of Total Column Water Vapour
tcwv_quality_flag (TBD – BC/SE)	dl	int8	Quality flag of Total Column Water Vapour
pixel_classif_flag	dl	uint16	pixel classification flag

3.1.2.2 TCWV L3 Products

The final TCWV L3 land products which will be delivered as CDR-1 dataset will be generated from the L2 products by

- temporal aggregation (daily and optionally monthly[1])
- spatial aggregation (global, WGS84, 0.5 and 0.05 degree resolution)

Table 3-2 provides an overview of the technical specifications.

Table 3-2: CDR-1 - Resolution and coverage in space and time.

Dimension	Specification
Temporal resolution	Daily and optionally monthly

[1] *The monthly L3 products are not part of the initially agreed products to be delivered, but have been identified as a quite useful add-on. Their generation needs to be confirmed.*

Dimension	Specification
Temporal coverage	July 2002 – December 2017
Spatial coverage	global
Spatial resolution	0.5 or 0.05 deg

3.1.3 Uncertainty estimates, quality indicators, and expected accuracy

After the iteration procedure of the TCWV algorithm, the retrieval uncertainty is calculated, considering the following sources of uncertainty:

- instrument uncertainty (SNR).
- uncertainty of the auxiliary aerosol optical depth over land (assumed to be 0.1).
- uncertainty of the surface pressure and –temperature (assumed to be 5 K and 5 hPa). It turned out, that this influence is insignificant.
- uncertainty due to the missing information about aerosol scale height by using as scattering factor f, belonging to a high aerosol layer.
- For MERIS and OLCI, using the forward operator, the uncertainty due to the estimation of the surface reflectance and spectral slope is quantified using an NDVI measure.

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

Table 3-3: Expected quality of CDR-1.

Quantity	Specification	Notes
Accuracy: Systematic component	1 kg/m^2 (initial estimate)	Bias or systematic difference to other data records, monthly means, at lower end of results from ESA DUE GlobVapour
Accuracy: Random component	3 kg/m^2 (initial estimate)	RMSD to other data records, monthly means, at lower end of results from ESA DUE GlobVapour
Stability	<0.02 (kg/m^2)/year (initial estimate)	This is the observed trend in MERIS time series.

3.1.4 Product layers, auxiliary output, format and metadata

Table 3-4 gives an overview of the product layers in CDR-1.

Table 3-4: Product layers in TCWV L3 product (CDR-1).

Name in product	Type	Description
tcwv	float32	Total Column Water Vapour
tcwv_uncertainty (TBD – BC/SE)	float32	Uncertainty of Total Column Water Vapour
tcwv_quality_flag (TBD – BC/SE)	int8	Quality flag of Total Column Water Vapour
tcwv_counts	int16	number of TCWV L2 retrievals contributing to L3 grid cell

An estimate of the file sizes is given in Table 3-5.

Table 3-5: 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 will follow the NetCDF Climate and Forecast (CF) Metadata Conventions version 1.7. CF standard names will be used for the main variables and global attributes required to ensure compliance with CCI Data Standards will be added. Compliance with the CCI Data Standards will be cross-checked and confirmed as the products are being generated.

3.2 CDR-2

The CDR-2 TCWV product will combine the land-based CDR-1 product and the ocean-based microwave imager HOAPS product from EUMETSAT CM SAF. Coastal areas and sea-ice regions will be filled with NIR-based products. This way, sensor specific advantages are 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 as to cover land, sea-ice and coastal areas. Input data specifications fro CDR-1 are described in section 3.1.

Over ocean TCWV from the CM SAF HOAPS product is used. 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 but can not be reliably retrieved in presence of strong scattering events such as in strong precipitation cases. At present CM SAF is preparing for the HOAPS v5. It is planned that this product will rely on SSM/I, SSMIS, AMSR-E, TMI, and GMI data. The currently foreseen specifications are: 0.5° spatial resolution, daily and monthly resolution, global ice-free coverage over the period July 1988 – December 2019.

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 an application of the 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 3-6.

Table 3-6: Expected quality of CDR-2.

Quantity	Specification	Notes
Accuracy: Systematic component	1 kg/m^2 (initial estimate)	Bias or systematic difference to other data records, monthly means, at lower end of results from ESA DUE GlobVapour
Accuracy: Random component	3 kg/m^2 (initial estimate)	RMSD to other data records, monthly means, at lower end of results from ESA DUE GlobVapour
Stability	<0.02 (kg/m^2)/year (initial estimate)	This is the observed trend in MERIS time series.

