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'AIRWAVE-SLSTR: an algorithm to retrieve TCWV from SLSTR measurements over water surfaces'

ATBD (Algorithm Theoretical Basis Document)

D6-AIRWAVE-SLSTR-ATBD

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1 Introduction

Acronyms and Abbreviations

AATSR	Advanced Along Track Scanning Radiometer
ADF	Auxiliary Data Files
ALTS	ATSR Long Term Stability
AIRWAVE	Advanced Infra-Red Water Vapour Estimator
ARSA	Analyzed RadioSounding Archive
ATBD	Algorithm Theoretical Basis Document
ATSR	Along Track Scanning Radiometer
BT	Brightness Temperature
DISORT	Discrete Ordinates Radiative Transfer Program
ECMWF	European Centre for Medium-Range Weather Forecasts
ECVs	Essential Climate Variables
ESA	European Space Agency
ESA DUE	ESA Data User Element programme (http://due.esrin.esa.int/)
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
ENVISAT	Environmental Satellite
FOV	Field of View
GCOS	Global Climate Observing System
GEWEX	Global Energy and Water Exchanges Project
GNSS	Global Navigation Satellite System
G-VAP	GEWEX Water Vapour Project
IFOV	Instantaneous Field Of View
IGRA	Integrated Global Radiosonde Archive
ILS	Instrumental Line Shape
IODD	Input Output Data Definition Document
IR	Infra-Red
IREMIS	IR emissivity
ISAC	Istituto di Scienze dell’Atmosfera e del Clima
JCSDA	Joint Center for Satellite Data Assimilation
LSWT	Lake Surface Water Temperature
LUT	Look-Up-Tables
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MWR	MicroWave Radiometer
NEΔT	Noise equivalent Delta Temperature
NWP	Numerical Weather Prediction

PSD	Product Specification Document
PSU	Practical Salinity Unit
PVP	Product Validation Plan
OLCI	Ocean and Land Colour Instrument on board Sentinel-.-3
PVR	Product Validation and evolution Report
QWG	Quality Working Group
RB	Requirements Baseline
RMSE	Root Mean Square Error
RTM	Radiative Transfer Model
RTTOV	Radiative Transfer for TOVS
RVD	Reference Validation Dataset
S3	Sentinel 3
SLSTR	Sea and Land Surface Temperature Radiometer
SSH	Sea Surface Height
SSM/I	Special Sensor Microwave/Imager
SSS	Sea Surface Salinity
SST	Sea Surface Temperature
SRF	Spectral Response Function
SWIR	Short Wave-Infrared
TCWV	Total Column of Water Vapor
TDS	Testing Data Set
TIR	Thermal Infrared
URD	User Requirements Document
VIS	Visible
WMO	World Meteorological Organization
WP	Work Package
WTC	Wet Tropospheric Correction

Purpose and Scope

This document describes the theoretical baseline of the algorithm to be used to retrieve the total column of water vapour above water surfaces from SLSR measurements (AIRWAVE-SLSTR) along with an overview of the product characteristics and requirements.

Accurate knowledge of the distribution and variability of the TCWV (vertically integrated atmospheric water vapour) is of vital importance in assessing climate change. Therefore, the Global Climate Observing System (GCOS) expert panels have identified TCWV as an essential climate variable (ECV). In the past years, in the frame of the ALTS project, a novel algorithm for the retrieval of TCWV over sea surface for the ATSR instrument series was developed [RD.1]. ATSR is a scanning radiometer that

observes the radiation emitted by the Earth surface with two viewing angles (nadir 90 deg and forward 55 deg) over a set of spectral bands, two of which (the TIR channels) have been operated in all the instrument series (ATSR-1, ATSR-2 and AATSR).
During the ALTS project, it was demonstrated that it is possible to retrieve the TCWV from ATSR-like instruments exploiting the top of the atmosphere Brightness Temperatures collected from nadir and forward views of the channels at 11 and 12 microns [RD.1]. The algorithm, called AIRWAVE, makes use of the clear-sky ATSR TIR BT above water surfaces, combining nadir and forward observation geometries. AIRWAVE adopts a linear solving equation that connects the TCWV above the earth surface covered by each pixel with the observed top of the atmosphere BTs in the two TIR channels. The equation exploits parameters calculated with a dedicated RTM and the emissivity of the surface in the used spectral ranges.
Because of the good knowledge and of the stability of the emissivity data above water surfaces as opposed to the uncertainty and variability of the emissivity above land, the algorithm makes use of pixels above water surfaces only.
In [RD.2] several shortcomings of the first version of the algorithm were highlighted and corrected in the second version of the algorithm AIRWAVEv2. When compared to independent TCWV products (i.e. using the SSM/I and the ARSA), the v2 products show very good agreement with almost no bias all over the ATSR missions, also in the polar and the coastal region [RD.3].
Copernicus Sentinel-3 (S3) SLSTR is a conical scanning imaging radiometer employing the along-track scanning dual-view technique to measure the radiance at the top of the atmosphere in nine spectral channels: six solar channels from the visible (554 nm) to the Short Wave-Infrared (3.74 nm), and two in the thermal infrared (10.85 and 12.02 µm). Each scene is observed twice: in nadir and backward views. SLSTR is an evolution of the ATSR instrument series (on board ERS-1 and 2) and AATSR (on board of ENVISAT). The major difference is that the SLSTR slant view points backward with respect to the satellite flight direction, while the ATSR slant view was pointing forward; moreover, SLSTR has a wider swath (1420 km in nadir, 750 km in backwards view) and an increased spatial resolution for the VIS channels (~500 m). Furthermore, SLSTR has two additional channels in the SWIR compared to AATSR: 1.3 µm and 2.2 µm.

