Water Vapour Climate Change Initiative (WV_cci) - CCI+ Phase 1

Product User Guide (PUG)

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Authors **:** Olaf Danne (Brockmann Consult), Michaela Hegglin (U. Reading), Hao Ye (U. Reading), Marc Schröder (DWD), Rene Preusker (Spectral Earth), Jürgen Fischer (Spectral Earth), Carsten Brockmann (Brockmann Consult)

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2.1	7 June 2022	Revision which addressed v2.0 RIDs
2.2	3 August 2022	Revision which addressed v2.1 RIDs

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1. INTRODUCTION

1.1 Purpose of the document

This document is the user guide for the data products produced by the ESA WV_cci project.

The main aim of the document is to aid a user in selecting a data product they require (including understanding its features and limitations) and then to enable them to read and use the data. A section on how the data are produced is also included for those who are interested.

The combined microwave and near-infrared imager based, global TCWV product (CDR-2) was generated within ESA WV_cci, except for the HOAPS data over ocean which was generated by EUMETSAT CM SAF. Following agreements between EUMETSAT, ESA and the project team, CDR-2 is owned by the EUMETSAT CM SAF. While this PUG describes all products developed within ESA WV_cci, including CDR-2, a dedicated Product User Manual for CDR-2 from CM SAF is available from https://doi.org/10.5676/EUM_SAF_CM/COMBI/V001, and it is recommended reading the PUM from CM SAF to get information on, e.g., access and license.

1.2 Background of the project

As one of the Essential Climate Variables (ECV) [1] produced in the frame of the ESA Climate Change Initiative (ESA CCI), the Water Vapour ECV includes Total Column Water Vapour (TCWV) and Vertically Resolved Water Vapour (VRWV) as primary variables. For TCWV retrieval, the project includes algorithms for the processing of MERIS, MODIS Terra, Sentinel-3 OLCI, and CM SAF HOAPS data. This combination of sensors is applied for the generation of merged products with global coverage over land only (CDR-1), but also over land and water (CDR-2), which allows the investigation of possible temporal, regional or systematic issues in order to improve the algorithms applied for the various sensors. CDR-2 is released by EUMETSAT CM SAF. For VRWV, the project includes the descriptions of two merging algorithms. The first describes the merging between the satellite limb sounders for SAGE II, UARS-MLS, HALOE, POAM III, SMR, SAGE III, SCIAMACHY, MIPAS, ACE-FTS, ACE-MAESTRO, Aura-MLS and SAGE III/ISS for a stratospheric zonal monthly mean climate data record (CDR-3). Here, corrections for handling spatio-temporal sampling differences and biases will be a focus. The second merging algorithm refers to the three-dimensional prototype version of the upper tropospheric/lower stratospheric (UTLS) climate data record (CDR-4), for which the input data consist of observations from the satellite limb sounders MIPAS, Aura-MLS, and a combined retrieval product (IMS) from the IASI/MHS/AMSU satellite instruments. Here, focus is primarily placed on how best to combine and bias-correct observations from nadir and limb sounders across the tropopause region in the merging process, despite their strongly differing viewing geometries.

1.3 Structure of the document

After this introduction, the document is divided into 10 further sections that are described briefly below:

Section 2	gives an overview of the WV_cci processing system as a whole.
Section 3	describes in detail all relevant products used and/or generated by the various steps of the WV_cci processing chains (separately for TCWV and VRWV products).
Section 4	gives a summary of the results from product validation and intercomparison.
Section 5	gives an overview of software tools to visualise and examine the WV_cci data products.
Section 6	describes how the WV_cci data products can be accessed.
Section 7	gives the terms of use of the WV_cci data products.
Sections 8, 9, 10, 11	are appendices containing references, glossary, merging rules and file content listings.

2. SYSTEM OVERVIEW

The WV_cci system interacts with various other entities as illustrated in Figure 2-1. This setup is quite similar to other CCIs such as Fire_cci or Landcover_cci, as described in [2] and [3]. In principle, this system context applies for both WV_cci subsystems for TCWV and VRWV generation (Figure 2-2). More details of this system context are given in [4].

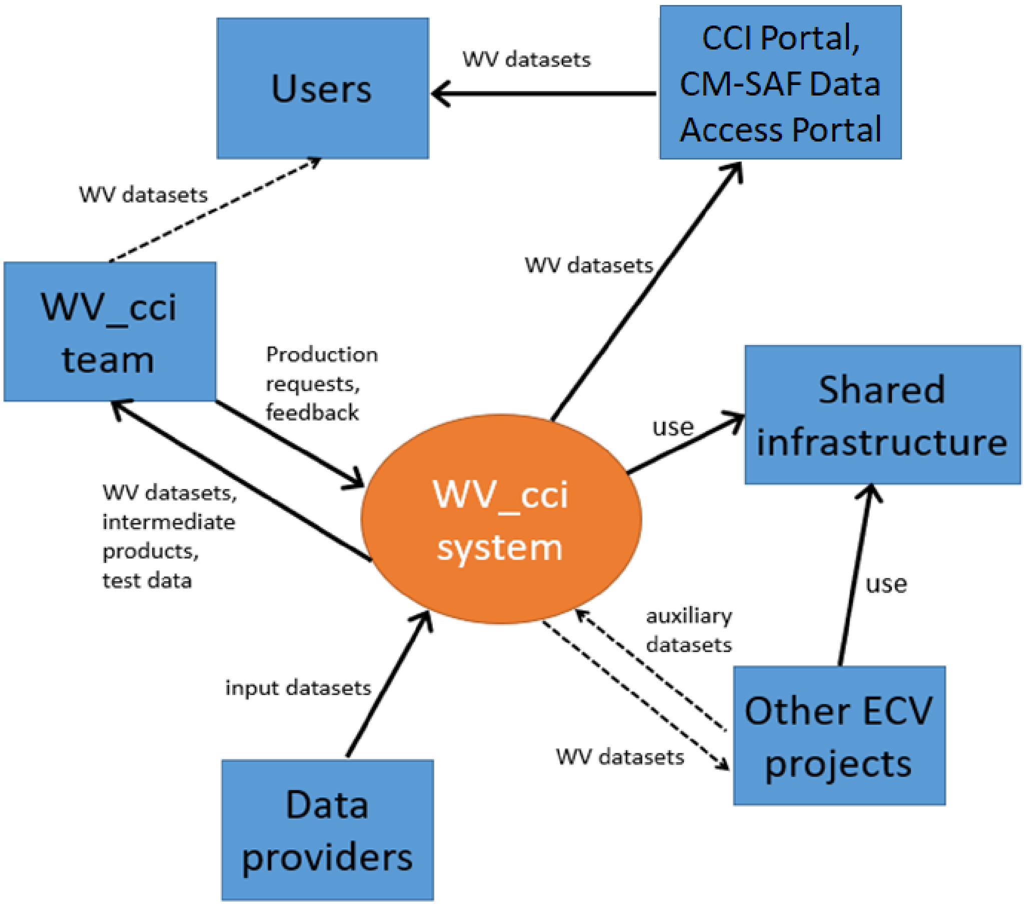

Figure 2-1: System context of the WV_cci system with team, data providers, and other entities. Taken from [4].

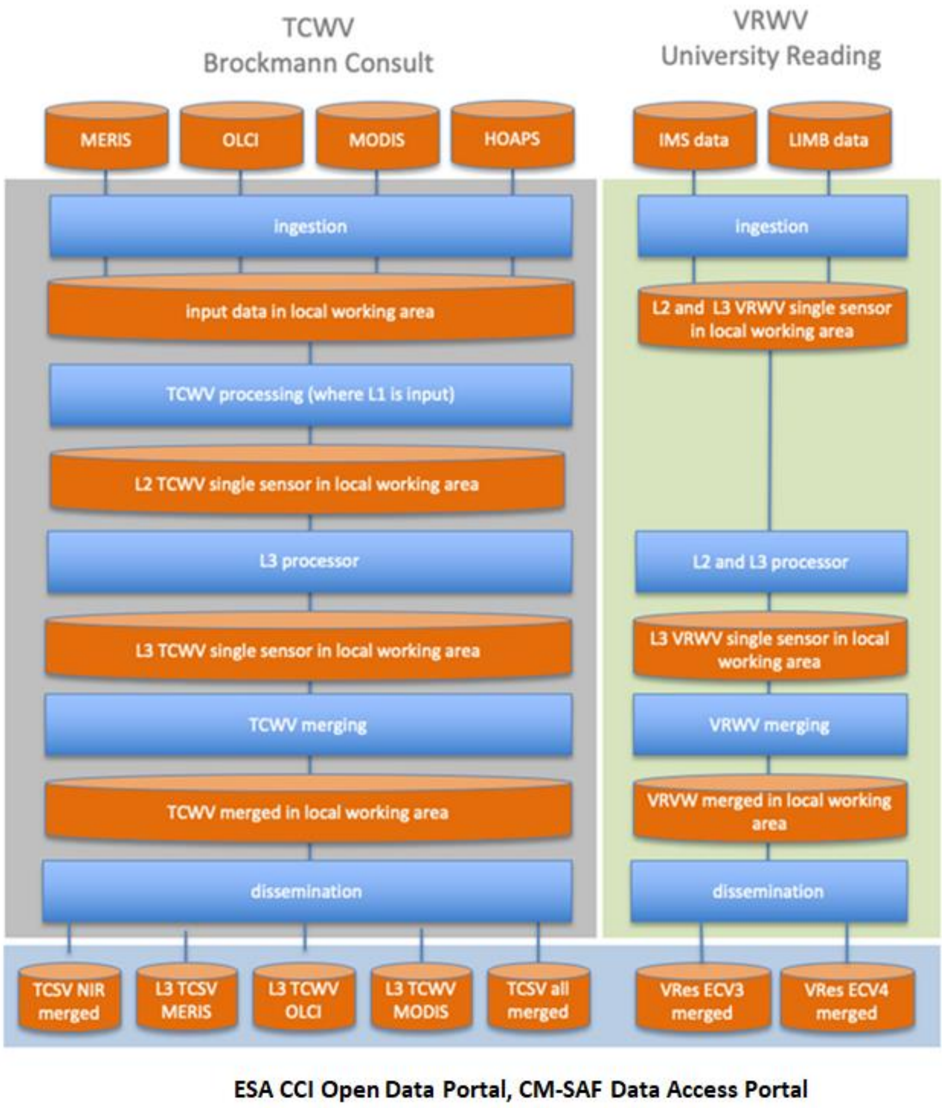

Figure 2-2: Symmetric system definition of the TCWV and VRWV processing systems.

3. WATER VAPOUR PRODUCTS

3.1 Total column products (CDR-1 and CDR-2)

3.1.1 Processing environment

From the system requirements [TR-30] in the SoW [5], it follows that the TCWV processing system shall ingest and process L1B input data from the MERIS, MODIS and OLCI instruments to retrieve finally global TCWV L3 products over land. These products in return shall be complemented by TCWV L3 products over oceans from CM SAF HOAPS (originally gathered from SSM/I, SSMIS, AMSR-E and TMI instruments). As outlined in detail in the SSD [4], the processing platforms

- Calvalus Linux cluster operated at Brockmann Consult, Germany, for MERIS and OLCI L2 processing, and for all L3 processing
- CEDA's JASMIN super-data-cluster operated at Harwell, UK, for MODIS L2 processing

were finally selected to generate the TCWV products which are described in detail in this PUG.

3.1.2 TCWV processing chain

The TCWV processing chain and the related processors for TCWV L2 and L3 retrieval, the merge of L3 products, and the generation of the final CF- and CCI compliant TCWV products are illustrated in Figure 3-1 and Figure 3-2. The single components of the workflows are described in detail in the SSD [4]; the input and output products of the various modules are described in Section 3.1.3 of this PUG.

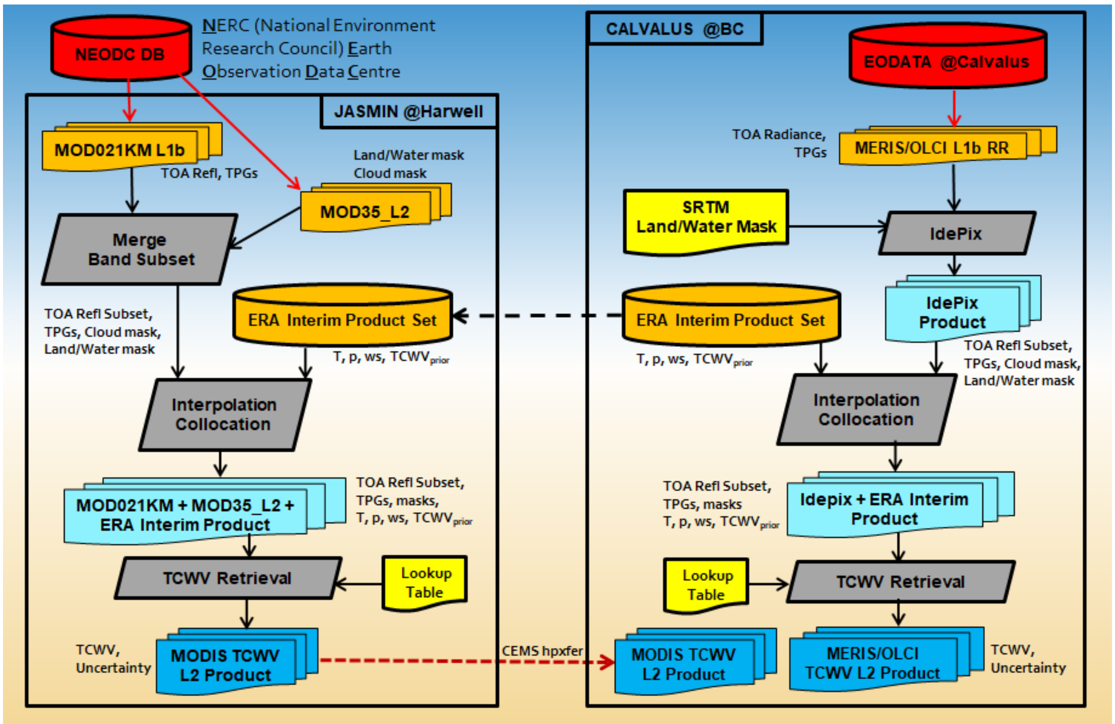

Figure 3-1: The TCWV L2 processing chains for MODIS, MERIS and OLCI. See details in [4].

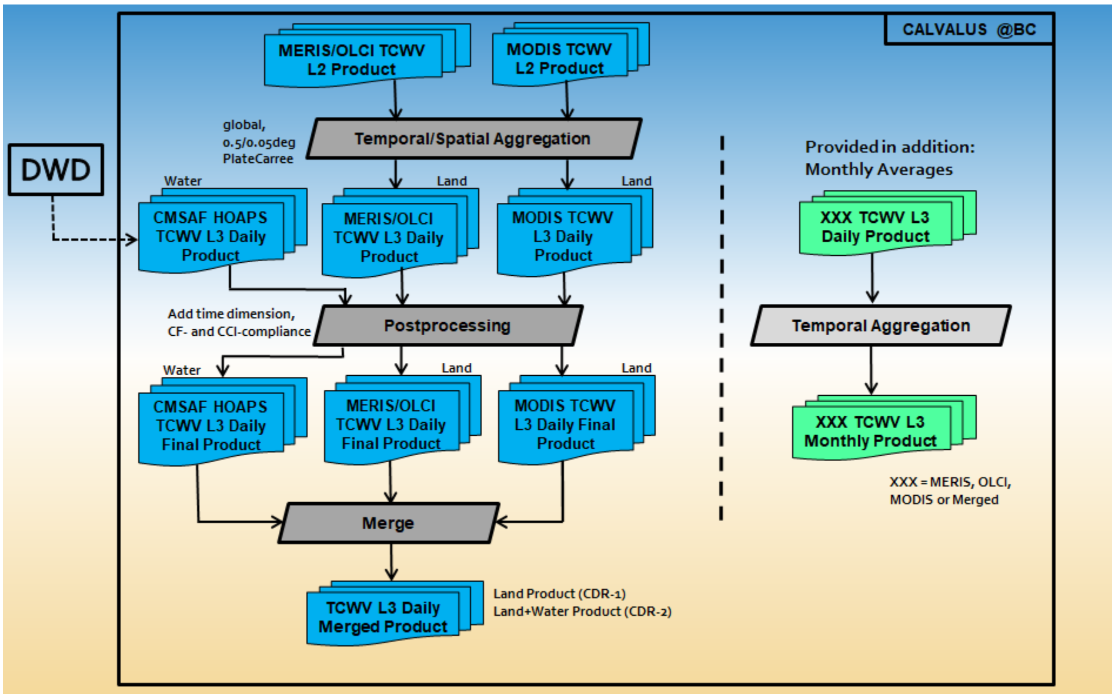

Figure 3-2: The TCWV L3 processing chains. See details in [4].

3.1.3 Description of products

3.1.3.1 Input products

3.1.3.1.1 Level-1 radiance/reflectance products

As satellite radiance/reflectance input for the TCWV retrieval algorithm used in WV_cci, Level-1 data products from the instruments

- Envisat MERIS
- MODIS Terra
- Sentinel-3 OLCI

are used. Details on these data products and more relevant information on these instruments can be found in [6], [7] (MERIS), [8], [9], [10] (MODIS Terra), and [11] (OLCI)

3.1.3.1.2 Auxiliary data products

Besides the satellite Level-1 radiance/reflectance input data sets, various auxiliary data products are needed for the TCWV retrieval in the WV_cci processing chain. These data products are described in brief in the following subsections.

3.1.3.1.2.1 SRTM Water Body Data (SWBD)

The SRTM Water Body Data (SWBD) is a geographical dataset encoding high-resolution worldwide coastline outlines in a vector format, published by NASA and designed for use in geographic information systems and mapping applications [12]. In the WV_cci processing chain, the SWBD is used to generate a land/water mask for the pixel classification as part of the Level-2 preprocessing towards the TCWV L2 retrieval, as outlined in more detail in the SSD [4].

3.1.3.1.2.2 Cloud mask products

For the TCWV retrieval from MODIS at Level-2, the MOD35 Cloud Mask [14] product is used for pixel classification (clouds, land, water) and for the exclusion of MODIS L1B night mode products. This product is a Level-2 product generated at 1-km and 250-m spatial resolutions. The cloud detection algorithm employs a series of visible and infrared threshold and consistency tests. In addition to the cloud flag, this product also provides a day/night flag and a land/water flag. The underlying cloud detection algorithm together with the encoding of the flags and a description of all cloud tests is described in great detail in [13].

For the TCWV retrieval from MERIS and OLCI at Level-2 (see Section 3.1.3.2.1), the IdePix (IDEntification of PIXels) plugin of the SNAP application (see Section 5.1) is used for pixel classification. Details on the definition of the various IdePix flags are given in the SNAP IdePix plugin documentation.

3.1.3.1.2.3 ERA Interim reanalysis dataset

ERA-Interim is an ECMWF global atmospheric reanalysis dataset that is available from 1 January 1979 to 31 August 2019. The data assimilation system includes a 4-dimensional variational analysis (4D-Var) with a 12-hour analysis window. The spatial resolution of the data set is approximately 80 km on 60 levels in the vertical from the surface up to 0.1 hPa.

In the WV_cci processing chain, ERA-Interim data are interpolated onto the grids of the satellite L1B products and used for prior estimates of reasonable quality for surface temperature, sea level pressure, wind speed (over ocean) and TCWV.

An introduction and instructions how to access ERA-Interim data is given on the ECMWF ERA-Interim web page [15]. For a detailed documentation of the ERA-Interim Archive see [16].

3.1.3.1.2.4 CM SAF global mask data

In the TCWV L3 final processing steps (Section 3.1.3.3), two types of global mask data are used:

- a static land/sea mask on a global plate carrée grid at 0.5 degree
- a sea ice mask on a global plate carrée grid at 0.5 and 0.05 degree spatial resolution, with one month temporal resolution (24 NetCDF products per year).

These data originate from CM SAF and were post-processed and provided by DWD for WV_cci.