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 3-7.

Table 3-7: Product layers in TCWV L3 product (CDR-2).

Name in product	Type	Description
tcwv	float32	Total Column Water Vapour
tcwv_uncertainty (TBD – BC/SE)	float32	Uncertainty of Total Column Water Vapour
tcwv_quality_flag (TBD – BC/SE)	int8	Quality flag of Total Column Water Vapour
tcwv_counts	int16	number of TCWV L2 retrievals contributing to L3 grid cell

An estimate of the file sizes is given in Table 3-8.

Table 3-8: 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 will follow the NetCDF Climate and Forecast (CF) Metadata Conventions version 1.7. CF standard names will be used for the main variables and global attributes required to ensure compliance with CCI Data Standards will be added. Compliance with the CCI Data Standards will be cross-checked and confirmed as the products are being generated.

3.3 CDR-3

3.3.1 Used input data

CDR-3 uses as input data observations from international satellite limb sounders as obtained directly from the different data providers as both single profile data (see

Section 3.3.1.1) and zonal monthly mean climatologies processed for the SPARC Data Initiative (see Section 3.3.1.2).

3.3.1.1 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, GOMOS, HALOE, MIPAS, POAM III, SAGE II, SCIAMACHY, and SMR.

These observations will be converted into a harmonized format, following the conventions of the HARMonized dataset of OZone profiles, HARMOZ (Sofieva et al., 2014). The harmonized 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 harmonized dataset will be processed into two versions: on a common fixed pressure grid and on 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.

3.3.1.2 L3 satellite limb sounder zonal mean climatologies

Intermediate L3 zonal monthly mean climatologies that are based on the L2 limb satellite profiles described in Section 3.3.1.1 will be used to produce the final CDR-3. These are provided to WV_cci via the SPARC Data Initiative (SPARC, 2017; Hegglin et al, 2013) and updated to include latest data versions, now also including climatologies from ACE-MAESTRO. The climatologies are based on L2 observations that are used for generating the homogenised L2 limb vertical profile, which are data described in Section 3.3.1.1.

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 is performed using retrieved temperature/pressure profiles or meteorological analyses (ECMWF, GEOS-5, or NCEP). Similarly, this information is 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.

Considered are a sub-selection of the available instrument that will achieve specified quality targets in the L2 limb vertical profile data Round Robin evaluation and as assessed from the SPARC Data Initiative (Hegglin et al., 2013). The instruments under selection include: SAGE II, SAGE III, HALOE, POAM 3, SMR, MIPAS, SCIAMACHY, ACE-FTS, ACE-MAESTRO, and Aura-MLS.

3.3.2 Resolution and coverage in space and time

The spatial, vertical and temporal resolution and coverage of CDR-3 mostly follow the SPARC Data Initiative convention using a latitude-pressure grid. Table 3-9 lists the associated technical specifications.

Table 3-9: CDR-3 (L3) - Resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	Monthly mean	
Temporal coverage	1985-2019	
Spatial coverage	Zonal mean	Latitude-pressure coordinates
Latitudinal resolution	SPARC Data Initative 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 Initative 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

3.3.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of CDR-3 is summarised in Table 3-10.

Table 3-10: Expected quality of CDR-3 (L3).

Quantity	Specification	Notes
Accuracy: Systematic component	10-20% (initial estimate)	For L3, the systematic component (bias) of the overall uncertainty will be defined based on an end-to-end error budget assessment that will include the uncertaintites of the input data (±10%), identified sampling biases, and the merging process that uses chemistry-climate models as transfer functions against reference dataset.
Accuracy: Random component	5-10% (initial estimate)	The random component of the overall uncertainty for L3 CDR-3 will be determined by the RMSE in the monthly mean values. The L2 product has an estimated precision of 5%.
Stability	2% per decade	Stability may not be able to be quanitifed over the full 1985-2019 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.

3.3.4 Product layers, auxiliary output, format and metadata

Table 3-11 and Table 3-12 compile the product layers, here separately for main and additional variables.