2 Product Overview (Requirement Baseline - D4 of SoW)

2.1 Product Description

Water vapour in the atmosphere is crucial for the Earth's energy balance since it is the most relevant greenhouse gas of natural source. Moreover, the concentration of water vapour in the atmosphere is a key element in the water cycle.

The water vapour distribution plays a major role for both meteorological phenomena and climate via its influence on the formation of clouds and precipitation, the growth of aerosols, and the reactive chemistry related to ozone and the hydroxyl radical [RD.4].

The TCWV is critical for understanding the impacts and risks of climate change, with global long time series being crucial for this task. In the Arctic, the rate of climate change is two times larger than the global one due to increment in greenhouse gases concentration. Being one of the major greenhouse gases, water vapour is responsible for this Arctic amplification [RD.5]. For all these reasons, the GCOS has therefore included TCWV among the ECVs. Satellite data are crucial for monitoring ECVs due to their global coverage and extended time of operations. In particular, for the TCWV ECV, satellite measurements are vital to achieve the desired global coverage and accuracy.

Due to the importance of TCWV in climate and atmospheric studies, several International bodies, such as GCOS and WMO, have assessed the requirements for the measurement of the TCWV.

Beside the aforementioned applications, the value of the TCWV is also crucial for applications such as the computation of WTC. WTC is a critical correction applied to altimetric measurements for the accurate (at centimetre level) retrieval of SSH, being one of its major error sources. WTC can be calculated from TCWV measurements or modelled with NWP. However, the accuracy of NWP models is still not sufficient for most altimetry applications. An accurate modelling of the effect of the WTC can, therefore, be achieved only through the use of concurrent measurements. For these reasons, in most recent altimetric missions, a MWR has been included. The spatial resolution of the MWR sensors ranges from 50 km to 10 km in most advanced instruments [RD.6].

The MWR spatial resolution allows for highly accurate WTC corrections in open ocean. However, in coastal regions, the accuracy of the correction is highly degraded by contamination from land and ice in the MWR FOV. Despite the minor coverage of coastal areas with respect to open ocean, the importance of altimetry measurements in this area is crucial because here the sea state has the larger effects on human society [RD.7].

Several approaches have been developed in recent years trying to overcome this issue. In the future the quality of WTC in coastal regions will rely on dedicated retrieval algorithms and from new generations of instruments with high spatial resolution.

2.2 Requirements analysis

The requirements of the users for the performance and characteristic that an observed quantity should have, and that will be applied to the TCWV product, are generally given in terms of:

1) Accuracy: reported in absolute or percentage value is "the closeness between a measured value and the true value of the measurand, including the effects of systematic errors". Often accuracy and measurements uncertainties are considered equivalent (see for example [RD.8]).
2) Precision: the random (unpredictable) variability of repeated measurements of the measurand.
3) Spatial resolution.
4) Temporal resolution.
5) Timeliness.

For long datasets, the requirement on the time length and stability of the records is also necessary.

Requirements can be defined through the use of different values:

1) **Threshold** (limit value for data to be useful for a given application).
2) **Target** value (limit value to get significant improvements for a specific application).
3) **Goal** (limit value below which no further improvement is foreseen).

2.3 *TCWV performance Requirements from Previous Studies*

In this section we analyse the requirements on TCWV on the basis of their applications: for NWP and/or climatological studies and for coastal altimetry applications.

2.3.1 GCOS, WMO, ESA DUE GlobVapour and GEWEX, GNSS, OLCI L3 baseline requirements

International organizations have set different requirements for temporal and spatial resolution for TCWV, depending on the different applications for which the dataset is used and on the needs of the identified end users. For this reason, the value of the requirements is not homogeneous and depends on the application for which the TCWV is used and on the organization that has set the requirement itself. The requirements reported in this section are mainly related to model application, both Global NWP and Regional or Local NWP or for Climate studies and atmospheric chemistry applications.

The requirements have been extracted from [RD.8, RD.9] for GCOS and GEWEX, from [RD.10] for GNSS and from [RD.11] for Sentinel/3 OLCI. The values of the requirements for a given application set by different agencies are quite similar in terms of accuracy and horizontal resolutions while for the observing cycle some difference exists.

Requirements set by various agencies are summarized in Table 1.

TCWV requirement	Threshold	Goal
Spatial resolution (global scale)	250 km	20 km
Spatial resolution (regional scale)	50-100 km	1-3 km
Stability	1%	0.3%
Observing cycle (temporal resolution)	daily	1 h
Accuracy	5 kg/m^2 (2%)	1 kg/m^2 (20%)
Precision	10%	1%

***Table 1**: TCWV Requirements from international organizations.*

These requirements are more applicable to averaged TCWV SLSTR products (Level 3) than to the TCWV SLSTR Level 2 products.

2.3.2 Coastal altimetry TCWV requirements from WTC

As reported in section 4.2, the accurate determination of TCWV at high spatial resolution is crucial for the calculation of the WTC correction, and thus for the SSH accurate retrieval, especially in coastal regions (but this is also true for inland water, some comments on that in section 6).