3.1.3.1.2.5 CM SAF HOAPS TCWV data

The EUMETSAT CM SAF HOAPS product relies on recalibrated, quality controlled and inter-calibrated microwave imager observations. In particular, it utilises the CM SAF Fundamental Climate Data Record (FCDR; [27], [28]) and AMSR-E and TMI observations, inter-calibrated to the CM SAF FCDR, following [28]. The retrieval of L2 TCWV and associated uncertainties from microwave imager observations is based on a 1D-Var retrieval scheme which was provided by NWP SAF. The HOAPS ATBD [29] describes the physical baseline for the retrieval of TCWV from microwave imager observations. Further reading on the 1D-Var retrieval is available at https://nwp-saf.eumetsat.int/site/software/1d-var/documentation/. L2 TCWV are first gridded onto a plate carrée longitude/latitude grid of 0.5° on hourly basis and per satellite. Then, for each hourly bin, averages over all available satellites are carried out. Finally, the daily average is computed based on the hourly bins. In order to generate a HOAPS based L3 product at 0.05°, the 0.5° product is oversampled. TCWV from HOAPS has global coverage, i.e. within ±180° longitude and ±80° latitude and are only defined over the ice-free ocean surface.

3.1.3.2 Intermediate products

3.1.3.2.1 Level-2 TCWV 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 [17]. 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. However, small subsets of those can be provided on demand for specific cases such as validation or other purposes.

3.1.3.2.2 Level-3 TCWV ‘raw’ products

This section describes the WV_cci Level-3 TCWV temporally and spatially aggregated products. This set of products consists of daily global TCWV products obtained from TCWV L2 products generated from MERIS, MODIS and OLCI measurements, as described in the previous sections, supplemented by Level-3 TCWV products from CM SAF HOAPS which were preprocessed by DWD for direct ingestion into the WV_cci TCWV L3 processing chain. The term ‘raw’ indicates that they are used in the processing chain ‘as they are’. These ‘raw’ NetCDF products do not yet fulfil all requirements for NetCDF-CF and CCI compliance. The conversion to fully CF- and CCI compliant products is done in a post-processing step (see Section 3.1.3.3.1). The ‘raw’ products are usually discarded afterwards and are not made publicly available, thus they are not described in more detail here.

3.1.3.3 Final products

This section describes in detail the WV_cci Level-3 TCWV final and publicly available products as specified in the PSD [18].

3.1.3.3.1 Level-3 TCWV daily final products

3.1.3.3.1.1 Common properties

The Level-3 TCWV products in their ‘raw’ versions were briefly summarised in Section 3.1.3.2.2. In a post-processing step, these products are converted into their final version which will be publicly available. The following modifications are applied to all Level-3 TCWV products:

- final flag bands are set
- final error terms are computed in a CCI conformant way as specified in the PSD [18]
- NetCDF global and variable attributes are added/updated in order to fulfil CCI compliance [19] and CF-conventions [20]
- CCI compliant filenames are set.

Table 3-1 lists the bands which are provided in all daily Level-3 TCWV products. The final flag codings for TCWV quality and for surface type are explained in Table 3-2 and Table 3-3.

Table 3-1: Bands in Level-3 TCWV daily product

Name in product	Unit	Type	Description
time	days since 1970-01-01	int32	Product dataset time
time_bnds	days since 1970-01-01	int32	Start and end times for the time period the data represent
lat	degrees_north	float32	Latitude
lat_bnds	degrees_north	float32	Northern and southern boundaries of the grid cells
lon	degrees_east	float32	Longitude

Name in product	Unit	Type	Description
lon_bnds	degrees_east	float32	Eastern and western boundaries of the grid cells
tcwv	kg/m^2	float32	Total column of water vapour[1]
stdv	kg/m^2	float32	Standard deviation of Total Column of Water Vapour
num_obs	none	int32	Number of TCWV retrievals contributing to L3 grid cell[2]
num_hours_tcwv	none	int32	Number of hours in day with a valid TCWV value in L3 grid cell
tcwv_err	kg/m^2	float32	Average retrieval uncertainty: $$\frac{1}{N}\sum_{i=1}^{N}\sigma_i$$ with N: number of TCWV L2 retrievals; σ_i: uncertainty of i-th TCWV L2 retrieval
tcwv_ran	kg/m^2	float32	Propagated retrieval uncertainty $$\sqrt{\frac{1}{N}\sum_{i=1}^{N}\sigma_i^2}$$ with N, σ_i as above

[1] *Calculated as mean average over the L2 values available in each L3 grid cell.*

[2] *There is no threshold number of observations used for the calculation of this standard deviation.*

Name in product	Unit	Type	Description
tcwv_quality_flag	none	byte	TCWV quality flag band
surface_type_flag	none	byte	Surface type flag band

Table 3-2: Level-3 TCWV quality flag coding

Value	Flag	Description
0	TCWV_OK	TCWV retrieval has no known issues
1	HIGH_COST_FUNCTION_1	Cost function value in TCWV retrieval is in [1.0, 2.0]
2	HIGH_COST_FUNCTION_2	Cost function value in TCWV retrieval is greater than 2.0
3	TCWV_INVALID	Invalid pixel (no TCWV retrieval)

Table 3-3: Level-3 TCWV Surface type flag coding

Value	Flag	Description
0	LAND	Pixel is over land
1	OCEAN	Pixel is over ocean[3]
2	CLOUD_OVER_LAND	Pixel is over land and totally cloudy (all contributing L2 pixels are cloudy)
3	HEAVY_PRECIPITATION_MW	Indicator of presence of heavy precipitation in HOAPS data over ocean

[3] *Note, inland waters cannot be mistaken as ocean. This flag is defined by the CM SAF L3 land/sea mask described in Section 3.1.3.1.2.4, which is too coarse to resolve inland waters.*

Value	Flag	Description
4	SEA_ICE	Sea ice pixel as given by CM SAF L3 sea ice mask
5	COAST	Pixel is in coastal zone as given by CM SAF L3 land/sea mask
6	PARTLY_CLOUDY_ OVER_LAND	Pixel is over land and partly cloudy (majority but not all contributing L2 pixels are cloudy)
7	PARTLY_SEA_ICE	Sea ice edge pixel as given by CM SAF L3 sea ice mask

3.1.3.3.1.2 Land products (CDR-1)

The Level-3 TCWV daily land products consist of the TCWV global daily aggregations for each separate NIR instrument (MERIS, MODIS or OLCI) as well as their possible merge products (MERIS+MODIS, OLCI+MODIS) for the processing periods with existing time overlaps. The rules for this merging are described in more detail in Appendix 3: TCWV L3 Merging Rules. For all of these 'land-only' products, the CM SAF land/sea mask is applied, thus all grid cells not classified as land are masked out.

The full set of these land products generated for all processing periods considered for WV_cci forms the 'CDR-1', see PSD [18].

Table 3-4 lists the main properties of the Level-3 TCWV daily land product.

Table 3-4: Level-3 TCWV daily land product fact sheet

Projectname	ESACCI-WATERVAPOUR
Shortname	CCI TCWV-land
Platforms	Envisat, Sentinel-3A, Terra
Instruments	MERIS, OLCI, MODIS
Processing Level	Level-3

Spatial Resolutions	0.5 and 0.05 degrees
Temporal Resolution	1 day[4]
Primary Data Format	NetCDF4
Product size	~1.5 MB for 0.5 deg, ~75 MB for 0.05 deg
Number of products	1 product per day per sensor (sensor combination)

File Naming Convention	as specified in detail in [19], section 2.7
	
	Examples:
	
	L3 TCWV from OLCI measurements on July 15th, 2016, 0.5 degree resolution, file version 2.2:
	`ESACCI-WATERVAPOUR-L3C-TCWV-olci-05deg-20160715-fv2.2.nc`
	
	L3 TCWV from OLCI and Terra MODIS measurements on May 8th, 2017, 0.05 degree resolution, file version 2.1:
	`ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-005deg-20170508-fv2.1.nc`

Collection	WV_cci CDR-1
Publisher	ESACCI
Citation	DOI 10.5285/a5c833831e26474bb1100ad3aa58bdf9

3.1.3.3.1.3 Land + Ocean products (CDR-2)

The Level-3 TCWV daily land + ocean products consist of the TCWV global daily aggregations for each separate NIR instrument (MERIS, MODIS or OLCI) as well as

[4] *'Day' is defined as 00:00-23:59 UTC for all L3 grid cells.*

their possible merged products (MERIS+MODIS, OLCI+MODIS), but each of them now merged with the corresponding CM SAF L3 daily TCWV products. This results in land + ocean products from the following combinations:

- MERIS + CM SAF HOAPS
- MODIS + CM SAF HOAPS
- (MERIS + MODIS) + CM SAF HOAPS
- OLCI + CM SAF HOAPS
- MODIS + CM SAF HOAPS
- (OLCI + MODIS) + CM SAF HOAPS

The merging is performed applying the rules described in detail in Appendix 3: TCWV L3 Merging Rules.

The full set of these land + ocean products generated for all processing periods considered for WV_cci forms the 'CDR-2', see PSD [18].

Table 3-4 lists the main properties of the Level-3 TCWV daily land + ocean product.

Table 3-5: Level-3 TCWV daily land + ocean product fact sheet

Projectname	ESACCI-WATERVAPOUR
Shortname	CM SAF / CCI TCWV-global (COMBI)
Platforms	Envisat, Sentinel-3, Terra, DMSP-F08, -F10, -F11, F13-15, F16-F18, AQUA, TRMM
Instruments	MERIS, OLCI, MODIS, SSM/I, SSMIS, AMSR-E, TMI
Processing Level	Level-3
Spatial Resolutions	0.5 and 0.05 degrees
Temporal Resolution	1 day

Primary Data Format	NetCDF4
Product size	~1.5 MB for 0.5 deg, ~75 MB for 0.05 deg
Number of products	1 product per day per sensor combination

File Naming Convention	as specified in detail in [19], section 2.7
	
	Examples:
	
	L3 TCWV from OLCI measurements merged with CM SAF HOAPS on July 15th, 2016, 0.5 degree resolution, file version 2.2:
	`ESACCI-WATERVAPOUR-L3C-TCWV-olci-cmsaf_hoaps-05deg-20160715-fv2.2.nc`
	
	L3 TCWV from OLCI and Terra MODIS measurements merged with CM SAF HOAPS on May 8th, 2017, 0.05 degree resolution, file version 2.1:
	`ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-cmsaf_hoaps-005deg-20170508-fv2.1.nc`

Collection	WV_cci CDR-2
Publisher	EUMETSAT CM SAF
Citation	DOI 10.5676/EUM_SAF_CM/COMBI/V001

3.1.3.3.2 Level-3 TCWV monthly products

In addition to the Level-3 TCWV daily products described above, monthly aggregates of the daily products are provided. They are generated by temporal aggregation of the daily products applying the following rules:

- for TCWV and error terms, the average from the daily products for the given month and the given instrument combination is computed
- no ‘monthly quality flag’ is computed
- the variable ‘num_hours_tcwv’ in the daily products is replaced by a variable ‘num_days_tcwv’, which is the number of days in month with a valid TCWV value in the L3 grid cell

- cloud cover in a given grid cell:

    a. CLOUDY_OVER_LAND in monthly products means that all daily aggregates are CLOUDY_OVER_LAND (i.e. there is no valid TCWV available for the whole month). This usually affects only very few grid cells;

    b. PARTLY_CLOUDY_OVER_LAND in monthly products means that at least one, but not all daily aggregates are CLOUDY_OVER_LAND. Thus there is at least one daily TCWV value available.

These rules apply for both land-only and land+ocean products.

Table 3-6 lists the main properties of the Level-3 TCWV monthly products.

Table 3-6: Level-3 TCWV monthly product fact sheet

Projectname	ESACCI-WATERVAPOUR
Shortname	CCI TCWV-land (for CDR-1) or CM SAF/CCI TCWV-global (COMBI) (for CDR-2)
Platforms	Envisat, Sentinel-3, Terra, F08, -F10, -F11, F13-15, F16 , DMSP-F17, DMSP--F18, AQUA, TRMM
Instruments	MERIS, OLCI, MODIS, SSM/I, SSMIS, AMSR-E, TMI
Processing Level	Level-3
Spatial Resolutions	0.5 and 0.05 degrees
Temporal Resolution	1 month
Primary Data Format	NetCDF4
Product size	~2 MB for 0.5 deg, ~120 MB for 0.05 deg
Number of products	1 product per month per sensor (sensor combination)

File Naming Convention	as specified in detail in [19], section 2.7
	
	Examples:
	
	L3 TCWV from OLCI measurements merged with CM SAF HOAPS from July 2016, 0.5 degree resolution, file version 2.2:
	`ESACCI-WATERVAPOUR-L3C-TCWV-olci-cmsaf_hoaps-05deg-201607-fv2.2.nc`
	
	L3 TCWV from OLCI and Terra MODIS measurements merged with CM SAF HOAPS from May 2017, 0.05 degree resolution, file version 2.1:
	`ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-cmsaf_hoaps-005deg-201705-fv2.1.nc`

Collection	WV_cci CDR-1, CDR-2
Publisher	ESACCI (CDR-1), EUMETSAT CM SAF (CDR-2)

3.1.3.3.3 NetCDF attributes

In the post-processing step for the generation of the final TCWV NetCDF products described above, global and variable attributes for each variable are set which fulfil CCI compliance [19] and CF-conventions [20]. The sections 2.5.1 and 2.5.2 in [20] list these attributes in detail together with their purpose and meanings. Explicit examples for WV_cci TCWV final products are given in Appendix 4: Listings of file contents.

3.1.3.3.4 Processing periods

It can be noted that key challenges of the project were to harmonise the time series due to issues around calibration performance, long-term stability, and inconsistency between records. Consequently, sub-periods with at least one year of temporal overlap between MERIS and MODIS as well as between MODIS and OLCI were selected for processing and generating CDR-1. With respect to CDR-2, the project takes advantage of the developments carried out within the ESA DUE GlobVapour project and makes use of the spatial complementarity of the land-based NIR and ocean-based microwave observations by SSM/I and SSMIS spanning the time period 2002 to 2017. Thus, the combined product has global coverage and was selected for processing for the whole time period 2002 to 2017. Key challenges were to fill the coastal and ice-covered areas and to improve consistency between all sensors.

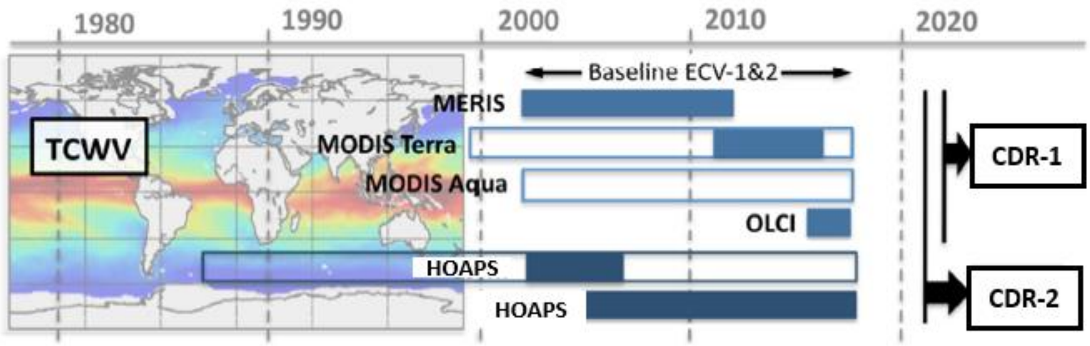

Figure 3-3: WV_cci TCWV instruments temporal coverage.

Figure 3-3 illustrates the temporal coverage of instruments used for the WV_cci TCWV retrievals, Table 3-7 lists the possible combinations of WV_cci TCWV instruments in the processing window 2002–2017.

Table 3-7: Possible WV_cci TCWV instruments combinations in the processing window 2002–2017

Processing period	Instrument combinations
07/2002 – 12/2010	MERIS MERIS + CMSAF HOAPS
01/2011 – 03/2012	MERIS MODIS MERIS + MODIS MERIS + CMSAF HOAPS MODIS + CMSAF HOAPS MERIS + MODIS + CMSAF HOAPS
01/2013 – 03/2016	MODIS MODIS + CMSAF HOAPS
04/2016 – 03/2017	OLCI MODIS OLCI + MODIS OLCI + CMSAF HOAPS MODIS + CMSAF HOAPS OLCI + MODIS + CMSAF HOAPS
04/2017 – 12/2017	OLCI OLCI + CMSAF HOAPS

3.1.3.3.5 Size of the data sets

Compared with the large volume of the input data sets used, the overall size of the final TCWV Level-3 daily and monthly products is much handier. The numbers for the different products are summarised in Table 3-8. The values are given per single instrument combination.

As an example, for the full data amount for one calendar year, we may look at Table 3-7 for 2016. We have two instrument combinations for Jan–Mar and six combinations for Apr–Dec. For one month, we have ~2.2 GB per combination. Thus we have 2x3x2.2 + 6x9x2.2 = 13.2 + 118.8 = 132 GB / year.

Another number of interest is the full size for each of the TCWV data sets CDR-1 and CDR-2. Table 3-9 summarises the numbers from the temporal coverage for each of the instrument combinations. We have a total of **~**520 GB for CDR-1. The value for CDR-2 should be very similar, as the instrument combination ‘xxx’ in CDR-1 is just replaced by ‘xxx + CM SAF HOAPS’ in CDR-2. Different sizes of products from CDR-1 compared to CDR-2 result from differences in the NetCDF4 compression over ocean (NaNs in CDR-1 vs ‘real’ CM SAF HOAPS values in CDR-2).

Thus we have a size of a bit more than **1 TB** for the full WV_cci TCWV data set which consists of CDR-1 and CDR-2.

Table 3-8: Size of the final TCWV Level-3 products (per instrument combination as given in Table 3-7)

Period	Resolution (degrees)	Size
daily	0.05	~ 2 GB / month
monthly	0.05	~ 120 MB / month
daily	0.5	~ 100 MB / month
monthly	0.5	~ 4 MB / month
total		**~ 2.2 GB / month**

Table 3-9: Approximate full size of the CDR-1 TCWV dataset

Instrument combination	Number of months	Size
MERIS 07/2002 – 03/2012	117	~ 257 GB
MODIS 01/2011 – 03/2017	75	~ 165 GB
OLCI 04/2016 – 12/2017	21	~ 44 GB
MERIS+MODIS 01/2011 – 03/2012	15	~ 33 GB
OLCI+MODIS 04/2016 – 03/2017	12	~ 26 GB
total		**~ 520 GB**

3.2 Vertically resolved products (CDR-3 and CDR-4)

From the system requirements [TR-30] in the SoW [5], it follows that the VRWV processing system shall ingest and process L3 input data from limb satellite sounders (SAGE II, UARS-MLS, HALOE, POAM III, SMR, SAGE III, SCIAMACHY, MIPAS, ACE-FTS, ACE-MAESTRO, Aura-MLS and SAGE III/ISS) for a homogeneous long-term zonal mean VRWV CDR-3, and from both L2 limb sounders (Aura-MLS and MIPAS) and nadir sounder (IMS) for a harmonised monthly prototype three-dimensional VRWV CDR-4. Input data products and product baseline (time coverage) are shown in Figure 3-4. As mentioned in the SSD [4], the whole processing will be performed on the RACC cluster system at University of Reading.

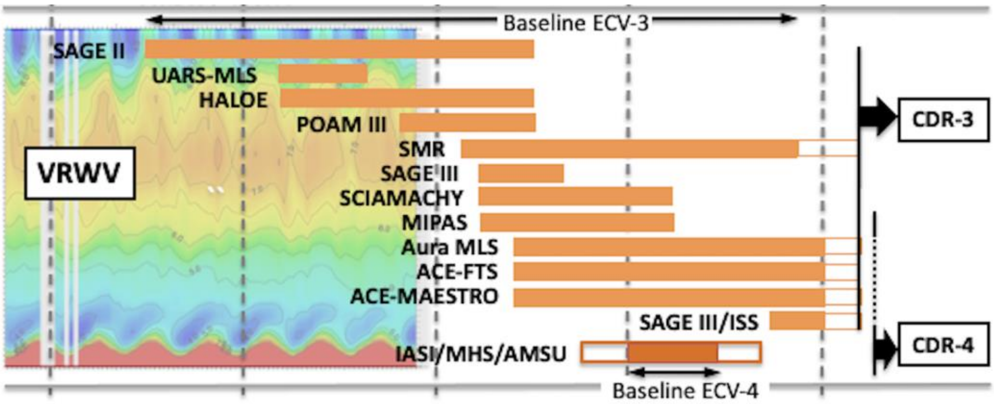

Figure 3-4: VRWV CDR-3 and CDR-4 input data and baseline.