Table 3-11: 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} x N_{lat} x $N_{pressure}$	zonal Mean Water Vapour Volume Mixing Ratio

Table 3-12: CDR-3 (L3) – Additional variable list and description.

Variable shortname	unit	Dimensions	Longname/description/comment
vmrh2o_std	mole mole-1	N_{lat} x $N_{pressure}$ x N_{time}	Water Vapour Volume Mixing Ratio Standard deviation
vmrh2o_nr	N/A	N_{lat} x $N_{pressure}$ x N_{time}	Number of values per climatological bin
vmrh2o_uncertainty	%	N_{lat} x $N_{pressure}$ x N_{time}	Overall uncertainty estimate of gridpoint value
Quality_flag	N/A	N_{lat} x $N_{pressure}$ x N_{time}	Threshold indicator that flags highly uncertain values

An estimate of the file sizes is given in Table 3-13.

Table 3-13: Estimate of final product output data volume (CDR-3).

	month	year	Full period
Size	25 MB	300 MB	7.5 GB

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

3.4 CDR-4

CDR-4 input data consist of L2 vertical profile data from RAL IMS satellite profiles (see product specification in Section 3.4.1.1) and limb sounders (MIPAS, ACE-FTS, ACE-MAESTRO, Aura-MLS), see product specification in Section 3.3.1.1).

3.4.1 Used input data

CDR-4 uses as input data for the stratosphere observations from international satellite limb sounders as obtained directly from the different data providers (see information in Section 3.3.1.1). However, for this prototype version we will focus only on ACE-FTS, ACE-MAESTRO, MIPAS, and Aura-MLS (apart from other instruments that may be identified from the UTLS validation work in WP2.7). For the troposphere, we will use 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. As part of the work in year 1, Level 3 files will be created for WV_cci from the existing L2 files (see DARD for further information).

3.4.2 Resolution and coverage in space and time

The spatial, vertical and temporal resolution and coverage of CDR-4 mostly follow the SPARC Data Initiative convention (see section 3.3.2) using a latitude-pressure grid. Table 3-14 lists the associated technical specifications.

Table 3-14: CDR-4 - Resolution and coverage in space and time.

Dimension	Specification	Notes
Temporal resolution	Monthly mean	
Temporal extent	2010-2014	Only short time period is provided since this is a prototype CDR
Spatial domain	Global	Latitude-longitude-pressure coordinates
Vertical resolution	1-2 (3-5) km	These values are estimates for the UTLS (deeper troposphere and stratosphere)
Vertical extent	1000-10 hPa	These values are estimates for the UTLS (deeper troposphere and stratosphere)
Latitudinal resolution	100 km	
Longitudinal resolution	100 km	

3.4.3 Uncertainty estimates, quality indicators, and expected accuracy

The expected quality of CDR-3 is summarised in Table 3-15.

Table 3-15: Expected quality of CDR-4.

Quantity	Specification	Notes
Accuracy: Systematic component	20-40% (initial estimate)	Value highly uncertain, since information is currently not available. Initial guess is based on Hegglin et al. (2013)

Quantity	Specification	Notes
Accuracy: Random component	10-20% (initial estimate)	Value highly uncertain, since information is currently not available. Initial guess is based on Hegglin et al. (2013)
Stability	2% dec^{-1} (initial estimate)	Value highly uncertain, since information is currently not available.

3.4.4 Product layers, auxiliary output, format and metadata

Table 3-16 and Table 3-17 compile the product layers, here separately for main and additional variables.

Table 3-16: 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	mole mole-1	N_{lon} x N_{lat} x $N_{pressure}$ x N_{time}	Water Vapour Volume Mixing Ratio

Table 3-17: CDR-4 (L3) – Additional variable list and description.

Variable shortname	unit	Dimensions	Longname/description/comment
vmrh2o_std	mole mole-1	N_{lon} x N_{lat} x $N_{pressure}$ x N_{time}	Water Vapour Volume Mixing Ratio Standard deviation
vmrh2o_nr	N/A	N_{lon} x N_{lat} x $N_{pressure}$ x N_{time}	Number of values per climatological bin
vmrh2o_uncertainty	%	N_{lon} x N_{lat} x $N_{pressure}$ x N_{time}	Overall uncertainty estimate of gridpoint value
Quality_flag	N/A	N_{lon} x N_{lat} x $N_{pressure}$ x N_{time}	Threshold indicator that flags highly uncertain values

An estimate of the file sizes is given in Table 3-18.