An estimate of the requirements for WTC is reported in the GMES Sentinel-3 Mission Requirement document [RD.12]. From this document the required accuracy for WTC from MWR on-board Sentinel-3 has a threshold correction accuracy of 2 cm with a goal of 1.2 cm in WTC for ground processing. Considering that a rough estimate of the ratio between WTC and TCWV can be given by [RD.6]:

$$WTC\ [m] \simeq -0.0067 \cdot TCWV\ [mm] \qquad \text{[Eq.1]}$$

And that 1 kg/m^2 of WV is equivalent to 1 mm of WV we can conclude that the requirement on TCWV for altimetry applications goes from 1.8 kg/m^2 to 3 kg/m^2. The TCWV requirements for coastal altimetry applications are reported in Table 2.

TCWV requirements for altimetry applications	Goal	Threshold
Accuracy	1.8 kg/m2	3 kg/m2
Spatial Resolution	order of km	10 km
Temporal resolution	coincident	6 h

***Table 2**: TCWV requirements for coastal altimetry applications.*

2.4 SLSTR TCWV estimated performances vs requirements

TCWV from SLSTR measurements can only have the spatial and temporal resolution equal or larger than the ones SLSTR pixels have. SLSTR measurements have a mean global coverage revisit time at the equator of 1.9 days (one spacecraft) or 0.9 days (two spacecraft) and global coverage for dual view and day and night measurements. The horizontal (pixel) resolution is about 1 km.

Due to their characteristics, and in particular of the high spatial resolution, the TCWVs from SLSTR should fit very well for coastal altimetry applications, provided that the required accuracy level is reached.

Up to now, we are not able to assess TCWV AIRWAVE SLSTR accuracy while we can have a rough estimate of the precision connected to the random error due to noise (about 0.02K in both channels). This value is about 3-5% depending on the used scenario [RD.13].

However, a rough estimate of the accuracy of AIRWAVE TCWV retrievals can be given extrapolating the results obtained from the validation of the AIRWAVEv2 ATSR dataset and reported in [RD.2]. In [RD.2] the performances of AIRWAVE have been evaluated against both satellite instrument (SSM/I) and radiosondes (ARSA archive). This exercise, performed over the whole ATSR mission (from 1991 to 2012), showed that AIRWAVE has a bias of 0.02 kg/m^2 with respect to SSM/I and of 0.19 kg/m^2 with respect to radiosondes. Both these values are below the goal accuracy required for both the altimetry and the climatological applications. While the bias calculated versus SSM/I is more representative at the global scale and is performed over TCWV values aggregated at SSM/I spatial resolution (0.25°x0.25°), the bias versus radiosondes, performed at native ATSR spatial resolution, is more representative of points near coastal areas/inland waters.

A further hint on the performances of AIRWAVE TCWV when applied to altimetry studies can come from [RD.14]. The objective of that work was to develop, assess and validate a GPD+ WTC computed with the AIRWAVE dataset of TCWV. GPD+ is an algorithm, developed by the University of Porto, aiming at computing WTC for coastal regions where MWR observations are invalid and for missions without an on-board MWR (e.g., CryoSat-2). GPD+ with AIRWAVE takes advantage of the high spatial resolution AIRWAVE TCWV (1x1 km^2) and of the existence of these data up to the coast. Results for the North-West Mediterranean Sea and for ENVISAT show that that GPD+ with AIRWAVE shows an improvement in coastal regions (0-100 km) when used instead of ESA-MWR- and ERA- derived WTC. Overall, the results underline the potential of AIRWAVE data for coastal altimetry applications (some strategy to reduce AIRWAVE noise should be applied to get even better results, [RD.15]).

2.5 Scientific state-of-the-art

The Along-Track Scanning Radiometer instrument series had, as its main objective, the accurate retrieval of sea surface temperature for climate studies. However, Casadio et al. (2016) in [RD.1] demonstrated that it is possible to retrieve accurate and precise TCWV from its daytime and night-time measurements, using the ATSR BTs collected from nadir and forward views in the channels at 10.8 and 12 µm in clear-sky daytime and night-time sea scenes. As already said in the introduction, the AIRWAVE algorithm exploits a sea emissivity dataset and calculations made with a dedicated RTM. A detailed description of the algorithm is given in [RD.1]. The first version of the AIRWAVE TCWV dataset (hereafter AIRWAVEv1), spanning from 1991 to 2012, is freely available from the GEWEX G-VAP website (G-VAP, 2018) in the form of monthly fields at 2°x2° regular grid resolution from 2003 to 2008 [RD.16] (Schroder et al., 2018). Due to the legacy of the ATSR series, and the fact that the radiances are a fundamental climate dataset record, the AIRWAVE dataset is an important resource for water vapour studies.

3 Brief Satellite Instrument Description

SLSTR is designed to maintain continuity with the ATSR instrument series. The ATSR mission was developed to provide a reference SST dataset. SLSTR aims at retrieving global coverage SST with zero bias and an uncertainty of ± 0.3 K for a 5° by 5° latitude–longitude area, having a temporal stability of 0.1 K/decade. For these reasons, SLSTR has been designed with characteristics similar to ATSR but with some advanced features. In particular, new spectral channels have been added: 2, at wavelengths of 2.25 and 1.375 μm, in support of cloud clearing for surface temperature retrieval; two more channels, with an extended dynamic range at 10.8 μm and 3.7 μm, were added to detect fires at ~650 K without saturation.