3.2.1 Vertically resolved stratospheric water vapour climatologies (CDR-3)

This section provides a description of the processing chain and data of the zonal monthly mean VRWV WV_cci CDR-3 product.

3.2.1.1 Processing chain

Figure 3-5 shows the processing chain for VRWV CDR-3, including the related processors for the SPARC Data Initiative (SDI) VRWV L3 products, the bias-corrected SDI L3 products, and the merging of the final VRWV CDR-3 product. The details of this processing chain can be found in the SSD [4]. Table 3-10 lists the different limb sounders, time period, and version number of the L3 SPARC Data Initiative input climatologies to the CDR-3 processing chain. Details of these input data are introduced in the DARD [22].

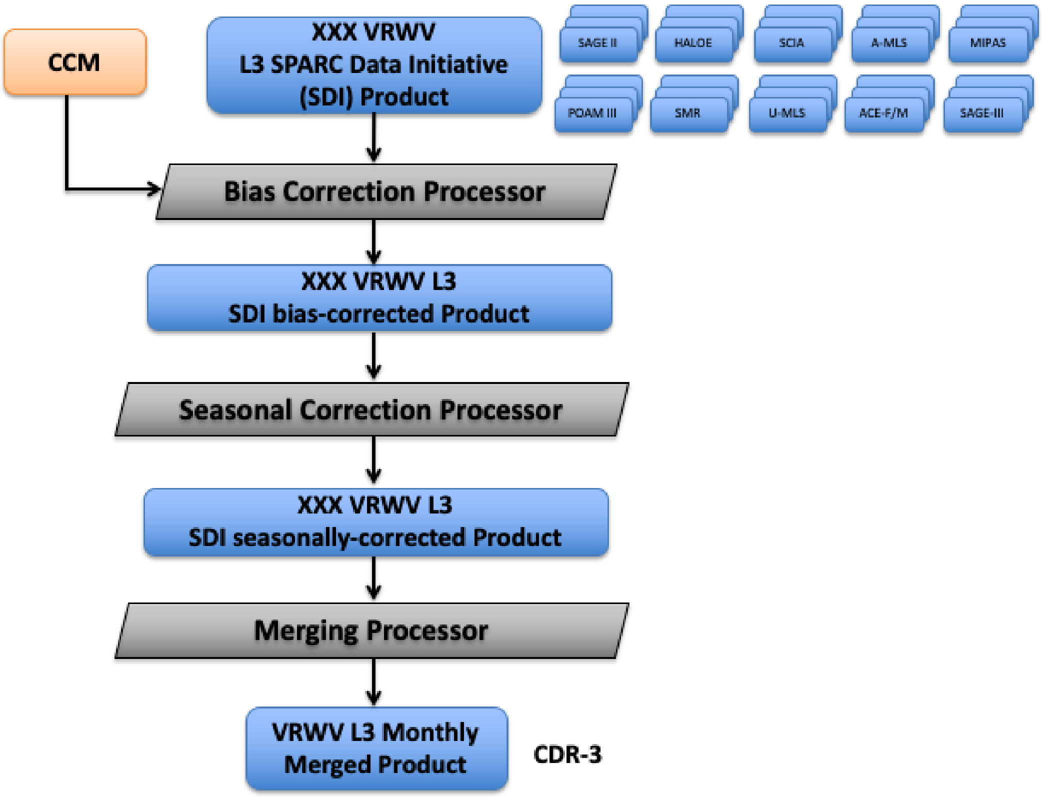

Figure 3-5: VRWV CDR-3 processing chain. See details in [4].

Table 3-10: SPARC Data Initiative L3 climatology inputs to the VRWV CDR-3 processing chain (see [23])

Product	Time Period	Data version
SAGE II	10/1984–08/2005	V7.0
UARS-MLS	10/1991–03/1993	V6
HALOE	10/1991–11/2005	V19
POAM III	04/1998–12/2005	V4.0
SAGE III	05/2002–12/2005	V4.0
SMR	07/2001–12/2019	V2-0 (16-20 km) and v2-1 (20-75 km)
MIPAS	03/2002–04/2012	V3o_H2O-21 (03/2002-03/2004) and V5r_H2O224 (01/2005-04/2012)
SCIAMACHY	09/2002–04/2012	V4.2
Aura MLS	08/2004–12/2019	V5.0
ACE-FTS	03/2004–12/2018	V3.6
ACE-MAESTRO	03/2004–12/2018	V31
SAGE III/ISS	06/2017–12/2019	V5.1

3.2.1.2 Description of products

This section describes the WV_cci L3 VRWV products that are part of the processing chain of CDR-3 and publicly accessible. This set of products consists of the L3 monthly zonal mean VRWV climatologies from the SPARC Data Initiative [23] and the final merged L3 VRWV CDR-3 product. The bias-corrected L3 VRWV datasets are not part of the distribution. Note the SDI input NetCDF files do not fulfil the formatting requirements for NetCDF-CF and CCI conventions. However, the final CDR-3 v3 NetCDF file is fully compliant as described in the following.

3.2.1.2.1 L3 SPARC Data Initiative L3 VRWV climatology products

The SPARC Data Initiative L3 VRWV climatology products are described in detail in [23]. The latitude and pressure grids of the individual instrument files thereby are the same as for the final product (see next section).

3.2.1.2.2 L3 merged L3 VRWV CDR-3 product

The final merged CDR-3 data product is available on a 5 degree latitude grid (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). Table 3-11 and Table 3-12 compile the product layers separately for main and additional variables. Table 3-13 offers the fact sheet for CDR-3.

Table 3-11: CDR-3 (L3) – Main variable list and description

Variable Name	Unit	Type	Description
lat	degrees_north	float32	Latitude given at grid cell centres
lat_bnds	degrees_north	float32	Latitude grid cell boundaries
plev	hPa	float32	Pressure levels
time	months since 1980-01-01	float32	Time for each month as months since reference time
time_bnds	months since 1980-01-01	float32	Latitude grid cell boundaries
zmh2o	mole mole-1	float32	Zonal mean of VRWV volume mixing ratio

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

Variable Name	Unit	Type	Description
zmh2o_stdv	mole mole-1	float32	Standard deviation of VRWV volume mixing ratio
zmh2o_nr	1	int32	Number of instrument values per climatological bin
zmh2o_err	%	float32	Estimated uncertainty of grid point value
quality_flag	1	int32	Threshold indicator that flags highly uncertain values

Table 3-13: Level-3 VRWV monthly zonal mean product (CDR-3 v3) fact sheet

Projectname	ESACCI-WATERVAPOUR
Shortname	CCI WV-strato
Platforms	ERBS, UARS, SPOT-4, Odin, Meteor-3M, EOS Aura, Envisat, SCISAT, ISS
Instruments	SAGE II, UARS-MLS, HALOE, POAM III, SMR, SAGE III, SCIAMACHY, MIPAS, ACE-FTS, ACE-MAESTRO, Aura-MLS, SAGE III/ISS
Processing Level	Level-3
Spatial Resolutions	5 degree (zonal mean)
Temporal Resolution	1 month
Primary Data Format	NetCDF4
Product size	Total of 7 MB
Number of products	1 for the time period 1985–2019
File Naming Convention	ESACCI-WATERVAPOUR-L3S-LP-MERGED-MZM-5deg-1985-2019_v3.3.nc
Collection	WV_cci CDR-3
Citation	doi: 10.5285/92824e3ec2e44a58b10048df3209b99c
Publisher	ESACCI (CDR-3)

3.2.1.2.3 NetCDF attributes

In the post-processing step for the generation of the final VRWV CDR-3 NetCDF product described above, global and variable attributes for each variable are set to ensure compliance with CCI data standards [19] and CF-conventions [20]. The sections 2.5.1 and 2.5.2 in [19] list these attributes in detail together with their purpose and meanings. Explicit examples for WV_cci VRWV final products are given in Appendix 4: Listings of file contents.

3.2.1.2.4 Processing periods

The goal of the project was to harmonise the time series of stratospheric limb sounders and resolve issues around calibration performance, long-term stability and inconsistency between records. For the current version CDR-3 v3.3, the key challenge was to apply an improved bias-correction scheme to the input data sets before merging. CDR-3 v3.3 is a merged product of 12 different input datasets over the time period 1985–2019 as listed in Table 3-14.

Table 3-14: WV_cci VRWV CDR-3 processing period

Processing period	Instrument combinations	CDR-3 data version
01/1985–12/2019	SAGE II UARS-MLS HALOE POAM III SMR SAGE III SCIAMACHY MIPAS ACE-FTS ACE-MAESTRO Aura-MLS SAGE III/ISS	**v3.3**

3.2.1.2.5 Size of the CDR-3 data set

The CDR-3 v3.3 product has a data volume of 8.5 MB, for the full-time range between 1985 and 2019.

3.2.2 Vertically resolved water vapour profiles in the UTLS (CDR-4)

3.2.2.1 Processing Chain

Figure 3-6 shows the processing chain for VRWV CDR-4, including the related processors for VRWV L2 products and the merging of L3 products for the generation of the final VRWV CDR-4 products. The details of this processing chain can be found in SSD [4]. Table 3-15 shows the time coverage of the L2 input data from Aura-MLS, MIPAS, and IMS to the CDR-4 processing chain. The details of these input data are introduced in the DARD [22].

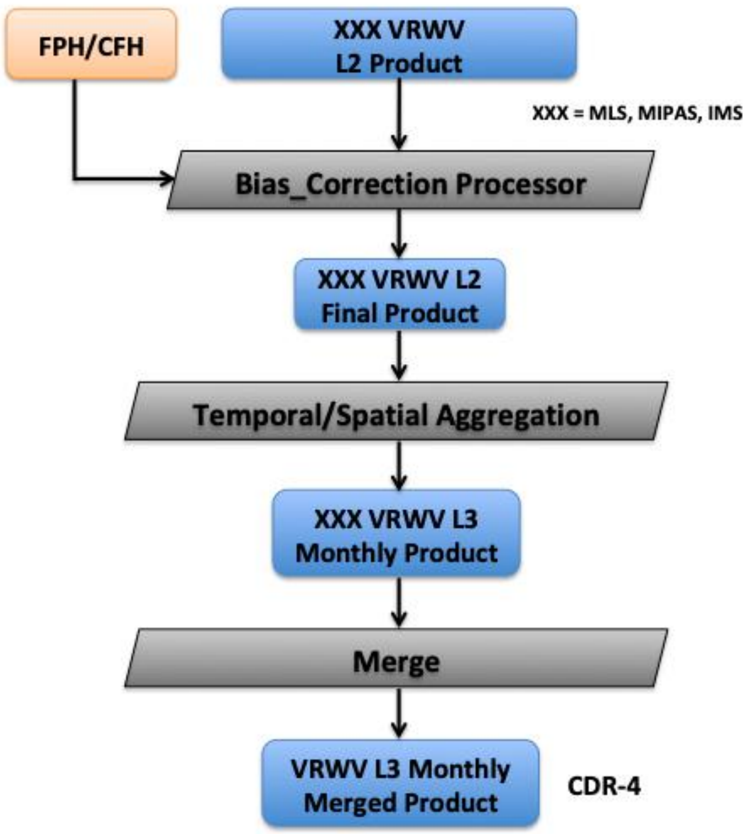

Figure 3-6: VRWV CDR-4 processing chain. See details in [4].

Table 3-15: Main inputs of the VRWV CDR-4 processing chain

Product	Coverage	Comment
Aura MLS L2	2010–2014	v5 from NASA JPL
MIPAS L2	2010–2011	v7R MIPAS-ESA
IMS L2	2010–2014	v2.1 from RAL

3.2.2.2 Description of products

3.2.2.2.1 L3 VRWV products

This section describes the WV_cci L3 VRWV temporally and spatially aggregated products in the processing chain of CDR-4. This set of products consists of the L3 monthly mean VRWV products obtained from original VRWV L2 input data and bias-corrected VRWV L2 data of Aura-MLS, MIPAS, and IMS. These NetCDF products do not fulfil all requirements for NetCDF-CF and CCI compliance.

3.2.2.2.1.1 Monthly L3 limb VRWV products from original L2 input data

All original L2 limb VRWV input data from Aura-MLS and MIPAS are taken for a temporal and spatial level 3 aggregation. The time aggregation window is the given month, and the spatial aggregation is done globally with a horizontal resolution of 5 degrees by 5 degrees in latitude and longitude. The vertical profiles are stored from 300 hPa to 10 hPa on 12 pressure levels: 300, 250, 225, 200, 175, 150, 125, 100, 70, 50, 30, 10 hPa. The VRWV profiles in log mixing ratio are linearly interpolated in log pressure to the desired pressure levels. The missing values are set to NaN.

Table 3-16 lists all the variables in the monthly L3 limb VRWV products from original L2 input data. It contains the average values of VRWV profiles in volume mixing ratio, number counts, and corresponding standard deviations. The estimated uncertainty of the VRWV volume mixing ratio would be updated in the next step.

Table 3-16: Variables in monthly L3 limb VRWV products from original L2 input data

Variable Name	Unit	Type	Description
lon	Degrees East	float32	Longitude given at grid cell centres
lon_bnds	Degrees East	float32	Longitude grid cell boundaries
lat	Degrees North	float32	Latitude given at grid cell centres
lat_bnds	Degrees North	float32	Latitude grid cell boundaries
time	Days since 1970-01-01	int32	Time for each month as days since reference time
time_bnds	Days since 1970-01-01	float32	Time boundaries for each month as days since reference time
level	hPa	float32	Pressure levels
vmrh2o	ppmv	float32	Average of the volume mixing ratio
vmrh2o_counts	none	int32	Number of L2 retrievals in given grid cell
vmrh2o_std (tbd)	ppmv	float32	Standard deviation of VRWV volume mixing ratio
vmrh2o_err (tbd)	ppmv	float32	Average uncertainty of VRWV volume mixing ratio

3.2.2.2.1.2 Monthly L3 nadir VRWV products from IMS (RAL)

The RAL Infra-red Microwave Sounder (IMS) scheme provides profiles of VRWV derived from combining measurements of Metop IASI, AMSU and MHS. As part of the work in year 1, Level 3 files were created for WV_cci from the existing L2 files (see DARD [22] for further information).

The time aggregation window is the given month, and the spatial aggregation is done globally with a horizontal resolution of 5 degrees by 5 degrees in latitude and longitude. Profiles are provided for 22 layers, with boundaries between the following levels (defined in variable p_bounds: 1000, 950, 900, 850, 800, 750, 700, 650, 600, 550, 500, 450, 400, 350, 300, 250, 225, 200, 175, 150, 125, 100 hPa. The IMS profiles are layer weighted to the desired pressure levels.

Table 3-17 lists the relevant variables in the monthly L3 VRWV product from original IMS input data. These are the variables related to the WV_cci project. The full list of file contents in L3 IMS products is attached in Appendix 4: Listings of file contents.

Table 3-17: Variables in monthly L3 VRWV products from original IMS

Variable Name	Unit	Type	Description
longitude	Degree East	float32	Longitude given at grid cell centres
lat	Degree North	float32	Latitude given at grid cell centres
time	second	int32	Mean time in s since 00:00 on 1 Jan 2000
p	hPa	float32	Mean pressure grid for retrieved profiles
w	ln(ppmv)	float32	Mean natural logarithm of the retrieved VRWV profile
w_median	ln(ppmv)	float32	Median natural logarithm of the retrieved VRWV profile
w_err	1	float32	Mean of the estimated uncertainty on the VRWV profile
w_std	ln(ppmv)	float32	Standard deviation in retrieved natural logarithm of VRWV profile
n	none	int32	Number of L2 retrievals in given grid cell

3.2.2.2.1.3 Monthly L3 VRWV products from bias-corrected L2 data

All original L2 VRWV input data from Aura-MLS, MIPAS, and IMS are processed with the bias-correction algorithm with reference to the VRWV profile observations at balloon-based hygrometer (BBH) sites in the tropopause-based coordinate. Within the tropopause-based coordinate, the profiles from L2 input data are adjusted to the seasonal profiles from BBH. The correction factors depend on latitude, altitude, and time. The details on the bias correction algorithm are in the ATBD [17].

The same as in Section 3.2.2.2.1.1, the bias-corrected L2 profiles are taken for temporal and spatial level 3 aggregation. The time aggregation window is the given month, and the spatial aggregation is done globally with a horizontal resolution of 5 degrees by 5 degrees in latitude and longitude. The vertical profiles for MLS and MIPAS are stored from 300 hPa to 10 hPa on 12 pressure levels: 300, 250, 225, 200, 175, 150, 125, 100, 70, 50, 30, 10 hPa and the vertical profiles for IMS are stored from 1000 hPa to 100 hPa on 22 pressure levels: 1000, 950, 900, 850, 800, 750, 700, 650, 600, 550, 500, 450, 400, 350, 300, 250, 225, 200, 175, 150, 125, 100 hPa. The VRWV profiles in log mixing ratio are linearly interpolated in log pressure to the desired pressure levels. The missing values are set to NaN. The list of variables is the same as shown in Table 3-16.

3.2.2.2.2 Merged L3 VRWV product (CDR-4)

As mentioned in SSD [4], the last processing step is to merge all the monthly L3 VRWV products into a global monthly prototype product (CDR-4) from 2010 to 2014. The merging rules applied are as follows:

- At and above 100 hPa (lower stratosphere), only use original VRWV L3 products from MLS and MIPAS before bias correction;
- Between 100 hPa and 300 hPa, include all bias-corrected VRWV L3 products from Aura-MLS, MIPAS, and IMS into the merged product;
- Below 300 hPa (troposphere), only use original VRWV L3 products from IMS before bias correction.

Table 3-18 lists the main properties of the Level-3 VRWV monthly products CDR-4 prototype v3 in 2010–2014.

Table 3-18: Level-3 VRWV monthly product (CDR-4 v3) fact sheet

Projectname	ESACCI-WATERVAPOUR
Shortname	CCI WV-UTLS
Platforms	EOS Aura, ENVISAT, EUMETSAT Metop
Instruments	MLS, MIPAS, IASI/MHS/AMSU
Processing Level	Level-3
Spatial Resolutions	5 degree
Temporal Resolution	1 month
Primary Data Format	NetCDF4
Product size	~ 20 MB for 2010–2014
Number of products	1 product for year 2010–2014
File Naming Convention	ESACCI-WATERVAPOUR-L3S-LP-NP-MERGED-MLS-MIPAS-IMS-5deg-2010-2014-v3.nc
Collection	WV_cci CDR-4
Citation	CDR-4 is available upon request. Please send email to: m.i.hegglin@reading.ac.uk and hao.ye@reading.ac.uk

3.2.2.2.3 NetCDF attributes

In the post-processing step for the generation of the final VRWV CDR-4 NetCDF products described above, global and variable attributes for each variable are set which fulfil CCI compliance [19] and CF-conventions [20]. Sections 2.5.1 and 2.5.2 in [19] list these attributes in detail together with their purpose and meanings. Explicit examples for WV_cci VRWV final products are given in Appendix 4: Listings of file contents.

3.2.2.2.4 Processing periods

Key challenges of the project were to harmonise the time series due to issues around calibration performance, long-term stability and inconsistency between records. For CDR-4 products, the key challenge was to merge the two types of VRWV sounders (limb and nadir) into a harmonised prototype climate data record. The currently available prototype version CDR-4 v3 covers the baseline period of 2010–2014. Table 3-19 lists the processing period for CDR-4 v3 and the input data.

Table 3-19: WV_cci VRWV CDR-4 processing period

Processing period	Instrument combinations	CDR-4 data version
01/2010 – 12/2014	Aura-MLS (2010–2014) MIPAS (2010–2011) IMS (2010–2014)	Prototype v3

3.2.2.2.5 Size of the data sets

As mentioned in Table 3-18, WV_cci VRWV prototype v3 CDR-4 data covering the full time range of 2010–2014, has a size of around 20 MB.

4. RESULTS FROM PRODUCT VALIDATION AND INTERCOMPARISON

4.1 TCWV products (CDR-1 and CDR-2)

4.1.1 Clear-sky bias

NIR based retrievals are predominantly applied under clear-sky conditions. Though instantaneous TCWV products from NIR show high quality and low uncertainty, gridded and temporally averaged data might exhibit a bias when compared to all-sky observations: conditions in clouds are typically more humid than the surrounding clear-sky areas, and are not observed by satellite-based NIR observations. This effect causes a clear-sky bias (CSB) and is of the order of 10% [26].