Table 3-18: Estimate of final product output data volume (CDR-4).

	month	**year**	**Full period**
Size	3 GB	36 GB	180 GB

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

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. At this stage the product specifications are partly initial estimates only.

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:

This product (with an expected resolution of 0.05°/0.5° and daily estimates) aims at fulfilling breakthrough requirements on spatial and temporal resolution. Note that the over ocean TCWV data will rely on microwave observations and will thus be oversampled for the 0.05° spatial grid. It is further noted that the daily estimates over land will 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 systematic (random) component of the uncertainty is estimated to be 1 kg/m^2 (3 kg/m^2) and based on the precursor, MERIS and SSM/I only product. This transforms into 4.5% (14%) when using an average global TCWV value of 22 kg/m^2 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 mans. Thus, the RMSD contains differences in sampling and not necessarily the clears-sky sampling bias which is however contributing to the total uncertainty. Further note that the RMSD of daily data will likely be larger due to larger natural variability.

Stability:

For the precursor version of the ESA GlobVapour project the stability has not been analysed. Thus, the provided value reflects the observed trend of the MERIS based TCWV product. When achieved this would be slightly below target requirement.

4.2 Level 2 input data to ECV-3

For Level 2 stratospheric profiles, compliance with the user requirements as defined in the URD are judged to be as follows.

Resolution:

The typical horizontal and vertical resolution of current stratospheric limb sounders (400-500 km and 3-4 km, respectively) are compliant with the threshold requirements, but do not achieve breakthrough requirements as defined in the URD.

Accuarcy:

A random error of 5% can be achieved for individual instruments, but the instruments are deviating from each other up to +- 10%, though in some cases it can go down to ±3%.

Stability:

Results of the WAVAS-II assessment show that the datasets can drift with respect to each other (not with respect to the truth) as small as 0.3% per decade. Hence, if the merged product will be produced out of these datasets only, than the drift of 0.3% would be realistic expectation. The absolute drift of these datasets is not known yet.

4.3 Level 3 CDR-3

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

Resolution:

As follows from the compliance assessement 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. The monthly time resolution also achieves the threshold requirements.

Accuracy:

The uncertainty in the systematic component is expected to be constraint to between 10-20% and hence should hence meet the threshold requirements easily. For the uncertainty in the random component, an expected 5-10% may only in the best case agree with the breakthrough requirement, however should be well within the threshold requirement.

Stability:

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

4.4 Level 2 input data to CDR-4

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

Resolution:

The vertical resolution of the RAL IMS product is about 3 km in the UTLS, hence does not meet the threshold requirements. The horizontal resolution however is relatively high (25 km), hence just about achieving breakthrough requirements.

Accuracy:

The uncertainty in the systematic component is estimated to be between 20 and 40%, which only would meet threshold requirements at its lower end of the range. However, UTLS specific validation may improve this assessement. For the uncertainty in the random component, an expected 15-30% (or 10-20% after accounting for averaging kernels) is meeting the threshold requirements.

Stability:

No measure of stability has yet been quantified for this product.

4.5 Level 3 CDR-4

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

Resolution:

The initial prototype of this product (with an expected resolution of 100 km / 1-2 (3-4) km for UTLS and deeper troposphere/stratosphere, respectively) aims at fulfilling threshold requirements. The same is currently envisaged for the time resolution (monthly).

Accuracy:

The uncertainty in the systematic component is estimated to be between 15 and 25%, which only marginally would meet threshold requirements. For the uncertainty in the random component, an expected 5-10% may achieve the breakthrough requirement, but should be well within the threshold requirement.

Stability:

The expected stability of 2% dec^{-1} is expected to be much better than the threshold (5%), but is far from being compliant with the breakthrough requirement (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 is based on initial estimates of the expected product uncertainties. Demonstrating the stability of all WV_cci products will be a challenge. Overall, the CDRs envisaged within WV_cci will be compliant with the new threshold and partly with the new target user requirements as newly defined by the URD.

APPENDIX 1: REFERENCES

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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 Receiver
BC	Brockmann Concult
CARIBIC	Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container
CCI	Climat 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)
ECCC	Environment and Climate Change Canada
ECMWF	European Centre for Medium Range Forecast
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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