The SLSTR swath is wider than the ATSR one: the width of the nominal image swath is 1400 km for the nadir view, and 740 km for the along track view. The spatial resolution is 500 m for visible 1km for TIR. The wider nadir swath and enhanced resolution are particularly important in coastal regions.

3.1 Assessment of Instrument Benefits and Capabilities with respect to the Product

The benefits and capabilities of AIRWAVE SLSTR TCWV for its applications in climatological and altimetric studies have already been reported in Section 2 - Requirement Baseline.

4 Algorithm Description

4.1 Processing Outline

The SLSTR-AIRWAVE algorithm derives total column water vapour products using all available SLSTR brightness temperature measurements in the thermal infrared (10.85 and 12.02 μm) both in nadir and backward views from the Sentinel 3-A and the Sentinel 3-B satellites. The primary inputs are the SLSTR Level-1b data files.

The SLSTR TCWV Level 2 generation is performed through the following processing chain:

1) Read SLSTR-AIRWAVE retrieval parameters and Type B uncertainties.
2) Read SLSTR Level 1B products.
3) Run the SLSTR-AIRWAVE retrieval algorithm.
4) Production of the NetCDF4 SLSTR TCWV Level 2 outputs.
5) Quality checks on the generated outputs.

4.2 Theoretical Description

In this section we describe the theoretical baseline for the algorithm used for the TCWV retrieval from SLSTR and the relative errors calculation.

4.2.1 Physical Description

The IR radiance that reaches the instrument onboard the satellite is given by:

$$J_t = \varepsilon J_S e^{-\tau_S} + L^{UP} + (1-\varepsilon) L_{DOWN} e^{-\tau_S} \qquad \text{Eq.1}$$

where J_t is the radiance at the sensor, ε is the Earth emissivity, J_S is the radiance emitted by the Earth at the sea surface temperature T, $e^{-\tau_S}$ accounts for the atmospheric transmittance, L^{UP} is the upward atmospheric radiance contribution, while L_{DOWN} is the downward atmospheric radiance contribution.

The J_t radiance measured by the instrument is the spectrally resolved TOA radiance "weighted" by the SRF of each instrument channel. In case of the SLSTR TCWV retrieval, we use the radiances measured by the S8 and S9 IR channels. The atmospheric Transmissivity of those channels is due to the atmospheric constituents with spectral features in the two spectral bands. In the S8 and S9 SLSTR bands the main spectral features are due to water vapour and, with a minor contribution, CO_2. Other species whose spectral features in the two bands are CFCs (-11 and -12) and HNO_3. However, those species have a very minor contribution and their impact on the atmospheric transmissivity can be neglected (see error analysis).

Therefore, the optical depth in the S8 and S9 channels is then a function of the TCWV and of the CO_2 total column amount:

$$\tau = \sigma\rho \approx \sigma_{H2O} TCWV + \sigma_{CO2}\rho_{CO2} \qquad \text{Eq.2}$$

where σ is the species-dependent absorption cross section and ρ is the total column amount of the atmospheric species. In the AIRWAVE ATSR and SLSTR TCWV retrieval, this relation is used to retrieve TCWV from the sensor radiances. In the following section we report the mathematical description used for the AIRWAVE TCWV retrieval.

4.2.2 Mathematical Description of the AIRWAVE algorithm

The expressions used to retrieve TCWV from AIRWAVE has been published in [RD.2], here we report the same expressions substituting "O" for "Oblique" view to the "F" for "Forward", for consistency with SLSTR nomenclature:

$$TCWV = \frac{\alpha}{\Delta\sigma_{NAD}} \left\{ ln \frac{L_{1N}^{\lambda 1}}{L_{2N}^{\lambda 2}} - \chi - E_N - \lambda 2\, \tau CO2_2^N + \lambda 1\, \tau CO2_1^N - \rho_{NAD} \right\} +$$

$$\frac{\beta}{\Delta\sigma_{OBL}}\left\{ln\frac{L_{1O}^{\lambda 1}}{L_{2O}^{\lambda 2}} - \chi - E_O - \lambda 2\, \tau CO2_2^O + \lambda 1\, \tau CO2_1^O - \rho_{OBL}\right\} \qquad \text{Eq.3}$$

where $\lambda 1$ is the central wavelength of the 11 micron channel, $\lambda 2$ is the central wavelength of the 12 micron channel, L_{1N}^1 is the radiance in the 11 micron channel at nadir , L_{1O}^1 is the radiance in the 11 micron channel in oblique view, L_{2N}^2 is the radiance in the 12 micron channel at nadir a, L_{2O}^2 is the radiance in the 12 micron channel in oblique view , χ is a constant, E_N and E_O are the ratio of the emissivities in the two channels in nadir and oblique view respectively , $\tau CO2_2^N$ and $\tau CO2_1^N$ are the optical depth due to CO_2 in the two channels at nadir and $\tau CO2_2^O$ and $\tau CO2_1^O$ are the optical depth due to CO_2 in the two channels for oblique view.