The CSB assessment carried out within WV_cci is based on the analysis of ERA5 data records and showed a distinct spatial distribution of wet and dry biases that are dominated by large-scale circulations for the mid to high latitudes and by the diurnal course of cloud coverage and the position of the ITCZ in tropical and subtropical regions. The area-weighted global average of the CSB is calculated to approximately -0.87 kg m-2 based on local time LT=10.

Due to the fairly large inherent variability in the TCWV, the CSB is hardly significant and thus not included in the final products as uncertainty information.

Further details are given in the CAR [24].

4.1.2 Recommended use in climate change analysis

Based on results from the PVIR, Part 1 [25] the following can be concluded:

TCWV from MERIS, MODIS and OLCI is retrieved under clear-sky conditions. The MODIS cloud mask is seemingly less conservative than the MERIS and OLCI cloud masks. Thus, the sampling differs between the sensors and this leads to relatively large regions with undefined values in the extra-tropics on a monthly scale for MERIS and OLCI. These regions are much smaller if present at all in MODIS TCWV monthly means. This can cause seeming instabilities when large scale averages (e.g. global) are considered due to the natural decrease in TCWV from tropics to poles. Thus, it is recommended to apply a conservative common cloud mask to the data record if (near) global average are computed for climate change analysis.

The TCWV time series is stable over ocean and over the MERIS and MODIS period over land, i.e. from 2002 until March 2016 if looking at clear-sky daily data. The clear-sky restriction can be explained by differences in the cloud mask between MERIS and

MODIS. This difference leads to different samples of the clear-sky bias and this in turn seems to cause a small change in the bias. We do not recommend to use the OLCI data from April 2016 onwards in climate change analysis because for unknown reasons a small change in bias between the MODIS and OLCI period is observed.

4.1.3 Cautionary note

Based on results from the PVIR, Part 1 [25], TCWV over inland water bodies as well as over coastal and sea-ice areas should be used with care.

4.2 VRWV-products (CDR-3 and CDR-4)

The VRWV products include the zonal mean monthly CDR-3 in the stratosphere from 1985 to 2019 and a three-dimensional monthly mean prototype CDR-4 in the UTLS region from 2010 to 2014. It needs to be noted that there is a lack of available observations that can be used as a well-defined reference for validation of the vertically resolved WV CDRs, especially in the UTLS but also in the stratosphere. The validation/comparison for VRWV CDRs thus have to be interpreted more as “consistency tests” between models and CDRs or between limited observational referenced datasets and CDRs.

4.2.1 CDR-3

VRWV CDR-3 has been compared to other similarly merged data products and chemistry–climate model simulations with specified dynamics from the SPARC/IGAC Chemistry–Climate Model Intercomparison (CCMI) Project, with the results being available in the PVIR, Part 2 [25]. The zonal mean monthly VRWV data agree with other references both in time series of absolute values and anomalies, especially from 2005 onwards. Caution has to be applied for the use in trend analysis below 100 hPa.

4.2.2 CDR-4

VRWV CDR-4 is a prototype version only and should generally be used with care. The new bias correction methodology introduced using quantile-mapping in tropopause coordinates is based on the “climatology” from limited measurements at balloon-based hygrometer stations only. Available reference data for the validation of the product in the UTLS are thus sparse. VRWV CDR-4 product has been compared to the BBH time series at individual sites and the comparison results indicate that the bias-correction method used in the CDR-4 production improves the VRWV in the UTLS region, especially during the summer season. Trend and stability analysis are not suitable for the CDR-4 product due to the short length of only 5 years.

5. SOFTWARE TOOLS

5.1 SNAP

The free Sentinel Application Platform software SNAP allows the visualisation and analysis of earth observation datasets including the ESA Water Vapour CCI products. It can be obtained from http://step.esa.int/main/toolboxes/snap/. In this section some example uses of SNAP are provided.

Each example makes use of the SNAP-Desktop application, a tool for displaying and analysing satellite data with an easy to use graphical user interface. Uses of the SNAP extend far beyond the examples shown here; users are encouraged to experiment with the software themselves.

5.1.1 Examining the contents of the WV_cci TCWV products

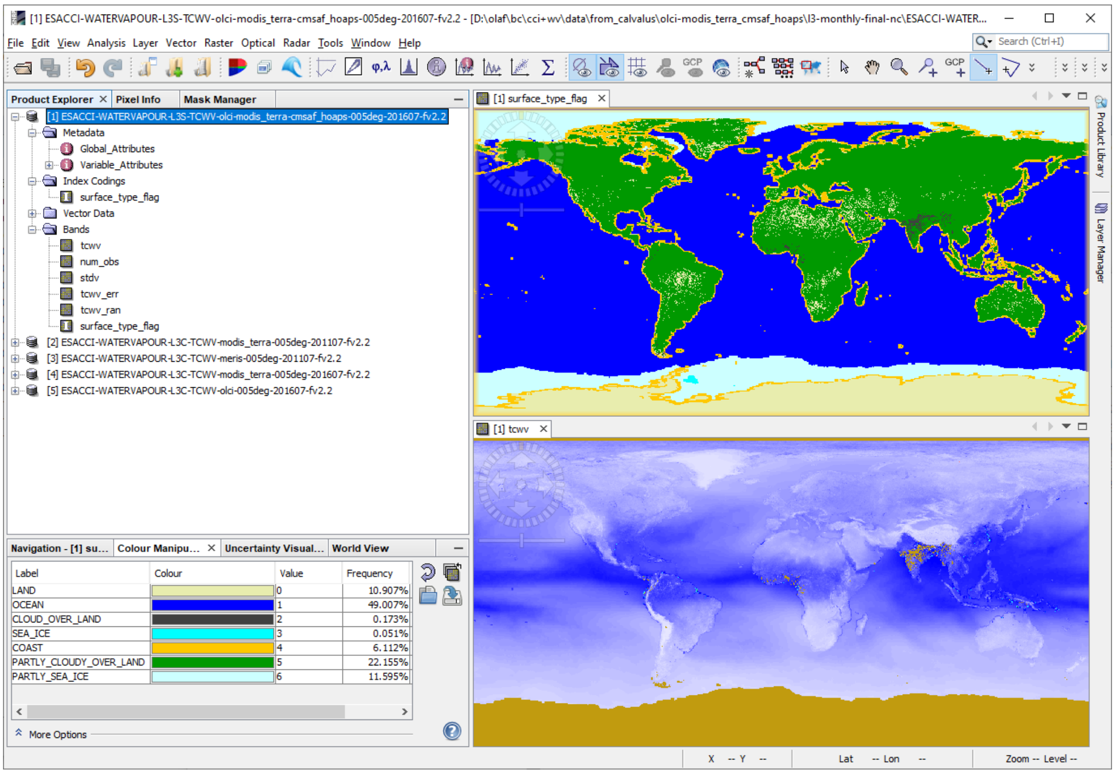

Figure 5-1: Visualising TCWV data with the SNAP Desktop application. See text for details.

Figure 5-1 shows the SNAP Desktop application with several tool windows arranged next to each other. The upper left tool window is the Product Explorer, listing several TCWV products which were opened from the File menu. For the first product, `ESACCI-`

`WATERVAPOUR-L3S-TCWV-olci-modis_terra-cmsaf_hoaps-005deg-201607-fv2.2.nc`, the content is listed in more detail. It is a TCWV L3 0.05-deg monthly product, thus the displayed bands are the same as given in Table 3-1. (Note that the 'Bands' tree node only displays the variables containing 2D raster data. 1D variables such as time, latitude, longitude can be listed by expanding the 'Variable_Attributes' tree node.) The two tool windows on the right show raster displays of the surface type flag (top) and TCWV (bottom). The colour scales were selected through the Colour Manipulation tool window in the lower left. Actually the selected discrete colours for the surface type flag are shown. As the surface_type_flag is recognised as an 'index band' (as interpreted from the corresponding NetCDF variable attributes), this tool window also provides a frequency distribution of the surface type in the given raster.

5.1.2 Working with TCWV data

With SNAP it is of course possible to investigate the TCWV data in greater detail, e.g. on regional scales. As an example, Figure 5-2, shows a cross-section through North America as set with the SNAP Line Drawing tool (upper part), and the corresponding TCWV as 1D profile plot. This plot gives a better impression of TCWV gradients, e.g. from land to water, or from the Rocky Mountains into the Great Plains.

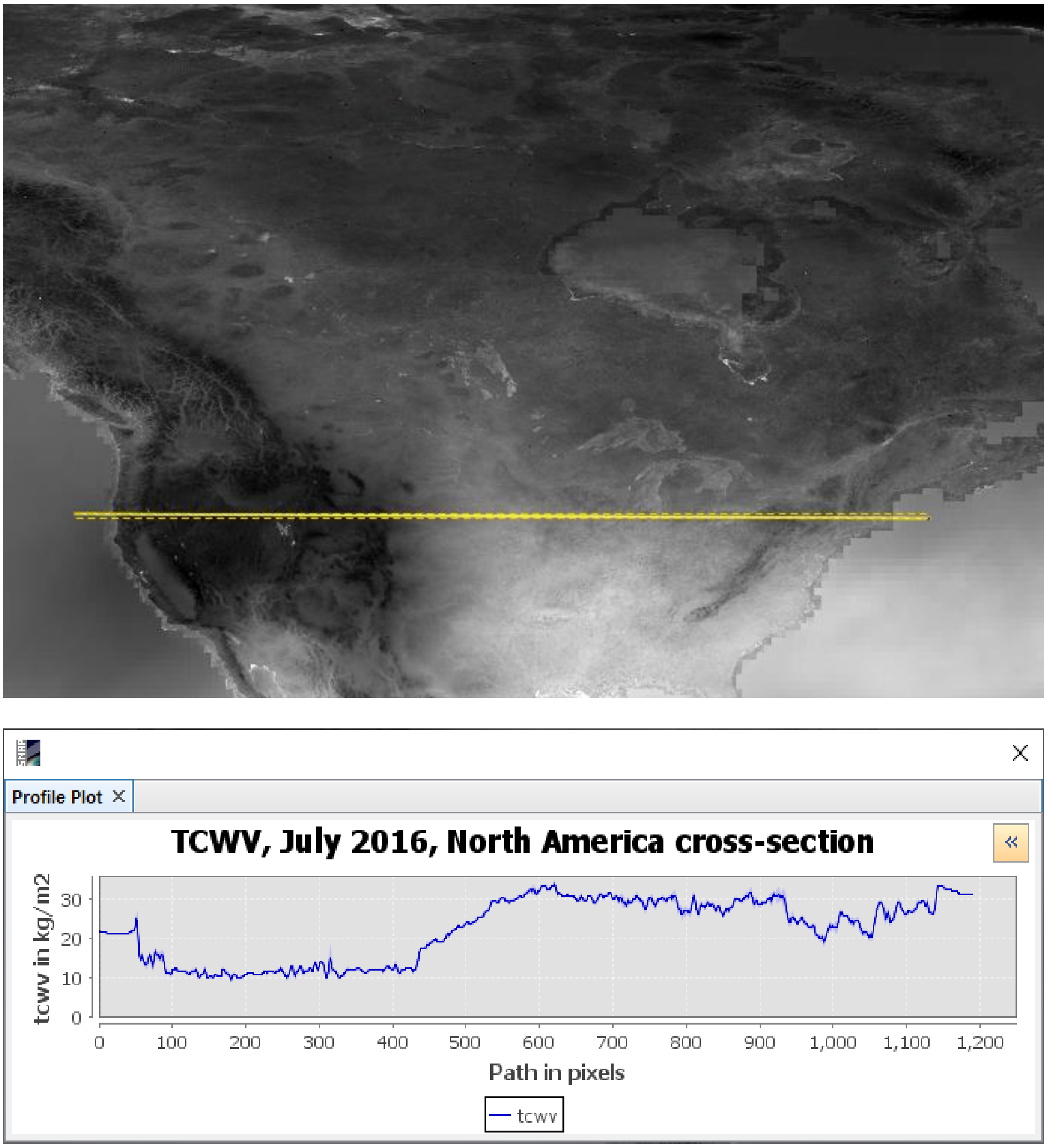

Figure 5-2: TCWV profile for a cross-section through North America.

Figure 5-3 shows a simple histogram for TCWV from July 2016 from the merge of all available sensors (OLCI, MODIS, CM SAF HOAPS).

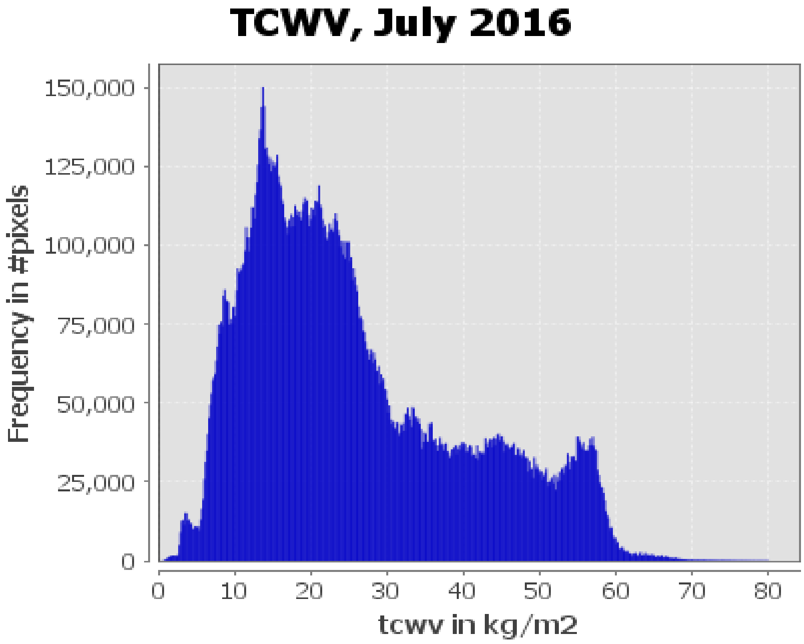

Figure 5-3: TCWV histogram for July 2016, merge of all sensors.

Figure 5-4 shows a scatter plot of TCWV over land from OLCI vs MODIS for July 2016 (0.05 degrees, 7200 x 3600 pixels). This is a very useful feature to investigate possible systematic differences in the TCWVs obtained from the different sensors, as the harmonisation of TCWV retrievals from different sensors was one of the major goals of the WV_cci project. Although there is quite some scatter especially towards higher TCWV values, it can be seen that by far most of the data points are located close to the 1:1 line for the two sensors.

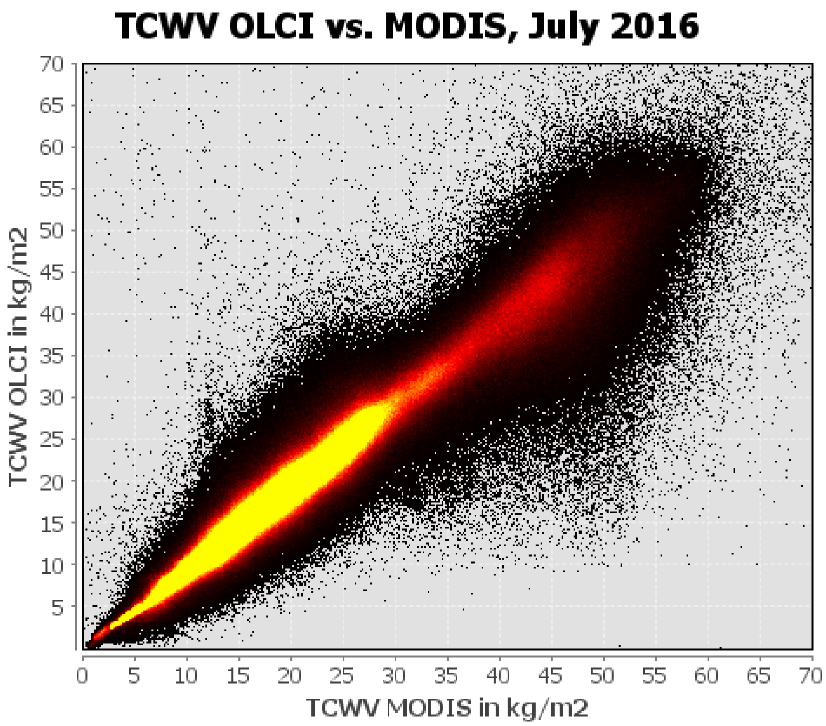

Figure 5-4: Scatter plot of TCWV over land from OLCI vs MODIS for July 2016.

5.2 Panoply

The free Panoply data viewer allows users to plot geo-referenced and other arrays from NetCDF, HDF, GRIB and other datasets. The software can be obtained from https://www.giss.nasa.gov/tools/panoply/ and can be installed on Macintosh, Windows, Linux and other desktop computers. For further information on this software, users are encouraged to check the details on the software website.

In this section, several examples on visualisation of VRWV products are provided below to show the ability and convenience of this software on desktop environment.

Figure 5-5 shows the Panoply application windows with the visualisation of VRWV data. The left side tool window shows the attributions and variables within the files and the panel in the middle shows the dataset/variable description details. The right side is the plotting window with L3 MLS VRWV 5 degrees monthly product in Jan. 2010. In the plotting window, the whole data plotted can be found in a table within the "Array 1" option. There are several options at the lower part of the plotting window provided to users to customise the plots. Not only does it plot the 2-D geo-referenced array in a map, Panoply also provides options to slice and plot 1-D arrays as lines from larger multidimensional variables.

Figure 5-6 shows the difference of VRWV between MLS and merged VRWV CDR-4 within the Panoply application. This is a very useful feature to compare easily the two datasets with a visual inspection. The application provides combined plot for two geo-referenced data sets by differencing, summing and averaging. It also provides a relative difference plot between two data sets. All the plots can be easily saved as image files to share.

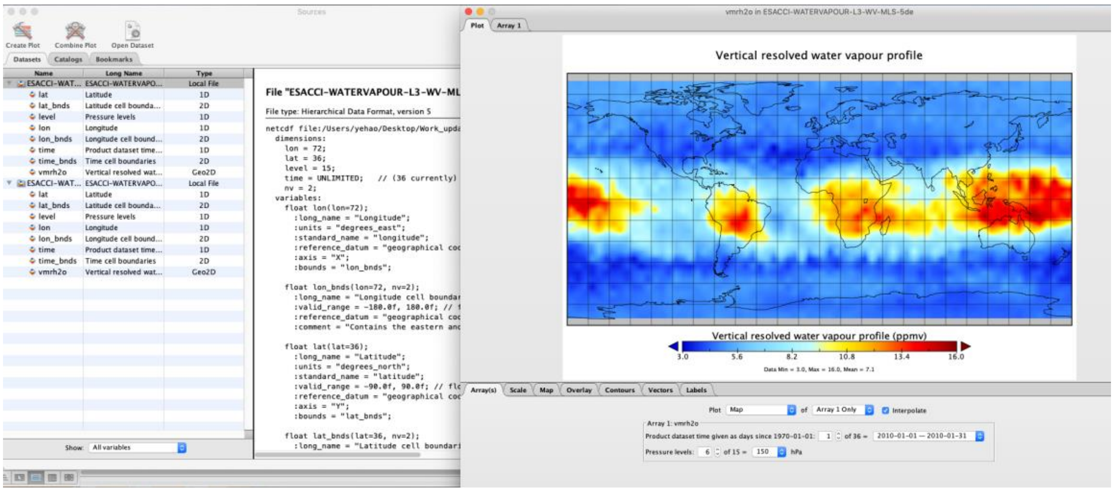

Figure 5-5: Visualising VRWV data with the Panoply Desktop application. See text for details.

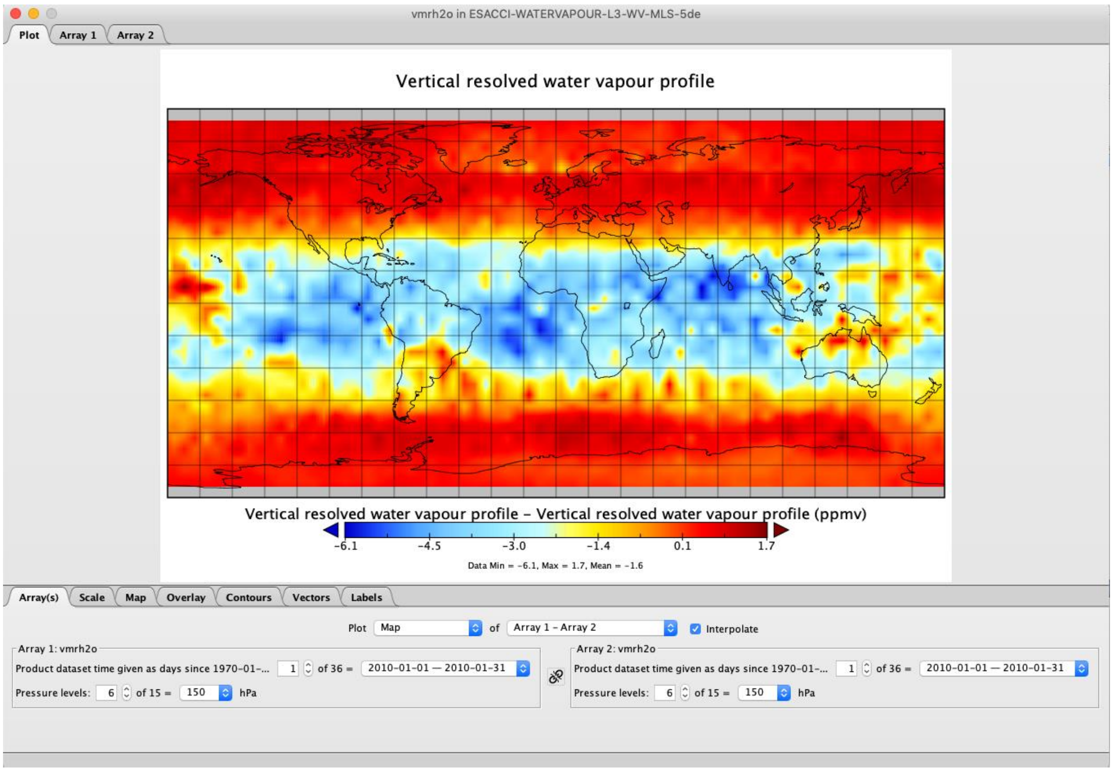

Figure 5-6: Difference of VRWV data between MLS and merged CDR-4 at 150 hPa in Jan. 2010.

5.3 The ESA Climate Analysis Toolbox (Cate)

The open source Climate Analysis Toolbox of the ESA Climate Change Initiative (Cate) allows users to ingest, analyse and visualise ESA's global satellite-derived climate observations including the ESA WV_cci products. Cate is a cloud-enabled computing environment geared for scientists who need to analyse, process, and visualise ESA's climate data and other spatio-temporal data. It can be used from an internet browser and perform all data access and processing needs on the cloud. There is no need for the user to download anything on a local computer.

The entry point to access the Cate services is: https://cate.climate.esa.int. New users will have to register for the use of the cloud service. There is also an option to use the Cate GUI as a local service. Instructions for this option are accessible from the web page given above.

After registration for the cloud service and successful login, the user will see the Cate GUI entry screen as shown in Figure 5-7.

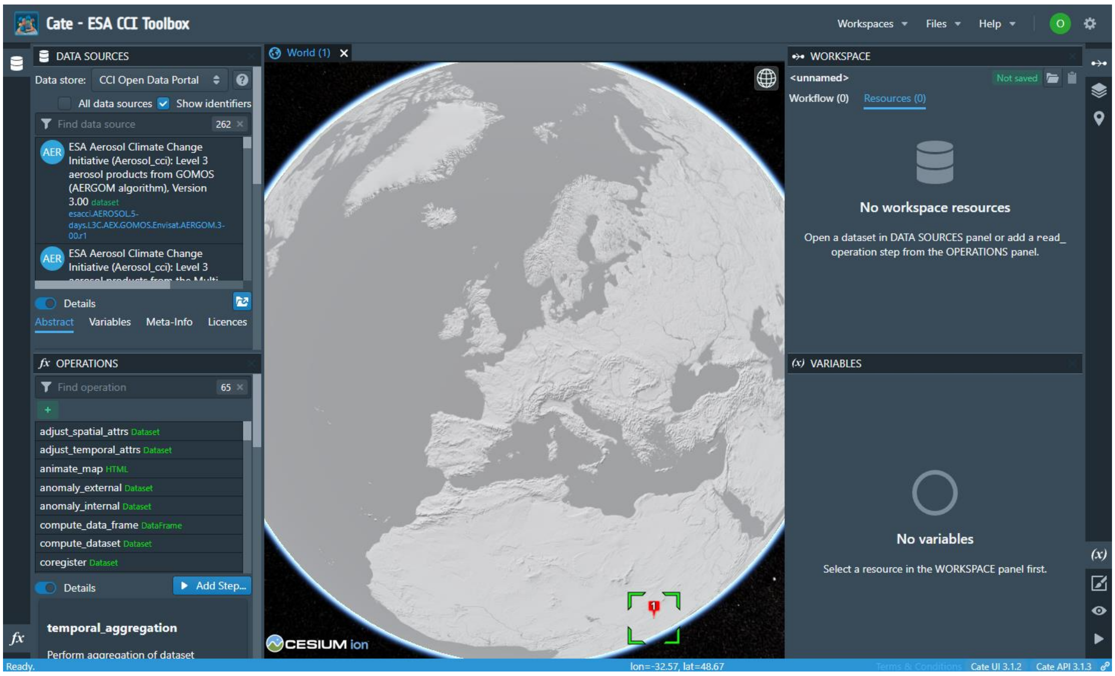

Figure 5-7: The entry screen of the Cate GUI.

The Cate GUI is basically divided in five areas:

- Data Sources (upper left): panel to browse, download and open both local and remote data sources, including data from ESA CCI Open Data Portal.
- Operations (lower left): panel to browse and apply operations and data processors for the analysis of the selected data.
- Workspace (upper right): panel to browse and select available resources and workflow steps resulting from opening data sources and applying operations.
- Variables (lower right): panel to browse and select the geo-physical variables contained in the selected resource.
- View area (centre): The active view on the data being analysed, which can be one of the following:
    - The world view (default), displaying imagery data originating from data variables and placemarks on either a 3D globe or a 2D map;
    - A table view, displaying tabular resource and variable data in a table;
    - A figure view, displaying plots from special figure resources resulting from the various plotting operations.

A full description of the capabilities available from these components is out of scope of this PUG. Instead, this detailed documentation is available from the Cate User Manual: https://cate.readthedocs.io/en/latest/user_manual.html#

which is part of the full Cate documentation:
https://cate.readthedocs.io/en/latest/index.html

A short overview of Cate is also given at the ESA Climate Office web page: https://climate.esa.int/en/explore/analyse-climate-data/

5.3.1 WV data ingestion and visualization

In Cate, CCI data can be ingested and visualized with the components described above. As a simple illustration, Figure 5-8 shows the view on a global TCWV dataset which was selected and ingested from the ‘Data Sources’ panel, temporarily aggregated over one month with the ‘temporal aggregation’ operation. The variable ‘TCWV’ was selected via the ‘Variables’ panel. This data analysis use case, which may contain e.g., many plots of many variables, is maintained in a dedicated workflow in the ‘Workspace’ panel.

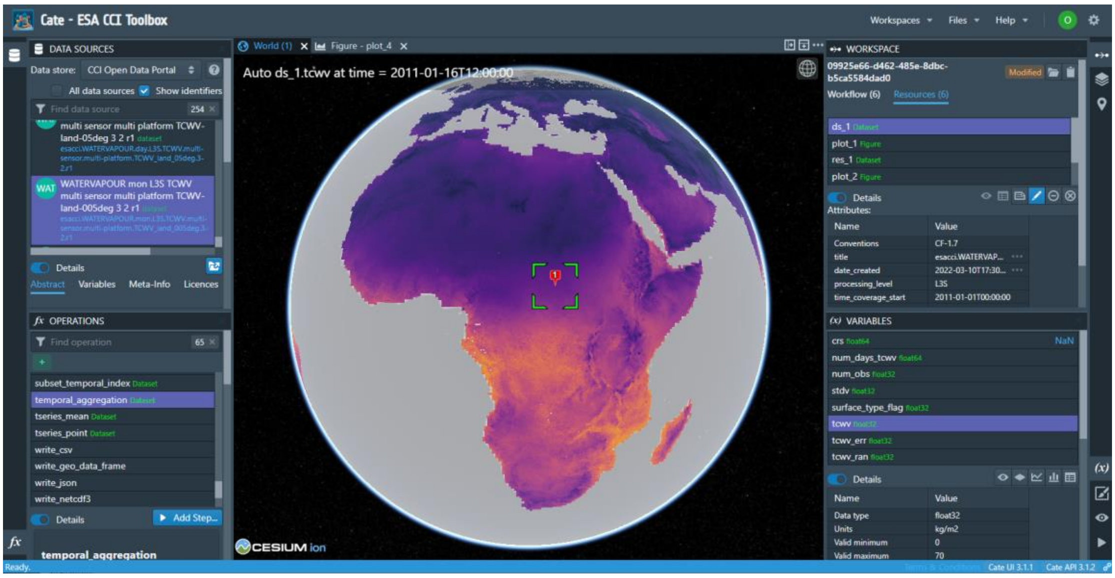

Figure 5-8: Cate: Global view of temporarily aggregated TCWV, January 2011.

5.3.2 WV data analysis

Cate offers a variety of data analysis capabilities, two simple examples are given below. Figure 5-9 shows a time series of TCWV over three years for the single location indicated by the ‘pin’ in Figure 5-8. For this tropical location, a distinct annual cycle of TCWV with a maximum in August/September is clearly illustrated. Figure 5-10 shows the TCWV histogram of the full dataset in Figure 5-8 (~6.7 million valid pixels).

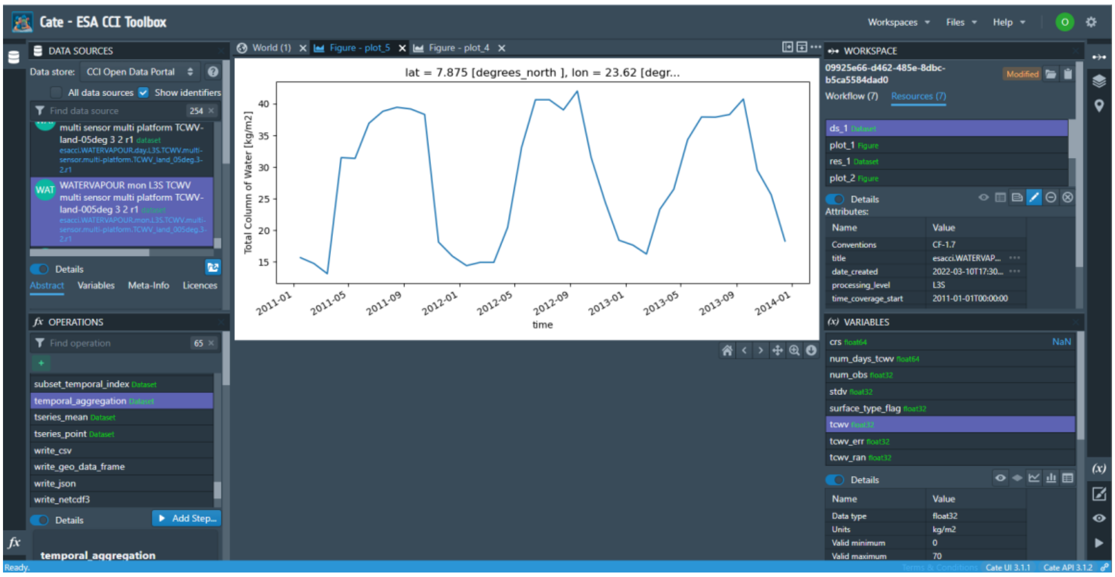

Figure 5-9: Cate: TCWV time series over 3 years for a tropical location indicated by the pin in Figure 5-8.

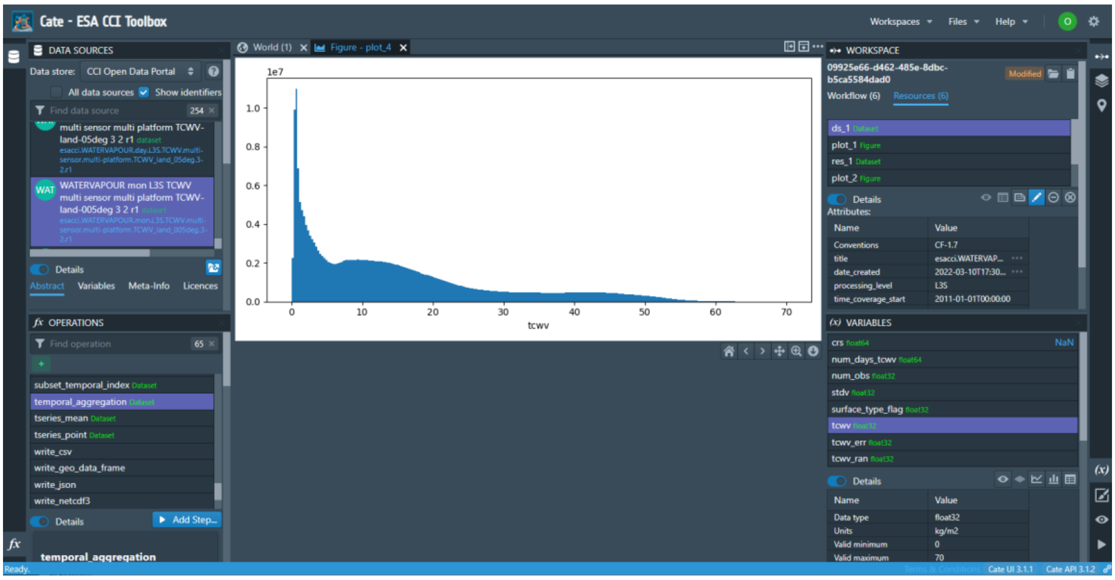

Figure 5-10: Cate: histogram of monthly global TCWV dataset shown in Figure 5-8.

5.4 Python tools

Python (http://www.python.org) is a free, general purpose programming language that is available on multiple operating systems including Linux, Windows and Mac OS. The core package can be extended using extra modules to increase its functionality. Modules are freely available that allow the use of Python for scientific data analysis and plotting and it is necessary to install these to e.g. try the read/plot example shown below.

Explicit use is made of the following modules:

- NetCDF4 – for reading and writing NetCDF files; see https://unidata.github.io/netcdf4-python/netCDF4/index.html
- Matplotlib – for scientific plotting; see http://matplotlib.org
- Iris – for analysing and visualising Earth science data, see https://scitools.org.uk/iris/docs/latest/index.html#

However, there are dependences on other modules (for example use of the NumPy module, http://www.numpy.org) that might be needed to be additionally installed. Python version 3.7 is used for the following examples which illustrate reading and plotting capabilities provided by the 'netcdf4', 'matplotlib' and 'iris' libraries. These examples were adapted from very similar ones shown in the SST CCI PUG [21]. This illustrates the high level of compatibility of data from different CCIs which makes them usable with very similar tools.

5.4.1 Reading with NetCDF4 and plotting with Matplotlib

The code shown below demonstrates how data can be read in from a file and plotted using Python; this example uses a TCWV L3 monthly product generated during a WV_cci test production cycle. Sections of text with a # symbol at the beginning are comments which explain what this code is doing in detail. The result is shown in Figure 5-11.

```
from netCDF4 import Dataset
import matplotlib.pyplot as plt
import matplotlib.colors as colors

# Open the ESA WV_cci file.
ncid = Dataset('ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-
                cmsaf_hoaps-005deg-201607-fv2.2.nc')

# Set up a large plotting window.
plt.figure(figsize=(14, 10))
```

```
# Do a line plot of the latitude coordinate in the upper left part of
# the plotting window. Metadata stored in the NetCDF file are used
# to define the y axis label.
var = 'lat'
latData = ncid.variables[var][:]
latLongName = ncid.variables[var].long_name
latUnits = ncid.variables[var].units
ax = plt.subplot(2, 2, 1)
ax.plot(latData)
ax.set_xlabel('Grid position')
ax.set_ylabel(latLongName + ' (' + latUnits + ')')
ax.set_title('Latitudes')

# Do a line plot of the longitude coordinate in the upper right part
# of the plotting window.(This is a replica of the code above except
# replacing latitude with longitude and changing the plot position).
var = 'lon'
lonData = ncid.variables[var][:]
lonLongName = ncid.variables[var].long_name
lonUnits = ncid.variables[var].units
ax = plt.subplot(2, 2, 2)
ax.plot(lonData)
ax.set_xlabel('Grid position')
ax.set_ylabel(lonLongName + ' (' + lonUnits + ')')
ax.set_title('Longitudes')

# Do a plot of the TCWV data array at the bottom left of the screen.
var = 'tcwv'
tcwvData = ncid.variables[var][::-1, :]
tcwvLongName = ncid.variables[var].long_name
tcwvUnits = ncid.variables[var].units
ax = plt.subplot(2, 2, 3)
tcwvPlot = ax.imshow(tcwvData, vmin=0, vmax=80,
                     origin='lower', cmap=plt.get_cmap('BuPu'),
                     extent=[-180,180,-90,90])
plt.xlabel('Longitude (degrees_east)')
plt.ylabel('Latitude (degrees_north)')
ax.set_title('TCWV')
cb = plt.colorbar(tcwvPlot, orientation='horizontal')
cb.set_label(tcwvLongName + ' (' + tcwvUnits + ')')

# Do a plot of the surface type flag data array.
```

```
var = 'surface_type_flag'
surfaceTypeData = ncid.variables[var][::-1, :]
surfaceTypeLongName = ncid.variables[var].long_name
ax = plt.subplot(2, 2, 4)

# Set colours from https://xkcd.com/color/rgb/ :
my_colors =['#e6daa6', '#0165fc', '#363737', '#00ffff', '#fac205',
            '#15b01a', '#d0fefe']
cmap = colors.ListedColormap(my_colors)
surfaceTypePlot = ax.imshow(surfaceTypeData, vmin=0, vmax=7,
              origin='lower', cmap=cmap, extent=[-180,180,-90,90])
plt.xlabel('Longitude (degrees_east)')
plt.ylabel('Latitude (degrees_north)')
ax.set_title('Surface type flag')
cb = plt.colorbar(surfaceTypePlot, orientation='horizontal')
cb.set_label(surfaceTypeLongName)

ncid.close() # Close the NetCDF file.
plt.show() # Show our completed plot.
```

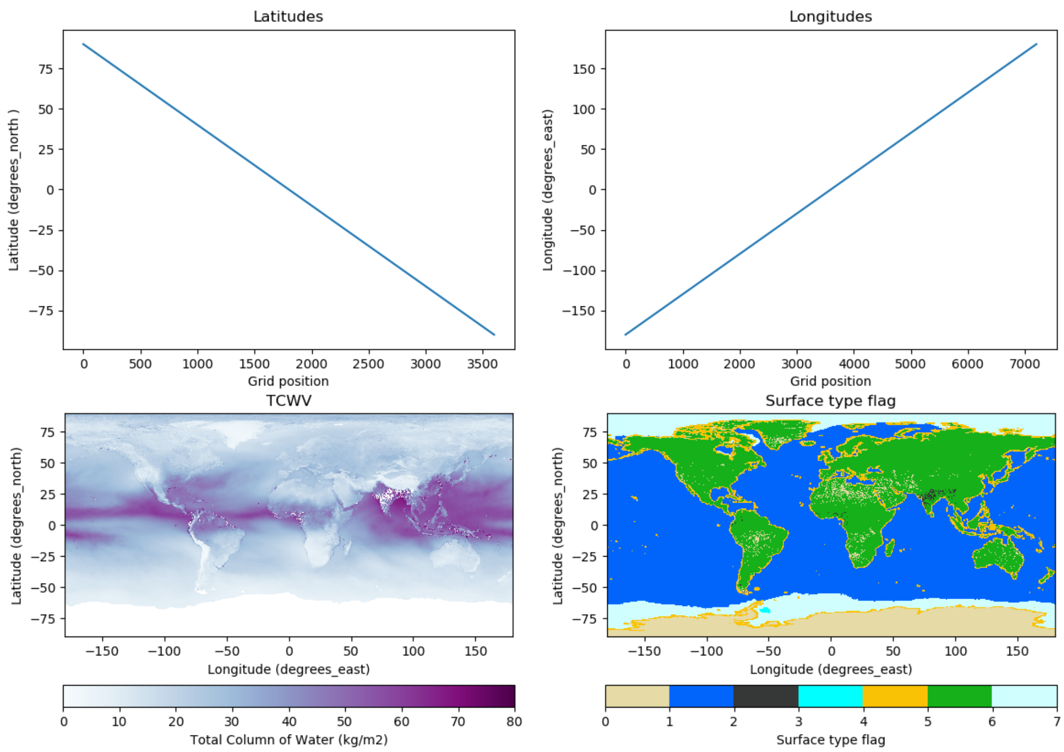

Figure 5-11: Result of applying the Python Matplotlib library to read and visualise TCWV data.