α,β, $\Delta\sigma_{NAD}$,$\Delta\sigma_{OBL}$,ρ_{NAD},ρ_{OBL} are the retrieval parameters. The description of their calculation is reported in [RD.2]. These parameters are computed a-priori for four seasons, six latitude bands and eleven viewing angles for Nadir and Forward views and then interpolated by the AIRWAVE retrieval code at the exact position, day and angles of measured radiances.

Some more details on the parameters calculations are given in the following section (Sect. 4.3.2.1).

The complete derivation of Eq. 3 from Eq. 1 can be found in [RD.2].

We recall here that the AIRWAVE retrievals only depend on the calculated retrieval coefficients and on the emissivity database (see section 4.2.2)

4.2.3 Retrieval Error Mathematical Description

A detailed description of the general definition of the errors and their treatment can be found in [RD.17] and [RD.18]. In particular, [RD.17] does not use the standard error separation in random and systematic but separates the types of errors in Type A (that can be evaluated statistically, e.g. the noise) and Type B (that are evaluated in all the other ways, e.g. scientifically based on natural variability of ancillary input quantities). In the case of AIRWAVE SLSTR TCWV retrieval, we need to evaluate these two types of errors.

According to equation 10 in [RD.7], the combined standard uncertainties for uncorrelated inputs are given by:

$$u_c^2(y) = \sum_{i=1}^{N} \left(\frac{\delta f}{\delta x_i}\right)^2 u^2(x_i) \qquad \text{Eq.4}$$

where the retrieved quantity y is given by $y = f(x_1 \dots x_N)$ and $u(x_i)$ is the standard uncertainty of the mean value of x_i. $\frac{\delta f}{\delta x_i}$ are the sensitivity coefficients and can also be calculated numerically.

Other quantities involved in the errors representations are:

1) the expanded uncertainties defined as:

$$U = k u_c(y) \qquad \text{Eq. 5}$$

where k is the coverage factor and it gives $Y = y \pm U$. Generally, k ranges between 2 and 3 (95% and 99% confidence level) depending on the degrees of freedom.

2) The degrees of freedom defined as:

$$v_{eff} = \frac{u_c^4}{\sum_{i=1}^{N} \frac{u^4(x_i)}{v_i}} \qquad \text{Eq.6}$$

where $v_i$are the degree of freedom for the single quantity x_i. Once we calculate v_{eff}, from table G.2 of [RD.18] we can obtain the value of *k* used to calculate *Y* via Eq. 5.

In the case of AIRWAVE SLSTR TCWV retrieval, the Type A errors are originated by the noise values on the BTs in the 11 and 12 µm channels in Nadir and Oblique views and by the radiometric uncertainties, and the Type B errors are originated by the errors on other assumptions, e.g. the emissivity variability, CO_2 and HNO_3 variability (1σ), the errors on the atmospheric temperature profile (about 1.5 K), on the surface temperature and on the SRF.

Regarding the Type A errors, we can evaluate the sensitivity coefficients of Eq.4 using the solving equation Eq.3 as:

$$\frac{\delta TCWV}{\delta BT_{1N}} = \frac{\delta TCWV}{\delta L_{1N}} \frac{\delta L_{1N}}{\delta BT_{1N}} = \frac{\alpha}{\Delta\sigma_{NAD}} \frac{\delta}{\delta L_{1N}} ln \frac{L_{1N}^{\lambda 1}}{L_{2N}^{\lambda 2}} \frac{\delta L_{1N}}{\delta L_{1N}} =$$
$$= \frac{\alpha}{\Delta\sigma_{NAD}} \frac{\delta}{\delta L_{1N}} \left(ln\left(L_{1N}^{\lambda 1}\right) - ln\left(L_{2N}^{\lambda 2}\right)\right) \frac{\delta L_{1N}}{\delta BT_{1N}} =$$
$$= \frac{\alpha}{\Delta\sigma_{NAD}} \frac{1}{L_{1N}^{\lambda 1}} \lambda 1\, L_{1N}^{\lambda 1-1} \frac{\delta L_{1N}}{\delta BT_{1N}} =$$
$$= \frac{\alpha\,\lambda 1}{\Delta\sigma_{NAD}} \frac{1}{L_{1N}} \frac{\delta L_{1N}}{\delta BT_{1N}}$$

here

$$\frac{\delta L_{1N}}{\delta BT_{1N}} = \frac{2hc^2}{\lambda 1^{\ 5}} \frac{b}{\lambda 1 (e^b - 1)^2} e^b \frac{1}{BT_{1N}}$$

with $b = \frac{hc}{K\,\lambda 1\, BT_{1N}}$ Eq.7

and

$$\frac{\delta TCWV}{\delta BT_{2N}} = \frac{\delta TCWV}{\delta L_{2N}} \frac{\delta L_{2N}}{\delta BT_{2N}} = \frac{\alpha}{\Delta\sigma_{NAD}} \frac{\delta}{\delta L_{2N}} ln \frac{L_{2N}^{\lambda 2}}{L_{2N}^{\lambda 2}} \frac{\delta L_{2N}}{\delta BT_{2N}} =$$
$$= \frac{\alpha}{\Delta\sigma_{NAD}} \frac{\delta}{\delta L_{2N}} \left(ln\left(L_{1N}^{\lambda 1}\right) - ln\left(L_{2N}^{\lambda 2}\right)\right) \frac{\delta L_{2N}}{\delta BT_{2N}} =$$
$$= \frac{\alpha}{\Delta\sigma_{NAD}} \frac{-1}{L_{2N}^{\lambda 2}} \lambda 2\, L_{2N}^{\lambda 2-1} \frac{\delta L_{2N}}{\delta BT_{2N}} =$$

$$= \frac{-\alpha\,\lambda 2}{\Delta\sigma_{NAD}} \frac{1}{BT_{2N}} \frac{\delta L_{2N}}{\delta BT_{2N}}$$

here

$$\frac{\delta L_{2N}}{\delta BT_{2N}} = \frac{2hc^2}{\lambda 2^{\;5}} \frac{b}{\lambda 2 (e^b - 1)^2} e^b \frac{1}{BT_{2N}}$$

$$\text{with } b = \frac{hc}{K\,\lambda 2\,BT_{2N}} \qquad \text{Eq.8}$$

thus follow for the Oblique view

$$\frac{\delta TCWV}{\delta BT_{1O}} = \frac{\delta TCWV}{\delta L_{1O}} \frac{\delta L_{1O}}{\delta BT_{1O}} = \frac{\beta}{\Delta\sigma_{OBL}} \frac{\delta}{\delta L_{1O}} ln \frac{L_{1O}^{\lambda 1}}{L_{2O}^{\lambda 2}} \frac{\delta L_{1O}}{\delta BT_{1O}} =$$

$$= \frac{\beta}{\Delta\sigma_{OBL}} \frac{\delta}{\delta L_{1O}} \left(ln\,(L_{1O}^{\lambda 1}) \; - ln\,(L_{2O}^{\lambda 2}) \right) \frac{\delta L_{1O}}{\delta BT_{1O}} =$$

$$= \frac{\beta}{\Delta\sigma_{OBL}} \frac{1}{L_{1O}^{\lambda 1}} \lambda 1\, L_{1O}^{\lambda 1 - 1} \frac{\delta L_{1O}}{\delta BT_{1O}} =$$

$$= \frac{\beta\,\lambda 1}{\Delta\sigma_{OBL}} \frac{1}{L_{1O}} \frac{\delta L_{1O}}{\delta BT_{1O}}$$

here

$$\frac{\delta L_{1O}}{\delta BT_{1O}} = \frac{2hc^2}{\lambda 1^{\;5}} \frac{b}{\lambda 1 (e^b - 1)^2} e^b \frac{1}{BT_{1O}}$$

$$\text{with } b = \frac{hc}{K\,\lambda 1\,BT_{1O}} \qquad \text{Eq.9,}$$

$$\frac{\delta TCWV}{\delta BT_{2O}} = \frac{\delta TCWV}{\delta L_{2O}} \frac{\delta L_{2O}}{\delta BT_{2O}} = \frac{\beta}{\Delta\sigma_{OBL}} \frac{\delta}{\delta L_{2O}} ln \frac{L_{1O}^{\lambda 1}}{L_{2O}^{\lambda 2}} \frac{\delta L_{2O}}{\delta BT_{2O}} =$$

$$= \frac{\beta}{\Delta\sigma_{OBL}} \frac{\delta}{\delta L_{2O}} \left(ln\,(L_{1O}^{\lambda 1}) \; - ln\,(L_{2O}^{\lambda 2}) \right) \frac{\delta L_{2O}}{\delta BT_{2O}} =$$

$$= \frac{\beta}{\Delta\sigma_{OBL}} \frac{-1}{L_{2O}^{\lambda 1}} \lambda 2\, L_{2O}^{\lambda 2 - 1} \frac{\delta L_{2O}}{\delta BT_{2O}} =$$

$$= \frac{-\beta\,\lambda 2}{\Delta\sigma_{OBL}} \frac{1}{L_{2O}} \frac{\delta L_{2O}}{\delta BT_{2O}}$$

here

$$\frac{\delta L_{2O}}{\delta BT_{2O}} = \frac{2hc^2}{\lambda 2} \frac{b}{\lambda 2 (e^b - 1)^2} e^b \frac{1}{BT_{2O}}$$

$$\text{with } b = \frac{hc}{K\,\lambda 2\,BT_{2O}} \qquad \text{Eq.10}$$

In these equations, *L* is the radiance (in W/(m2.sr.m)), *BT* the brightness temperature (in K).

Then combining the values in equations Eq.7-10 we get for Type A errors:

$$u^2_{TypeA}(TCWV) = \sum_{i=1}^{4} \left(\frac{\delta TCWV}{\delta BT}_i\right)^2 (noise_i^2 + rad.unc\ _i^2)$$

Eq.11

with $i = 1N, 2N, 1O, 2O$

For Type B errors we have:

$$u^2_{TypeB}(TCWV) = \sum_{i=1}^{N} \left(\frac{\delta TCWV}{\delta x}_i\right)^2 \sigma_{xi}^2 \qquad \text{Eq.12}$$

here x_i are the different quantities that can affect TCWV retrievals and σ^2_{xi} are related errors/variability. N here is the number of different quantities that can affect the TCWV retrieval. In Eq.12 the evaluation of sensitivity coefficient is performed through the analysis of synthetic BTs simulated with a perturbed state of x_i.