5.4.2 Reading and plotting with Iris

The ‘iris’ Python module is being developed at the Met Office for the purpose of analysing and visualising geophysical data. The simple example below demonstrates the use of Iris to read and plot the same data used for the Matplotlib example above. The result is shown in Figure 5-12.

```
import iris

import iris.quickplot as qplt

import matplotlib.cm as mpl_cm

import matplotlib.pyplot as plt


# Load the tcwv data into an iris structure known as a ‘cube’.

file = ‘ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-cmsaf_hoaps-
        05deg-201607-fv2.2.nc’

WVCube = iris.load_cube(file, ‘tcwv’)


# Also read the ‘surface_type_flag’ data array so that ice and
# land and ocean can be distinguished.

maskCube = iris.load_cube(file, iris.Constraint(cube_func=lambda
                         cube: cube.var_name == ‘surface_type_flag’))


# Find the TCWV values which are not ocean, seaice or coastal zone
# and mask them in the surface type flag data array. This is any
# point where the mask is not equal to 1, 3 or 4.

WVCube.data.mask[(maskCube.data != 1) & (maskCube.data != 3) &
                 (maskCube.data != 4)] = True


# Do a quick plot of the data. In this case a contour plot is done;
# qplt.pcolormesh could be used instead to do a block plot.
# For the colours, load a Cynthia Brewer palette
# (see http://colorbrewer.org/).

# Draw a countour line to highlight the coastlines.

brewer_cmap = mpl_cm.get_cmap(‘brewer_Blues_09’)

qplt.contourf(WVCube, brewer_cmap.N, cmap=brewer_cmap, vmin=0,
vmax=80)

plt.gca().coastlines()

plt.show()
```

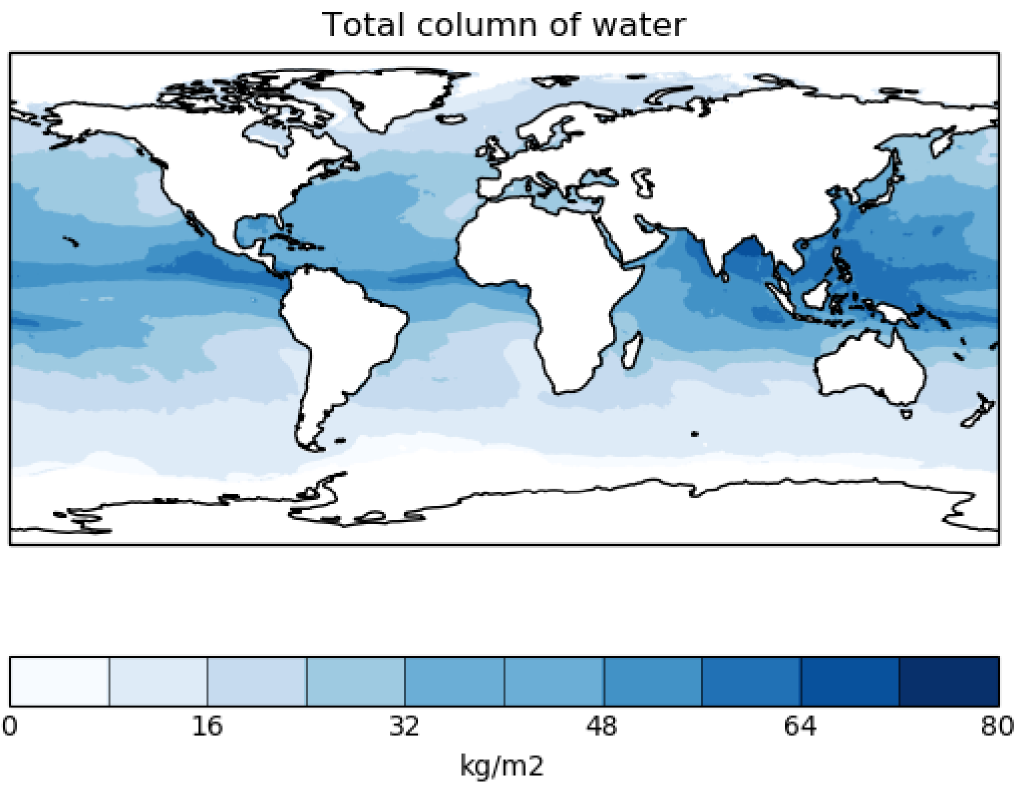

Figure 5-12: Result of applying the Python Matplotlib and Iris libraries to read and visualise TCWV data.

It is also possible to view metadata about the variable using Iris. Printing the TCWV Cube variable gives this information, which is automatically read by the software.

```
print WVCube
```

The output is shown below. It is very similar to a NetCDF ncdump (see Appendix 4: Listings of file contents).

```
Total Column of Water / (kg/m2)     (latitude: 3600; longitude: 7200)
     Dimension coordinates:
          latitude                          x                  -
          longitude                         -                  x
     Attributes:
          Conventions: CF-1.7
          actual_range: [0.0  78.372  ]
          cdm_data_type: grid
```

comment: These data were produced in the frame of the Water Vapour ECV (Water_Vapour_cci)…

creator_email: info@brockmann-consult.de; contact.cmsaf@dwd.de

creator_name: Brockmann Consult GmbH; EUMETSAT/CMSAF

creator_url: www.brockmann-consult.de; http://www.cmsaf.eu

date_created: 2020-04-07 10:18:32 UTC

format_version: CCI Data Standards v2.0

geospatial_lat_max: 90.0

geospatial_lat_min: -90.0

geospatial_lat_resolution: 0.05

geospatial_lat_units: degrees_north

geospatial_lon_max: 180.0

geospatial_lon_min: -180.0

geospatial_lon_resolution: 0.05

geospatial_lon_units: degrees_east

geospatial_vertical_max: 0.0

geospatial_vertical_min: 0.0

history: python nc-compliance-py-process.py /ssd1/yarn/local/usercache/olaf/app…

id: ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-cmsaf_hoaps-005deg-201607…

institution: Brockmann Consult GmbH; EUMETSAT/CMSAF

invalid_standard_name: atmosphere_water_vapor_content

key_variables: tcwv

keywords: EARTH SCIENCE > ATMOSPHERE > ATMOSPHERIC WATER VAPOR > WATER VAPOR,EARTH…

keywords-vocabulary: GCMD Science Keywords, Version 8.1

license: ESA CCI Data Policy: free and open access. Products containing CM SAF data…

naming-authority: brockmann-consult.de

platform: Envisat, Terra, DMSP-F16, DMSP-F17, DMSP-F18

product_version: 2.2

project: Climate Change Initiative - European Space Agency

references: WV_cci D2.2: ATBD Part 1 - MERIS-MODIS-OLCI L2 Products, Issue 1.1, 3 April…

sensor: MERIS, MODIS, SSMIS

source: MERIS RR L1B 3rd Reprocessing; MODIS MOD021KM L1B; HOAPS-S version 4.0…

spatial_resolution: 5.6km at Equator

standard_name_vocabulary: NetCDF Climate and Forecast (CF) Metadata Convention version 67

summary: Water Vapour CCI TCWV Dataset 1 (2010-2012)

```
time_coverage_duration: P1M
time_coverage_end: 201607-31 23:59:59 UTC
time_coverage_resolution: P1M
time_coverage_start: 201607-01 00:00:00 UTC
title: Water Vapour CCI Total Column of Water Vapour
       Product
tracking_id: 225dde06-78b9-11ea-9930-0cc47a950a6a
valid_range: [ 0. 80.]
```

Iris includes many other functions – data analysis, aggregation, mathematical operations etc. – and is constantly being improved with new functionality.

6. DATA ACCESS

CDR-1, CCI TCWV-land, is available via the ESA Open Data Portal at https://climate.esa.int/en/odp/#/project/water-vapour.

CDR-2, **CCI TCWV-global (COMBI)**, i.e. global TCWV from HOAPS and NIR measurements, is owned by the EUMETSAT CM SAF and is accessible via https://wui.cmsaf.eu. A dedicated Product User Manual for CDR-2 from CM SAF contains more details and is available from https://doi.org/10.5676/EUM_SAF_CM/COMBI/V001.

CDR-3, CCI WV-strato, is available via the ESA Open Data Portal at https://climate.esa.int/en/odp/#/project/water-vapour.

CDR-4, CCI WV-UTLS, is available upon request via email to: m.i.hegglin@reading.ac.uk and hao.ye@reading.ac.uk.

7. TERMS OF USE

CDR-1: ESA Climate Change Initiative Data Policy: free and open access, however, citation of the data-doi is requested.

CDR-2: All intellectual property rights of the CM SAF products belong to EUMETSAT. The use of these products is granted to every interested user, free of charge. If you wish to use these products in publications, presentations, web pages etc., EUMETSAT's copyright credit must be shown by displaying the words "copyright (2022) EUMETSAT" on each of the products used.

When exploiting EUMETSAT/CM SAF data you are kindly requested to acknowledge this contribution accordingly and make reference to the CM SAF, e.g. by stating "The work performed was done (i.a.) by using data from EUMETSAT's Satellite Application Facility on Climate Monitoring (CM SAF)". It is highly recommended to clearly identify the product version used. An effective way to do this is the citation of CM SAF data records via the digital object identifier (DOI).

Please do not re-distribute CM SAF data to 3rd parties and register as a user at https://www.cmsaf.eu/ to receive latest information on CM SAF services and to get access to the CM SAF User Help Desk

CDR-3: ESA Climate Change Initiative Data Policy: free and open access, however, citation of the data-doi is requested.

CDR-4: is available upon request. Usage should be discussed with data producers.

8. APPENDIX 1: REFERENCES

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9. APPENDIX 2: GLOSSARY

Term	Definition
AATSR	Advanced Along Track Scanning Radiometer
ACE-FTS	Atmospheric Chemistry Experiment Fourier Transform Spectrometer
AMSU	Advanced Microwave Sounding Unit
ATBD	Algorithm Theoretical Basis Document
BC	Brockmann Consult
BEAM	Basic Toolbox for Envisat AATSR and MERIS
Calvalus	Cal/Val and User Services
Cate	Climate Analysis Toolbox of the ESA Climate Change Initiative
CCI	Climate Change Initiative
CDR	Climate Data Record
CEDA	Centre for Environmental Data Analysis
CF	Climate and Forecast
CM SAF	Satellite Application Facility on Climate Monitoring
CSB	Clear-Sky Bias
DMSP	Defense Meteorological Satellite Program
DWD	Deutscher Wetterdienst (German Meteorological Service)
ECMWF	European Centre for Medium Range Weather Forecast
ECV	Essential Climate Variable
EO	Earth Observation
EOS	Earth Observing System
ERA	European Re-Analysis
ESA	European Space Agency
ESRI	Environmental Systems Research Institute
FCDR	Fundamental Climate Data Record
FTP	File Transfer Protocol
HALOE	Halogen Occultation Experiment
HDF	Hierarchical Data Format
HOAPS	Hamburg Ocean Atmosphere Parameters and Fluxes from Satellites data
IASI	Infrared Atmospheric Sounder Interferometer
IMS	Infrared Microwave Sounding
JASMIN	Joint Analysis System Meeting Infrastructure
MERIS	Medium Resolution Imaging Spectrometer
MHS	Microwave Humidity Sounder

Term	Definition
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder
MODIS	Moderate Resolution Imaging Spectroradiometer
NaN	Not a Number
NASA	National Aeronautics and Space Administration
NCAS	National Centre for Atmospheric Science
NEODC	NERC Earth Observation Data Centre
NERC	National Environment Research Council
NetCDF	Network Common Data Form
NGA	National Geospatial-Intelligence Agency
NIR	Near Infrared
OLCI	Ocean and Land Colour Instrument
PSD	Product Specification Document
PUG	Product User Guide
RAL	Rutherford Appleton Laboratory
RefSB	Reflective Solar Bands
RR	Reduced Resolution
SAFE	Standard Archive Format for Europe
SAGE	Stratospheric Aerosol and Gas Experiment
SCRIP	Spherical Coordinate Remapping and Interpolation Package
SDI	SPARC Data Initiative
SE	Spectral Earth
SNAP	Sentinel Application Platform
SoW	Statement of Work
SPARC	Stratosphere-troposphere Processes and their Role in Climate
SRD	System Requirements Document
SRTM	Shuttle Radar Topography Mission
SSD	System Specification Document
SSM/I	Special Sensor Microwave/Imager
SSMIS	Special Sensor Microwave Imager Sounder
SST	Sea Surface Temperature
STFC	Science and Technology Facilities Council
SWBD	SRTM Water Body Data
TB	TeraByte
TCWV	Total Column of Water Vapour
TOA	Top of Atmosphere

Term	**Definition**
UoR	University of Reading
UTLS	Upper tropospheric/lower stratospheric
VRWV	Vertically Resolved Water Vapour
VM	Virtual Machine
WGS-84	World Geodetic System 1984
WV	Water Vapour

10. APPENDIX 3: TCWV L3 MERGING RULES

10.1 Merge of products from NIR instruments (CDR-1)

The Level-3 TCWV CDR-1 products are generated for all single NIR instruments for periods with only one instrument available, and for combinations of instruments if there is a time overlap. This means that the following two merges are possible:

- MERIS + MODIS
- OLCI + MODIS

For a given grid cell, the merge is performed applying the following rules:

- merged TCWV and uncertainty terms are computed from the average of the two sensors, weighted by the corresponding numbers of L2 retrievals;
- flag values are merged 'by majority': the value from the sensor with the higher number of L2 retrievals is taken;
- the merged number of observations is the sum of the numbers of L2 retrievals from both sensors.

10.2 Merge of products from NIR instruments with CM SAF HOAPS (CDR-2)

The Level-3 TCWV CDR-2 products are generated for the combination of one or two NIR instruments with CM SAF HOAPS. This means that the following merges are possible in addition:

- MERIS + CM SAF HOAPS
- MODIS + CM SAF HOAPS
- (MERIS + MODIS) + CM SAF HOAPS
- OLCI + CM SAF HOAPS
- MODIS + CM SAF HOAPS
- (OLCI + MODIS) + CM SAF HOAPS

For a given grid cell, the merge is performed applying the following rules:

- if TCWV from CM SAF HOAPS is available, set merged TCWV to this value. This applies over ocean excluding 'coastal zone' (< 50km away from any coastline including islands[5]) and sea ice as given from the CM SAF L3 masks;

- if TCWV from CM SAF HOAPS is not available (land, coastal zone or sea ice), set merged TCWV to value from NIR instrument(s). If that value is not available either, set TCWV to NaN;

- if TCWV from CM SAF HOAPS is not available over open ocean because of lack of coverage, set TCWV to NaN;

- the merged number of observations is the value from CM SAF HOAPS if available, otherwise the value from NIR instrument(s).

[5] *Note that only if islands are large enough to be resolved in the CM SAF L3 land mask, a related coastline for this island is given in the mask product. This coastline is then treated as any other coastline.*

11. APPENDIX 4: LISTINGS OF FILE CONTENTS

This appendix contains listings of the headers of NetCDF files for examples of the ESA WV_cci final data products. The listings were produced using the ‘ncdump’ tool that is provided with the NetCDF library. The format of the listings is ‘network Common data form Description Language’ (CDL), which is described at http://www.unidata.ucar.edu/software/netcdf/docs/netcdf/CDL-Syntax.html

11.1 Header from a WV_cci TCWV L3 daily product

```
netcdf ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-cmsaf_hoaps-
05deg-20160716-fv3.1 {
dimensions:
	lat = 360 ;
	lon = 720 ;
	time = UNLIMITED ; // (1 currently)
	nv = 2 ;
variables:
	int time_bnds(time, nv) ;
		time_bnds:long_name = "Time cell boundaries" ;
		time_bnds:comment = "Contains the start and end times for
                                    the time period the data represent." ;
	int time(time) ;
		time:long_name = "Product dataset time given as days since
                                 1970-01-01" ;
		time:standard_name = "time" ;
		time:units = "days since 1970-01-01" ;
		time:calendar = "gregorian" ;
		time:axis = "T" ;
		time:bounds = "time_bnds" ;
	float lat(lat) ;
		lat:long_name = "Latitude" ;
```

```
        lat:standard_name = "latitude" ;
        lat:units = "degrees_north" ;
        lat:valid_range = -90.f, 90.f ;
        lat:reference_datum = "geographical coordinates,
                                WGS84 projection" ;
        lat:axis = "Y" ;
        lat:bounds = "lat_bnds" ;
    float lon(lon) ;
        lon:long_name = "Longitude" ;
        lon:standard_name = "longitude" ;
        lon:units = "degrees_east" ;
        lon:valid_range = -180.f, 180.f ;
        lon:reference_datum = "geographical coordinates,
                                WGS84 projection" ;
        lon:axis = "X" ;
        lon:bounds = "lon_bnds" ;
    float lat_bnds(lat, nv) ;
        lat_bnds:long_name = "Latitude cell boundaries" ;
        lat_bnds:valid_range = -90.f, 90.f ;
        lat_bnds:reference_datum = "geographical coordinates,
                                    WGS84 projection" ;
        lat_bnds:comment = "Contains the northern and southern
                             boundaries of the grid cells." ;
    float lon_bnds(lon, nv) ;
        lon_bnds:long_name = "Longitude cell boundaries" ;
        lon_bnds:valid_range = -180.f, 180.f ;
        lon_bnds:reference_datum = "geographical coordinates,
                                    WGS84 projection" ;
        lon_bnds:comment = "Contains the eastern and western
                             boundaries of the grid cells." ;
    byte tcwv_quality_flag(time, lat, lon) ;
        tcwv_quality_flag:_FillValue = -128b ;
```

```
        tcwv_quality_flag:long_name = "Quality flag of Total Column
                                       of Water Vapour" ;
        tcwv_quality_flag:units = " " ;
        tcwv_quality_flag:standard_name = "status_flag " ;
        tcwv_quality_flag:valid_range = 0b, 3b ;
        tcwv_quality_flag:flag_values = 0b, 1b, 2b, 3b ;
        tcwv_quality_flag:flag_meanings = "TCWV_OK
                                           HIGH_COST_FUNCTION_1
                                           HIGH_COST_FUNCTION_2
                                           TCWV_INVALID" ;
    byte surface_type_flag(time, lat, lon) ;
        surface_type_flag:_FillValue = -128b ;
        surface_type_flag:long_name = "Surface type flag" ;
        surface_type_flag:units = " " ;
        surface_type_flag:standard_name = "status_flag " ;
        surface_type_flag:valid_range = 0b, 7b ;
        surface_type_flag:flag_values = 0b, 1b, 2b, 3b, 4b,
                                        5b, 6b, 7b ;
        surface_type_flag:flag_meanings = "LAND OCEAN
               CLOUD_OVER_LAND HEAVY_PRECIP_OVER_OCEAN
               SEA_ICE COAST PARTLY_CLOUDY_OVER_LAND
               PARTLY_SEA_ICE" ;
    int num_obs(time, lat, lon) ;
        num_obs:_FillValue = -1 ;
        num_obs:long_name = "Number of Total Column of Water Vapour
                  retrievals contributing to L3 grid cell" ;
        num_obs:units = " " ;
        num_obs:coordinates = "lat lon" ;
    int num_hours_tcwv(time, lat, lon) ;
        num_hours_tcwv:_FillValue = -1 ;
        num_hours_tcwv:long_name = "Number of hours in day with
                       a valid TCWV value in L3 grid cell" ;
        num_hours_tcwv:units = " " ;
```

```
     num_hours_tcwv:coordinates = "lat lon" ;
float tcwv(time, lat, lon) ;
     tcwv:_FillValue = NaNf ;
     tcwv:long_name = "Total Column of Water" ;
     tcwv:units = "kg/m2" ;
     tcwv:standard_name = "atmosphere_water_vapor_content " ;
     tcwv:ancillary_variables = "stdv num_obs" ;
     tcwv:valid_range = 0.f, 70.f ;
     tcwv:actual_range = 0.009999999f, 70.f ;
float stdv(time, lat, lon) ;
     stdv:_FillValue = NaNf ;
     stdv:long_name = "Standard deviation of Total Column
                       of Water Vapour" ;
     stdv:units = "kg/m2" ;
float tcwv_err(time, lat, lon) ;
     tcwv_err:_FillValue = NaNf ;
     tcwv_err:long_name = "Average retrieval uncertainty" ;
     tcwv_err:units = "kg/m2" ;
float tcwv_ran(time, lat, lon) ;
     tcwv_ran:_FillValue = NaNf ;
     tcwv_ran:long_name = "Propagated retrieval uncertainty" ;
     tcwv_ran:units = "kg/m2" ;
int crs ;
     crs:wkt = "GEOGCS[\"WGS84(DD)\", \n  DATUM[\"WGS84\", \n
          SPHEROID[\"WGS84\", 6378137.0, 298.257223563]], \n
          PRIMEM[\"Greenwich\", 0.0], \n  UNIT[\"degree\",
          0.017453292519943295], \n  AXIS[\"Geodetic
          longitude\", EAST], \n  AXIS[\"Geodetic latitude\",
          NORTH]]" ;
     crs:i2m = "0.5,0.0,0.0,-0.5,-180.0,90.0" ;
     crs:long_name = "Coordinate Reference System " ;
```

```
        crs:comment = "A coordinate reference system (CRS) defines
                       how the georeferenced spatial data relates to
                       real locations on the Earth\'s surface " ;


// global attributes:
        :title = "Global Total Column of Water Vapour Product from
                 Microwave and Near Infrared Imagers" ;
        :institution = "EUMETSAT/CM SAF" ;
        :publisher_name = "EUMETSAT/CM SAF" ;
        :publisher_email = "contact.cmsaf@dwd.de" ;
        :publisher_url = "http://cmsaf.eu" ;
        :source = "Near-infrared Level 3 data (land, sea-ice and
                  coast) from Brockmann Consult and Spectral Earth:
                  microwave imager Level 3 data (ice-free ocean)
                  from EUMETSAT CM SAF : combined NIR and MW data
                  from Brockmann Consult and Spectral Earth : the
                  combined product was funded by and generated
                  within the ESA Water_Vapour_cci project" ;
        :history = "python nc-compliance-py-process.py
/hd1/yarn/local/usercache/olaf/appcache/application_1608030060513_158
912/container_1608030060513_158912_01_000002/l3_tcwv_olci-
modis_terra-cmsaf_hoaps_05deg_2016-07-16_2016-07-16.nc" ;
        :references = "WV_cci D2.2: ATBD Part 1 - MERIS-MODIS-OLCI
                      L2 Products, Issue 1.1, 3 April 2019; WV_cci
                      D4.2: CRDP Issue 2.1, 30 September 2020 " ;
        :tracking_id = "390aa76c-4f67-11eb-9359-00259074eaa6" ;
        :Conventions = "CF-1.7" ;
        :product_version = "3.1" ;
        :format_version = "CCI Data Standards v2.0" ;
        :summary = "This global TCWV data record makes use of the
                   complementary spatial coverage of near infrared
                   (NIR) and microwave imager (MW) observations:
                   SSM/I observations were used to generate TCWV
                   data over the global ice-free ocean while
                   MERIS, MODIS and OLCI observations were used
```

```
            over land, coastal areas and sea-ice. The
            product covers the period 2002-2017 with daily
            and montlhy as well as 0.05° and 0.5° temporal
            and spatial resolutions, respectively." ;
:keywords = "EARTH SCIENCE > ATMOSPHERE > ATMOSPHERIC WATER
             VAPOR > WATER VAPOR,EARTH SCIENCE > ATMOSPHERE
           > ATMOSPHERIC WATER VAPOR > PRECIPITABLE WATER" ;
:id = "10.5676/EUM_SAF_CM/COMBI/V001" ;
:naming-authority = "EUMETSAT/CM SAF" ;
:filename = "ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-
              cmsaf_hoaps-05deg-20160716-fv3.1.nc" ;
:keywords-vocabulary = "GCMD Science Keywords, Version 8.1"
;
:cdm_data_type = "grid" ;
:comment = "These data were produced in the frame of the
             Water Vapour ECV (Water_Vapour_cci) of the ESA
             Climate Change Initiative Extension (CCI+)
             Phase 1. They include CM SAF products over the
             ocean." ;
:date_created = "2021-01-05 15:03:52 UTC" ;
:creator_name = "ESA Water_Vapour_cci; Brockmann Consult;
                 DWD; EUMETSAT/CM SAF; Spectral Earth" ;
:creator_url = "http://cci.esa.int/watervapour" ;
:creator_email = "contact.cmsaf@dwd.de" ;
:project = "CM SAF" ;
:acknowledgement = "The combined MW and NIR product was
                    initiated and funded by the ESA
                    Water_Vapour_cci project. The NIR
                    retrieval was developed by Spectral
                    Earth. The NIR data was processed and
                    combined with the MW data by Brockmann
                    Consult. NIR data is owned by Brockmann
                    Consult and Spectral Earth." ;
:geospatial_lat_min = "-90.0" ;
:geospatial_lat_max = "90.0" ;
```

```
:geospatial_lon_min = "-180.0" ;

:geospatial_lon_max = "180.0" ;

:geospatial_vertical_min = "0.0" ;

:geospatial_vertical_max = "0.0" ;

:time_coverage_duration = "P1D" ;

:time_coverage_resolution = "P1D" ;

:time_coverage_start = "20160716 00:00:00 UTC" ;

:time_coverage_end = "20160716 23:59:59 UTC" ;

:standard_name_vocabulary = "NetCDF Climate and Forecast
                     (CF) Metadata Convention version 67" ;

:license = "The CM SAF data are owned by EUMETSAT and are
            available to all users free of charge and with
            no conditions to use. If you wish to use these
            products, EUMETSATs copyright credit must be
            shown by displaying the words \"Copyright (c)
            ([release-year]) EUMETSAT\" under/in each of
            these SAF Products used in a project or shown
            in a publication or website. Please follow the
            citation guidelines given at [DOI landing-page]
            and also register as a user at http://cm-
            saf.eumetsat.int/ to receive latest information
            on CM SAF services and to get access to the CM
            SAF User Help Desk." ;

:platform = "Environmental Satellite; Earth Observing
            System, Terra (AM-1); Defense Meteorological
            Satellite Program-F16; Defense Meteorological
            Satellite Program-F17; Defense Meteorological
            Satellite Program-F18" ;

:sensor = "Medium Resolution Imaging Spectrometer;
           Moderate-Resolution Imaging Spectroradiometer;
           Ocean and Land Colour Instrument; Special Sensor
           Microwave Imager/Sounder" ;

:spatial_resolution = "56km at Equator" ;

:geospatial_lat_units = "degrees_north" ;

:geospatial_lon_units = "degrees_east" ;
```

```
          :geospatial_lat_resolution = "0.5" ;
          :geospatial_lon_resolution = "0.5" ;
          :key_variables = "tcwv" ;
}
```

11.2 Header from a WV_cci TCWV L3 monthly product

```
netcdf ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-cmsaf_hoaps-
05deg-201607-fv3.1 {
dimensions:
     lat = 360 ;
     lon = 720 ;
     time = UNLIMITED ; // (1 currently)
     nv = 2 ;
variables:
     int time_bnds(time, nv) ;
          time_bnds:long_name = "Time cell boundaries" ;
          time_bnds:comment = "Contains the start and end times for
the time period the data represent." ;
     int time(time) ;
          time:long_name = "Product dataset time given as days since
                            1970-01-01" ;
          time:standard_name = "time" ;
          time:units = "days since 1970-01-01" ;
          time:calendar = "gregorian" ;
          time:axis = "T" ;
          time:bounds = "time_bnds" ;
     float lat_bnds(lat, nv) ;
          lat_bnds:long_name = "Latitude cell boundaries" ;
          lat_bnds:valid_range = -90.f, 90.f ;
          lat_bnds:reference_datum = "geographical coordinates, WGS84
                                      projection" ;
```

```
        lat_bnds:comment = "Contains the northern and southern
                            boundaries of the grid cells." ;
    float lon_bnds(lon, nv) ;
        lon_bnds:long_name = "Longitude cell boundaries" ;
        lon_bnds:valid_range = -180.f, 180.f ;
        lon_bnds:reference_datum = "geographical coordinates,
                                   WGS84 projection" ;
        lon_bnds:comment = "Contains the eastern and western
                            boundaries of the grid cells." ;
    byte surface_type_flag(time, lat, lon) ;
        surface_type_flag:long_name = "Surface type flag" ;
        surface_type_flag:units = " " ;
        surface_type_flag:standard_name = "status_flag " ;
        surface_type_flag:valid_range = 0b, 6b ;
        surface_type_flag:flag_values = 0b, 1b, 2b, 3b, 4b, 5b, 6b;
        surface_type_flag:flag_meanings = "LAND OCEAN
           CLOUD_OVER_LAND SEA_ICE COAST PARTLY_CLOUDY_OVER_LAND
           PARTLY_SEA_ICE" ;
    int num_days_tcwv(time, lat, lon) ;
        num_days_tcwv:_FillValue = -1 ;
        num_days_tcwv:coordinates = "lat lon" ;
        num_days_tcwv:long_name = "Number of days in month with a
                                  valid TCWV value in L3 grid cell" ;
        num_days_tcwv:units = " " ;
    float tcwv(time, lat, lon) ;
        tcwv:_FillValue = NaNf ;
        tcwv:coordinates = "lat lon" ;
        tcwv:long_name = "Total Column of Water" ;
        tcwv:units = "kg/m2" ;
        tcwv:standard_name = "atmosphere_water_vapor_content " ;
        tcwv:ancillary_variables = "stdv num_obs" ;
        tcwv:valid_range = 0.f, 70.f ;
```

```
        tcwv:actual_range = 1.28901f, 65.60595f ;
    float num_obs(time, lat, lon) ;
        num_obs:_FillValue = NaNf ;
        num_obs:coordinates = "lat lon" ;
        num_obs:long_name = "Number of Total Column of Water Vapour
                      retrievals contributing to L3 grid cell" ;
        num_obs:units = " " ;
    float stdv(time, lat, lon) ;
        stdv:_FillValue = NaNf ;
        stdv:coordinates = "lat lon" ;
        stdv:long_name = "Standard deviation of Total Column of
                      Water Vapour" ;
        stdv:units = "kg/m2" ;
    float tcwv_err(time, lat, lon) ;
        tcwv_err:_FillValue = NaNf ;
        tcwv_err:coordinates = "lat lon" ;
        tcwv_err:long_name = "Average retrieval uncertainty" ;
        tcwv_err:units = "kg/m2" ;
    float tcwv_ran(time, lat, lon) ;
        tcwv_ran:_FillValue = NaNf ;
        tcwv_ran:coordinates = "lat lon" ;
        tcwv_ran:long_name = "Random retrieval uncertainty" ;
        tcwv_ran:units = "kg/m2" ;
    double lat(lat) ;
        lat:long_name = "Latitude" ;
        lat:units = "degrees_north " ;
        lat:standard_name = "latitude" ;
        lat:valid_range = -90.f, 90.f ;
        lat:reference_datum = "geographical coordinates,
                           WGS84 projection" ;
        lat:axis = "Y" ;
```

```
          lat:bounds = "lat_bnds" ;

     double lon(lon) ;

          lon:long_name = "Longitude" ;

          lon:units = "degrees_east" ;

          lon:standard_name = "longitude" ;

          lon:valid_range = -180.f, 180.f ;

          lon:reference_datum = "geographical coordinates,
                                 WGS84 projection" ;

          lon:axis = "X" ;

          lon:bounds = "lon_bnds" ;

     int crs ;

          crs:wkt = "GEOGCS[\"WGS84(DD)\", \n  DATUM[\"WGS84\", \n
            SPHEROID[\"WGS84\", 6378137.0, 298.257223563]], \n
            PRIMEM[\"Greenwich\", 0.0], \n  UNIT[\"degree\",
            0.017453292519943295], \n  AXIS[\"Geodetic longitude\",
            EAST], \n  AXIS[\"Geodetic latitude\", NORTH]]" ;

          crs:i2m = "0.5,0.0,0.0,-0.5,-180.0,90.0" ;

          crs:long_name = "Coordinate Reference System " ;

          crs:comment = "A coordinate reference system (CRS) defines
                         how the georeferenced spatial data relates to
                         real locations on the Earth\'s surface " ;


 // global attributes:

          :title = "Global Total Column of Water Vapour Product from
                    Microwave and Near Infrared Imagers" ;

          :institution = "EUMETSAT/CM SAF" ;

          :publisher_name = "EUMETSAT/CM SAF" ;

          :publisher_email = "contact.cmsaf@dwd.de" ;

          :publisher_url = "http://cmsaf.eu" ;

          :source = "Near-infrared Level 3 data (land, sea-ice and
                    coast) from Brockmann Consult and Spectral Earth:
                    microwave imager Level 3 data (ice-free ocean)
                    from EUMETSAT CM SAF : combined NIR and MW data
```

```
                 from Brockmann Consult and Spectral Earth : the
                 combined product was funded by and generated
                 within the ESA Water_Vapour_cci project" ;
          :history = "python nc-compliance-py-process.py
/hd1/yarn/local/usercache/olaf/appcache/application_1608030060513_507
80/container_1608030060513_50780_01_000002/l3_tcwv_olci-modis_terra-
cmsaf_hoaps_05deg_2016-07-01_2016-07-31.nc" ;
          :references = "WV_cci D2.2: ATBD Part 1 - MERIS-MODIS-OLCI
                   L2 Products, Issue 1.1, 3 April 2019; WV_cci
                   D4.2: CRDP Issue 2.1, 30 September 2020 " ;
          :tracking_id = "cb005ab0-453d-11eb-8b45-0025900890e5" ;
          :Conventions = "CF-1.7" ;
          :product_version = "3.1" ;
          :format_version = "CCI Data Standards v2.0" ;
          :summary = "This global TCWV data record makes use of the
                  complementary spatial coverage of near infrared
                  (NIR) and microwave imager (MW) observations:
                  SSM/I observations were used to generate TCWV
                  data over the global ice-free ocean while
                  MERIS, MODIS and OLCI observations were used
                  over land, coastal areas and sea-ice. The
                  product covers the period 2002-2017 with daily
                  and montlhy as well as 0.05° and 0.5° temporal
                  and spatial resolutions, respectively." ;
          :keywords = "EARTH SCIENCE > ATMOSPHERE > ATMOSPHERIC WATER
                   VAPOR > WATER VAPOR,EARTH SCIENCE > ATMOSPHERE
                 > ATMOSPHERIC WATER VAPOR > PRECIPITABLE WATER" ;
          :id = "10.5676/EUM_SAF_CM/COMBI/V001" ;
          :naming-authority = "EUMETSAT/CM SAF" ;
          :filename = "ESACCI-WATERVAPOUR-L3S-TCWV-olci-modis_terra-
                  cmsaf_hoaps-05deg-201607-fv3.1.nc" ;
          :keywords-vocabulary = "GCMD Science Keywords, Version 8.1"
;
          :cdm_data_type = "grid" ;
```

```
:comment = "These data were produced in the frame of the
            Water Vapour ECV (Water_Vapour_cci) of the ESA
         Climate Change Initiative Extension (CCI+) Phase 1.
         They include CM SAF products over the ocean." ;

:date_created = "2020-12-23 16:42:06 UTC" ;

:creator_name = "ESA Water_Vapour_cci; Brockmann Consult;
                 DWD; EUMETSAT/CM SAF; Spectral Earth" ;

:creator_url = "http://cci.esa.int/watervapour" ;

:creator_email = "contact.cmsaf@dwd.de" ;

:project = "CM SAF" ;

:acknowledgement = "The combined MW and NIR product was
                    initiated and funded by the ESA
                    Water_Vapour_cci project. The NIR
                    retrieval was developed by Spectral
                    Earth. The NIR data was processed and
                    combined with the MW data by Brockmann
                    Consult. NIR data is owned by Brockmann
                    Consult and Spectral Earth." ;

:geospatial_lat_min = "-90.0" ;

:geospatial_lat_max = "90.0" ;

:geospatial_lon_min = "-180.0" ;

:geospatial_lon_max = "180.0" ;

:geospatial_vertical_min = "0.0" ;

:geospatial_vertical_max = "0.0" ;

:time_coverage_duration = "P1M" ;

:time_coverage_resolution = "P1M" ;

:time_coverage_start = "20160701 00:00:00 UTC" ;

:time_coverage_end = "20160731 23:59:59 UTC" ;

:standard_name_vocabulary = "NetCDF Climate and Forecast
                    (CF) Metadata Convention version 67" ;

:license = "The CM SAF data are owned by EUMETSAT and are
            available to all users free of charge and with
            no conditions to use. If you wish to use these
            products, EUMETSATs copyright credit must be
```

```
                 shown by displaying the words \"Copyright (c)
                 ([release-year]) EUMETSAT\" under/in each of
                 these SAF Products used in a project or shown in
                 a publication or website. Please follow the
                 citation guidelines given at [DOI landing-page]
                 and also register as a user at http://cm-
                 saf.eumetsat.int/ to receive latest information
                 on CM SAF services and to get access to the CM
                 SAF User Help Desk." ;

        :platform = "Environmental Satellite; Earth Observing
                  System, Terra (AM-1); Defense Meteorological
                  Satellite Program-F16; Defense Meteorological
                  Satellite Program-F17; Defense Meteorological
                  Satellite Program-F18" ;

        :sensor = "Medium Resolution Imaging Spectrometer;
                Moderate-Resolution Imaging Spectroradiometer;
                Ocean and Land Colour Instrument; Special Sensor
                Microwave Imager/Sounder" ;

        :spatial_resolution = "56km at Equator" ;

        :geospatial_lat_units = "degrees_north" ;

        :geospatial_lon_units = "degrees_east" ;

        :geospatial_lat_resolution = "0.5" ;

        :geospatial_lon_resolution = "0.5" ;

        :key_variables = "tcwv" ;

}
```

11.3 Header from original IMS monthly L3 product

Dimensions:

- nlat: Number of latitude bins (360)
- nlon: Number of longitude bins (180)
- nz: Number of vertical layers for profiles (24)
- nz1: Number of vertical levels for profiles (24)
- nbounds: Number of values needed to define layer boundaries (2)
- nsc_o: Number of reported sub-column amounts (10)
- nwn: Number of spectral points at which emissivity reported
- navhrr: Number of AVHRR channels
- nbcf: Number of spectal bias correction spectra fitted in retrieval

Global attributes:

- version: 1
- title: RAL IASI/AMSU/MHS (IMS) Temperature/Humidity/Ozone/Emissivity/Cloud L3 Product
- licence: TBC
- sensor: IASI/MHS/AMSU
- platform: Metop A
- institution: STFC Rutherford Appleton Laboratory / NCEO
- funding: TBC
- filename: TBC
- sensing_date: Nominal date of the L3 data; year, month as [YYYYMM]
- input_filenames: List of all L2 filename
- processing_flags: List of processing flags used at L3
- processing_flags_l2: List of processing flags used at L2
- conventions: CF-1.6
- source: TBC
- history: TBC
- references: doi:10.5194/amt-8-385-2015,http://www.rsg.rl.ac.uk,http://www.esa-ozoe-cci.org,http://climate.copernicus.eu
- tracking_id:
- product_version: v01
- summary: This dataset contains RAL Level-3 retrievals from the Infra-red + Microwave Sounder scheme (IMS) on a regular latitude/longitude grid. Retrievals are generated using the RAL optimal estimation scheme. The files include the individual profile uncertainties and averaging kernels (observational operators) which must be applied for appropriate comparison with other data sets, e.g. models or ozone sondes. See product user guide for information on file content and application of averaging kernels
- id: TBC
- naming_authority: uk.ac.rl.rsg
- cmd_data_type: Grid
- project: UK National Centre for Earth Observation (NCEO)
- acknowledgement: This data product has been developed at RAL with funding from NERC/NCEO and the ESA CCI. Data production supported by NERC, UKSA, ESA-CCI and EU-C3S. Metop L1 data was provided by Eumetsat
- comment: TBC
- date_created: TBC
- creator_name: Richard Siddans
- creator_url: www.rsg.rl.ac.uk
- creator_email: richard.siddans@stfc.ac.uk
- creator_address: Rutherford Appleton Laboratory, Harwell Campus, Didcot, Oxfordshire. OX11 0QX. UK
- NetCDF_Format: 4
- geospatial_lat_min: -90
- geospatial_lat_max: 90
- geospatial_lon_min: -180
- geospatial_lon_max: 180
- geospatial_vertical_min: 0
- geospatial_vertical_max: 80
- geospatial_lat_units: degrees_north
- geospatial_lon_units: degrees_east
- spatial_resolution: TBC
- string_date_format: YYYYMMDDTHHmmssZ UTC