$$TCWV(x_i + pert.) = \frac{\alpha}{\Delta\sigma_{NAD}}\left\{ln\frac{BT + pert^{\lambda1}_{1N}}{BT + pert^{\lambda2}_{2N}} - \chi - \varepsilon_N - \lambda2\,\tau CO2^N_2 + \lambda1\,\tau CO2^N_1 - \rho_{NAD}\right\} + \frac{\beta}{\Delta\sigma_{OBL}}\left\{ln\frac{BT+pert^{\lambda1}_{1O}}{BT+pert^{\lambda2}_{2O}} - \chi - \varepsilon_O - \lambda2\,\tau CO2^O_2 + \lambda1\,\tau CO2^O_1 - \rho_{OBL}\right\} \qquad \text{Eq.13}$$

where $BT + pert_i$ is the values of the BT obtained with perturbed xi state.

then

$$TCWV(x_i + pert.) - TCWV(x_i) = \frac{\alpha}{\Delta\sigma_{NAD}}\left\{ln\frac{BT + pert^{\lambda1}_{1N}}{BT + pert^{\lambda2}_{2N}} - ln\frac{BT^{\lambda1}_{1N}}{BT^{\lambda2}_{2N}}\right\} + \frac{\beta}{\Delta\sigma_{OBL}}\left\{ln\frac{BT + pert^{\lambda1}_{1O}}{BT + pert^{\lambda2}_{2O}} - ln\frac{BT^{\lambda1}_{1O}}{BT^{\lambda2}_{2O}}\right\}$$

$$= \frac{\alpha}{\Delta\sigma_{NAD}}\left\{\lambda1\,ln\frac{BT+pert_{1N}}{BT_{1N}} - \lambda2\,ln\frac{BT+pert^{\lambda2}_{2N}}{BT^{\lambda2}_{2N}}\right\} + \frac{\beta}{\Delta\sigma_{OBL}}\left\{\lambda1\,ln\frac{BT+pert_{1O}}{BT_{1O}} - \lambda2\,ln\frac{BT+pert_{2O}}{BT_{2O}}\right\}$$

Eq.14

Alternatively, since the retrieval code is really fast, the retrieval with perturbed BTs can be performed and the sensitivity functions can thus be evaluated numerically using directly the TCWV retrieval.

We have adopted the latter strategy for the calculation of Type B errors.

As already said, Type A errors are the measurement noise affecting the BTs in the 11 and 12 µm channels in Nadir and Oblique views and the radiometric uncertainties. Type B errors (both random and systematic) are given by the other assumptions e.g. emissivity variability, atmospheric variability and trends, error on atmospheric temperature profile on surface temperature or on SRF. We consider all these error sources as uncorrelated and provide the final TOTAL error. The description of the treatment of the errors due to noise and the extraction of the noise information from the SLSTR L1B files is given in the following section.

For the evaluation of Type B errors, an a-priori information of the variability of the assumptions made is required. For example, the variability of the atmospheric Temperature profile in one season can be of the order of 3K, while for the atmospheric gases we can use an evaluation of their atmospheric variability (e.g. from IG2).

The two errors components in Eq.11 and Eq.12, are evaluated separately and can be reported separately or summed up. While the Type A errors(Eq.11) differs for each pixel, since the they are given per pixel the Type B errors, that are introduced in the TCWV computation through the retrieval parameters evaluation, follow the coefficients behaviour and their interpolation rules. Regarding the degrees of freedom, since we retrieve only one value per pixel we should consider to have 1 degree of freedom. Therefore, the expanded uncertainties should coincide with the standard uncertainty.

4.3.3.1 Type A errors computation strategy

Type A errors are extracted using a tool provided by RAL, described in [RD.19, RD.20]. The tool is written in python and is named “mapnoiS3.ph”. It extracts per-pixel noise NEΔT and NEΔL, and radiometric uncertainty information from the SLSTR Level-1 products. The inputs of the tool are the Level 1B data files and some Auxiliary data (ADF). The outputs are reported in a netcdf file.

In particular, for our purposes, the tool requires for both S8 and S9 channels and for both nadir and oblique views, the following inputs:

1) the BTs
2) the quality flags (containing estimates of detector noise measured from the blackbody signals, and the LUT of radiometric calibration uncertainty estimates)
3) indices of scan, pixel and detector in original instrument coordinates
4) SLSTR Level-1 TIR ADF used in the L1 processing, containing temperature-to-radiance LUT (blackbody emissivity and non-linearity LUT).
5) SLSTR Level-2 ADF (LUT of detector noise as a function of scene temperature and detector temperature).

In order to compute the radiometric uncertainties, the tool uses the Level-1 quality products, which contain a LUT with uncertainty estimates in the radiometric calibration as a function of the scene temperature.
For the computation of the NEΔT values, SLSTR L2 TIR Noise Data file are used. They contain LUTs of NEΔT vs Temperature for each detector and as a function of detector temperature. These tables act as a reference model that allow us to scale the NEΔTs measured at the two internal BBs to the full range of scene temperatures.

The algorithm uses the input files described above and computes two Level-1 images, one image containing the radiometric calibration uncertainties (systematic effects) and a second image containing the radiometric noise (random) at the pixel level. For a full description of the tool we recommend [RD.20].

The AIRWAVE-SLSTR code, first check on the existence and the size of the output of the mapnoiS3.ph tool. If the output generation fails, the back-up solution, using default values (mean values inside a random chunk), is adopted and, in the L2 output file, the global attribute '*unc_availability*' is set to specifically track this occurrence.