- time_coverage_start: TBC
- time_coverage_end: TBC
- time_coverage_duration: TBC
- time_coverage_resolution: TBC
- Lv1b_File_version: TBC
- L2_data_version: -999
- File_creation_date: TBC
- Data_date: TBC

Variables:

- NC_FLOAT longitude (nlon)
    - long_name: Longitude
    - standard_name: longitude
    - units: degree_east
- NC_FLOAT latitude (nlat)
    - long_name: Latitude
    - standard_name: latitude
    - units: degree_north
- NC_FLOAT n (nlon,nlat)
    - long_name: Number of retrievals in each bin
    - units: 1
- NC_FLOAT p (nlon,nlat,nz)
    - long_name: Mean pressure grid for retrieved profiles
    - standard_name: air_pressure
    - units: hPa
- NC_FLOAT satzen (nlon,nlat)
    - long_name: Mean satellite zenith angle
    - units: degrees
- NC_FLOAT solzen (nlon,nlat)
    - long_name: Mean solar zenith angle
    - units: degrees
- NC_DOUBLE time (nlon,nlat)
    - long_name: Mean time in s since 00:00 on 1 Jan 2000
    - units: s
- _FillValue: -9.99e+11
- NC_FLOAT p_mid (nz)
    - long_name: Mean pressure of layer
    - units: hPa
- NC_FLOAT p_bounds (nbounds,nz)
    - long_name: Bounding pressures of layer
    - units: hPa
- NC_FLOAT sc_o (vertices,nsc_o)
    - long_name: Bounding pressure levels of reported ozone sub-columns (1000 hPa means surface)
    - standard_name: 1
    - units: hPa
- NC_FLOAT sc_c (vertices,nsc_c)
    - long_name: Bounding pressure levels of reported carbon monoxide sub-columns (1000 hPa means surface)
    - standard_name: 1
    - units: hPa
- NC_FLOAT t (nlon,nlat,nz)
    - long_name: Mean Retrieved atmospheric temperature profile
    - standard_name: air_temperature
    - units: K
- NC_FLOAT t_err (nlon,nlat,nz)

  - long_name: Mean of the estimated uncertainty on the retrieved atmospheric temperature profile
  - standard_name: air_temperature
  - units: K
- NC_FLOAT t_nwp (nlon,nlat,nz)
  - long_name: NWP atmospheric temperature profile
  - standard_name: air_temperature
  - units: K
- NC_FLOAT t_dofs (nlon,nlat)
  - long_name: Degrees of Freedom for Signal of temperature
  - units: 1
- NC_FLOAT w (nlon,nlat,nz)
  - long_name: Mean natural logaritm of the retrieved atmospheric water vapour profile in parts per million by volume
  - units: ln(ppmv)
- NC_FLOAT w_median (nlon,nlat,nz)
  - long_name: Median natural logaritm of the retrieved atmospheric water vapour profile in parts per million by volume
  - units: ln(ppmv)
- NC_FLOAT w_ap (nlon,nlat,nz)
  - long_name: A priori water vapour
  - units: ln(ppmv)
- NC_FLOAT w_apc (nlon,nlat,nz)
  - long_name: A priori contribution to retrieved water vapour
  - units: ppmv
- NC_FLOAT w_err (nlon,nlat,nz)
  - long_name: Mean of the estimated uncertainty on the atmospheric water vapour profile
  - units: 1
- NC_FLOAT w_std (nlon,nlat,nz)
  - long_name: Standard deviation in retrieved natural logarithm of the atmospheric water vapour profile
  - units: 1
- NC_FLOAT w_nwp (nlon,nlat,nz)
  - long_name: Natural logaritm of the atmospheric water vapour profile in parts per million by volume from NWP model
  - units: ln(ppmv)
- NC_FLOAT w_nwp_ak (nlon,nlat,nz)
  - long_name: Natural logaritm of the atmospheric water vapour profile in parts per million by volume from NWP model with averaging kernels applied
  - units: ln(ppmv)
- NC_FLOAT w_dofs (nlon,nlat)
  - long_name: Degrees of Freedom for Signal of water vapour
  - units: 1
- NC_FLOAT tpw (nlon,nlat)
  - long_name: Mean retrieved Total precipitable water vapour
  - units: mm
- NC_FLOAT tpw_median (nlon,nlat)
  - long_name: Median retrieved Total precipitable water vapour
  - units: mm
- NC_FLOAT tpw_err (nlon,nlat)
  - long_name: Mean of the estimated uncertainty on the Total precipitable water vapour
  - units: mm
- NC_FLOAT tpw_std (nlon,nlat)
  - long_name: Standard deviation in retrieved Total precipitable water vapour
  - units: mm

- NC_FLOAT tpw_nwp (nlon,nlat)
    - long_name: Total precipitable water vapour from NWP model
    - units: mm
- NC_FLOAT o (nlon,nlat,nsc_o)
    - long_name: Mean ozone sub-column amount
    - units: DU
- NC_FLOAT o_median (nlon,nlat,nsc_o)
    - long_name: Median ozone sub-column amount
    - units: DU
- NC_FLOAT o_std (nlon,nlat,nsc_o)
    - long_name: Standard deviation in retrieved ozone sub-columns
    - units: DU
- NC_FLOAT tsk (nlon,nlat)
    - long_name: Retrieved surface (skin) temperature
    - standard_name: surface_temperature
    - units: K
- NC_FLOAT tsk_ap (nlon,nlat)
    - long_name: A priori surface temperature
    - units: K
- NC_FLOAT tsk_err (nlon,nlat)
    - long_name: Mean of the estimated uncertainty on retrieved surface temperature
    - units: K
- NC_FLOAT tsk_std (nlon,nlat)
    - long_name: Standard deviation in the retrieved surface temperature
    - units: K
- NC_FLOAT tsk_nwp (nlon,nlat)
    - long_name: Model surface temperature
    - standard_name: surface_temperature
    - units: K
- NC_FLOAT t2 (nlon,nlat)
    - long_name: Retrieved 2m atmospheric temperature
    - standard_name: surface_temperature
    - units: K
- NC_FLOAT t2_nwp (nlon,nlat)
    - long_name: Model 2m atmospheric temperature
    - standard_name: surface_temperature
    - units: K
- NC_FLOAT dt2 (nlon,nlat)
    - long_name: Retrived surface - air temperature contrast (at 2m)
    - standard_name: surface_temperature
    - units: K
- NC_FLOAT dt2_nwp (nlon,nlat)
    - long_name: Model surface - air temperature contrast (at 2m)
    - standard_name: surface_temperature
    - units: K
- NC_FLOAT dt1000 (nlon,nlat)
    - long_name: Retrived surface - air temperature contrast (at 1km)
    - standard_name: surface_temperature
    - units: K
- NC_FLOAT dt1000_nwp (nlon,nlat)
    - long_name: Model surface - air temperature contrast (at 1km)
    - standard_name: surface_temperature
    - units: K
- NC_FLOAT cfr (nlon,nlat)
    - long_name: Retrieved effective cloud fraction
    - units: 1
- NC_FLOAT cfr_err (nlon,nlat)

  - long_name: Mean of the estimated uncertainty on retrieved cloud fraction
  - units: 1
- NC_FLOAT cfr_std (nlon,nlat)
  - long_name: Standard deviation in retrieved cloud fraction
  - units: 1
- NC_FLOAT cth (nlon,nlat)
  - long_name: Retrieved cloud top pressure in z-star scae-height.
  - units: km
  - comment: z-star is related to pressure by pressure=10^(3-zstar/16)
- NC_FLOAT cth_err (nlon,nlat)
  - long_name: Mean of the estimated uncertainty on retrieved cloud top height
  - units: km
- NC_FLOAT cth_std (nlon,nlat)
  - long_name: Standard deviation in the retrieved cloud top height
  - units: km
- NC_FLOAT bcf (nlon,nlat,nbcf)
  - long_name: Retrieved bias correction factor
  - units: 1
- NC_FLOAT bcf_err (nlon,nlat,nbcf)
  - long_name: Mean of the estimated uncertainty on retrieved bias correction factors
  - units:
- NC_FLOAT bcf_std (nlon,nlat,nbcf)
  - long_name: Standard deviation in the retrieved bias correction factors
  - units: 1
- NC_FLOAT em (nlon,nlat,nwn)
  - long_name: Retrieved emissivity
  - units: 1
- NC_FLOAT em_dofs (nlon,nlat)
  - long_name: Degrees of Freedom for Signal of surface emissivity
  - units: 1
- NC_FLOAT avhrr (nlon,nlat,navhrr)
  - long_name: Mean of co-located AVHRR radiances
  - units: 1
- NC_FLOAT jx (nlon,nlat)
  - long_name: State vector component of cost
  - units: 1
- NC_FLOAT jy (nlon,nlat)
  - long_name: Measurement component of cost
  - units: 1
- NC_FLOAT n_step (nlon,nlat)
  - long_name: The average number of retrieval steps (number of calls to the forward model)
  - units: 1
- NC_FLOAT cwn (nwn)
  - long_name: Wavenumbers associated with retrieved emissivity
  - units: cm-1
- NC_FLOAT sp (nlon,nlat)
  - long_name: Mean surface pressure in retrieval
  - units: hPa
- NC_FLOAT btd (nlon,nlat)
  - long_name: Brightness temperature difference between observed and simulated measurements for first guess state, in a window channel at 955.25 cm-1
  - units: K
- NC_FLOAT ak_w (nlon,nlat,nz,nz)

- long_name: Water vapour averaging kernel
- units: ppmv/ppmv

11.4 Header from WV_cci L3 monthly zonal mean VRWV CDR-3 v3

```
netcdf ESACCI-WATERVAPOUR-L3S-LP-MERGED-MZM-5deg-1985-2019_v3.3 {
dimensions:
        lat = 36 ;
        plev = 28 ;
        time = UNLIMITED ; // (420 currently)
        bnds = 2 ;
variables:
        float lat(lat) ;
                lat:units = "degrees_north" ;
                lat:bounds = "lat_bnds" ;
                lat:long_name = "Latitude" ;
                lat:standard_name = "latitude" ;
                lat:axis = "Y" ;
        float plev(plev) ;
                plev:units = "Pa" ;
                plev:long_name = "Pressure" ;
                plev:standard_name = "air_pressure" ;
                plev:positive = "down" ;
                plev:axis = "Z" ;
        double time(time) ;
                time:units = "months since 1980-01-01 00:00" ;
                time:bounds = "time_bnds" ;
                time:long_name = "Time" ;
                time:standard_name = "time" ;
                time:calendar = "standard" ;
                time:axis = "T" ;
        float lat_bnds(lat, bnds) ;
        double time_bnds(time, bnds) ;
        float zmh2o(time, plev, lat) ;
                zmh2o:units = "moles mole-1" ;
                zmh2o:long_name = "Zonal Mean Water Vapour Volume
Mixing Ratio" ;
                zmh2o:cell_methods = "time: mean longitude: mean" ;
                zmh2o:standard_name =
"mole_fraction_of_water_vapor_in_air" ;
        float zmh2o_std(time, plev, lat) ;
                zmh2o_std:units = "moles mole-1" ;
                zmh2o_std:long_name = "Standard Deviation of Zonal
Mean Water Vapour Volume Mixing Ratio" ;
        float zmh2o_err(time, plev, lat) ;
                zmh2o_err:units = "moles mole-1" ;
                zmh2o_err:long_name = "Uncertainty of Zonal Mean
Water Vapour Volume Mixing Ratio" ;
        float zmh2o_nr(time, plev, lat) ;
                zmh2o_nr:units = "1" ;
                zmh2o_nr:long_name = "Number of Instrument Values per
Climatological Bin" ;
        float quality_flag(time, plev, lat) ;
                quality_flag:units = "1" ;
                quality_flag:flag\ values = "0, 1, 2" ;
                quality_flag:flag\ meanings = "bad, good, use with
caution" ;
```

```
                quality_flag:comment = "only quality flags with value
of 1 should be used" ;
                quality_flag:long_name = "Quality Flag of Zonal Mean
Water Vapour Volume Mixing Ratio" ;

// global attributes:
                :title = "ESA CCI level 3 vertically resolved merged
monthly zonal mean water vapour product" ;
                :institution = "Reading University" ;
                :source = "SPARC Data Initiative water vapour
climatologies, see Hegglin et al. (ESSD, 2021)" ;
                :references = "Hegglin et al., ESSD,
https://doi.org/10.5194/essd-2020-342, 2021 (input datasets); Hegglin
et al., Nature Geosc., DOI: 10.1038/NGEO2236, 2014 (merging
algorithm)." ;
                :history = "Product generated using updated merging
algorithm by Hegglin et al. (2014)." ;
                :tracking_id = "ee307c3a-9d50-4140-b66e-9de5f818f4db"
;
                :Conventions = "CF-1.7" ;
                :product_version = "v3.3" ;
                :doi = "10.5285/92824e3ec2e44a58b10048df3209b99c" ;
                :format_version = "CCI Data Standards v2.2" ;
                :summary = "This dataset contains a timeseries of
monthly zonal mean water vapour fields merged from stratospheric limb
satellite observations." ;
                :keywords = "satellite, observation, atmosphere,
stratosphere, limb sounder" ;
                :id = "ESACCI-WATERVAPOUR-L3S-LP-MERGED-MZM-5deg-
1985-2019_v3.3.nc" ;
                :naming\ authority = "https://www.reading.ac.uk/met/"
;
                :comment = "This data was merged within the
Water_Vapour_cci using the merging algorithm" ;
                :date_created = "20220305T120000Z" ;
                :creator-name = "University of Reading, Department of
Meteorology" ;
                :creator-url = "https://www.reading.ac.uk/met/" ;
                :creator-email = "m.i.hegglin@reading.ac.uk" ;
                :project = "Water Vapour Climate Change Initiative -
European Space Agency" ;
                :geospatial_lat_min = "-90" ;
                :geospatial_lat_max = "90" ;
                :geospatial_vertical_min = "0.1" ;
                :geospatial_vertical_max = "300" ;
                :geospatial_vertical_units = "pressure" ;
                :time_coverage_start = "1985-01" ;
                :time_coverage_end = "2019-12" ;
                :time_coverage_duration = "P34M6" ;
                :standard_name_vocabulary = "CF Standard Name Table
v75" ;
                :licence = "ESA Climate Change Initiative Data
Policy: free and open access" ;
                :platform = "ERBS, UARS, SPOT-4, Odin, Meteor-3M,
Envisat, SCISAT, EOS Aura, ISS" ;
                :sensor = "SAGE II (v7), UARS-MLS (v6), HALOE (v19),
SAGE III (v4.0), POAM III (v4.0), SMR (v2), MIPAS (v20/v220),
SCIAMACHY (v4),ACE-FTS (v3.6), ACE-MAESTRO (v31), Aura-ML (v5), SAGE
III/ISS (v5.1)" ;
```

```
                :key_variables =
"mole_fraction_of_water_vapor_in_air" ;
                :geospatial_lat_units = "degrees_north" ;
                     :geospatial_lat_resolution = "\005" ;
```

11.5 Header from WV_cci L3 monthly VRWV CDR-4 v3

```
netcdf file ESACCI-WATERVAPOUR-L3S-LP-NP-MERGED-MLS-MIPAS-IMS-
5deg-2010-2014-v3.nc {
   dimensions:
     lon = 72;
     lat = 36;
     level = 22;
     time = UNLIMITED;   // (60 currently)
     nv = 2;
   variables:
     float lon(lon=72);
       :long_name = "Longitude";
       :units = "degrees_east";
       :standard_name = "longitude";
       :reference_datum = "geographical coordinates, WGS84
projection";
       :axis = "X";
       :bounds = "lon_bnds";

     float lon_bnds(lon=72, nv=2);
       :long_name = "Longitude cell boundaries";
       :valid_range = -180.0f, 180.0f; // float
       :reference_datum = "geographical coordinates, WGS84
projection";
       :comment = "Contains the eastern and western boundaries
of the grid cells.";

     float lat(lat=36);
       :long_name = "Latitude";
       :units = "degrees_north";
       :standard_name = "latitude";
       :valid_range = -90.0f, 90.0f; // float
       :reference_datum = "geographical coordinates, WGS84
projection";
       :axis = "Y";
       :bounds = "lat_bnds";

     float lat_bnds(lat=36, nv=2);
       :long_name = "Latitude cell boundaries";
       :valid_range = -90.0f, 90.0f; // float
       :reference_datum = "geographical coordinates, WGS84
projection";
       :comment = "Contains the northern and southern boundaries
of the grid cells.";

     float level(level=15);
       :long_name = "Pressure levels";
       :units = "hPa";
       :standard_name = "level";
       :valid_range = 30.0f, 500.0f; // float
       :axis = "Z";
```

```
     int time(time=60);
       :long_name = "Product dataset time given as days since
1970-01-01";
       :standard_name = "time";
       :units = "days since 1970-01-01";
       :calendar = "gregorian";
       :axis = "T";
       :bounds = "time_bnds";
       :_ChunkSizes = 1024; // int

     int time_bnds(time=60, nv=2);
       :long_name = "Time cell boundaries";
       :comment = "Contains the start and end times for the time
period the data represent.";
       :_ChunkSizes = 1, 2; // int

     float vmrh2o(time=60, level=15, lat=36, lon=72);
       :long_name = "Vertical resolved water vapour profile";
       :units = "ppmv";
       :standard_name = "atmosphere water vapour profile";
       :_ChunkSizes = 1, 15, 36, 72; // int

   // global attributes:
   :_NCProperties =
"version=1|netcdflibversion=4.6.1|hdf5libversion=1.10.2";
   :title = "Water Vapour CCI vertical resolved profile of Water
Vapour Product";
   :institution = "University of Reading";
   :source = "MLS L2 v4.2; MIPAS IMK v7; IMS L2 v2.1";
   :references = "XXXX";
   :Conventions = "CF-1.7";
   :product_version = "0";
   :format_version = "CCI Data Standards v3";
   :summary = "Water Vapour CCI VRWV Dataset 4 (2010-2014)";
   :keywords = "EARTH SCIENCE > ATMOSPHERE > ATMOSPHERIC WATER
VAPOR > WATER VAPOR";
   :id = " ESACCI-WATERVAPOUR-L3S-LP-NP-MERGED-MLS-MIPAS-IMS-
5deg-2010-2014-v3.nc";
   :keywords_vocabulary = "GCMD Science Keywords, Version 8.1";
   :cdm_data_type = "grid";
   :comment = "These data were produced in the frame of the
Water Vapour ECV (Water_Vapour_cci) of the ESA Climate Change
Initiative Extension (CCI+) Phase 1.";
   :creator_name = "University of Reading Department of
Meteorology";
   :creator_url = "https://www.reading.ac.uk/met/";
   :project = "Climate Change Initiative - European Space
Agency";
   :geospatial_lat_min = "-90.0";
   :geospatial_lat_max = "90.0";
   :geospatial_lon_min = "-180.0";
   :geospatial_lon_max = "180.0";
   :geospatial_vertical_min = "10 hPa";
   :geospatial_vertical_max = "1000 hPa";
   :time_coverage_duration = "P1M";
   :time_coverage_resolution = "P1M";
   :time_coverage_start = "2010-01-01 00:00:00 UTC";
   :time_coverage_end = "2014-12-31 23:59:59 UTC";
```

```
    :standard_name_vocabulary = "NetCDF Climate and Forecast (CF)
Metadata Convention version 67";
    :license = "ESA CCI Data Policy: free and open access.";
    :platform = "NASA\'s EOS Aura; ENVISAT; SCISAT; SCISAT;
Eumetsat Metop";
    :sensor = "MLS; MIPAS; ACE-FTS; ACE MAESTRO; IASI/MHS/AMSU";
    :spatial_resolution = "556km at Equator";
    :geospatial_lat_units = "degrees_north";
    :geospatial_lon_units = "degrees_east";
    :geospatial_lat_resolution = "5";
    :geospatial_lon_resolution = "5";
    :key_variables = "vrwv";
 }
```