The following table reports the used default values (units [K]):

	S8 Nadir	S8 Oblique	S9 Nadir	S9 Oblique
NEΔT	0.013	0.013	0.020	0.020
Radiometric Uncertainties	0.034	0.033	0.033	0.032

Table 3*: Default NEDT values.*

In the AIRWAVE-SLSTR Type A solving formula, the two components are summed at pixel level as reported in Eq.11.

4.3.2.2 Type B errors computation

Type B errors used in this study are mainly the same identified for AIRWAVEv2 and reported in [RD.2]. Among them we can list errors due to variability of atmospheric scenario (Temperature profiles and interfering species) and of surface conditions (emissivity variations due to wind and salinity).

The calculation of Type B errors has been performed for the following error sources: 1) Wind effect over emissivity; 2) Salinity effect over emissivity; 3) Variability of Temperature profiles (3K); 4) Variability of CO_2 profiles, 5) Trend per year of CO_2; 6) Variability of F11 profiles, 7) Trend per year of F11; 8) Variability of F12 profiles, 9) Trend per year of F12; 10) HNO_3 variability, 11) Type A errors on the SRF, 12) Type B errors on the SRF.

Wind effects: The mean winds on the global scale are reported in Figure 1. As can be seen the maximum value over ocean is at about 10 m/s. For this reason we used the emissivity tabulated for 10 m/s to calculate the maximum error due to wind effect on emissivity. The retrieval parameters are calculated using the emissivity tabulated for 3 m/s.

Salinity: Regarding the salinity effect we have computed the error due to a 3 PSU deviation from the average sea salinity. Annual salinity variations are negligible (below 0.7 PSU) and thus no seasonal salinity effect has been considered.

Atmospheric variability and SST Temperatures: The maximum atmospheric Temperature variability is considered to be 3K globally and the SST is perturbed accordingly while all the 1 sigma atmospheric variabilities are extracted from the MIPAS IG2 database. To model the effects of the annual trends we have used the data observed from Mauna Loa (+2 ppm/year for CO_2, -2.2 ppt/year for CFC-11 and -2.8 ppt/year for CFC-12 [RD.20]).

SRF uncertainties: The SRF Type A and Type B errors are reported into [RD.21] by RAL.

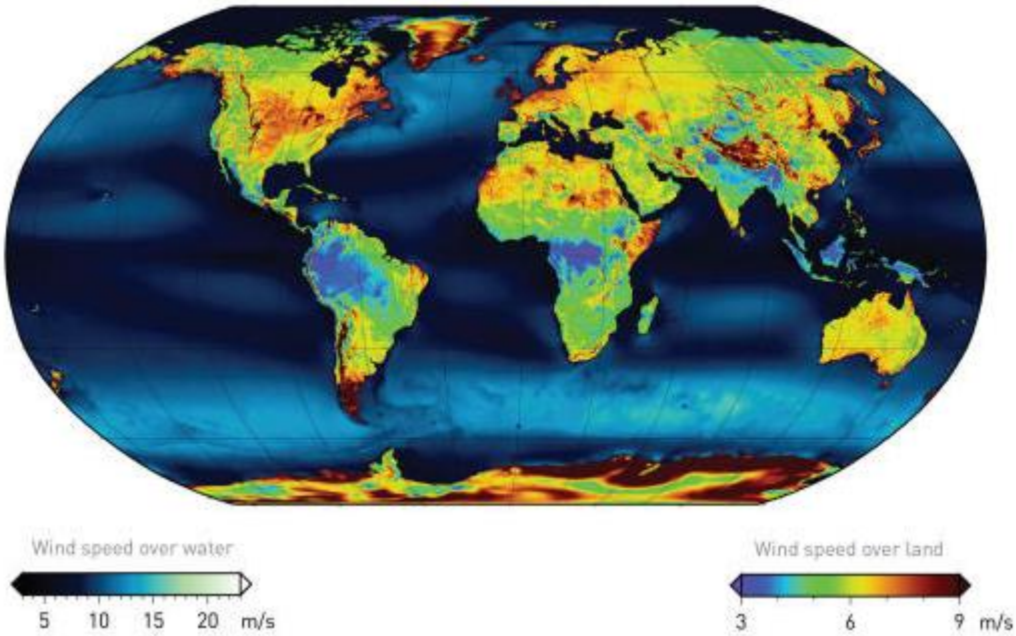


***Figure 1**: Global wind atlas (from http://www.energybc.ca/wind.html).*

As said, Type B errors are calculated by perturbing the desired quantity, simulating the BTs and performing the retrieval. Results are compared with the retrievals in the unperturbed case. Calculations are performed off-line using the same coefficients used into the retrieval code. As done for the retrieval coefficients, we used six latitude bands, four seasons but, due to computing time, we performed our calculations only for 3 across track positions (in the centre and at the two edges of the swath). This produces more than 1000 simulations.

An example of the results of Type B errors for each latitude band is reported in Figure 2 for a January on the along track position, the total error, calculated as the quadratic sum of all the Type B components is given in black. As can be noticed, the errors due to a 3K error on atmospheric temperature are more relevant in the tropics due to the atmospheric opacity, while errors due to surface effects on emissivity are higher in the polar regions, where the atmosphere is more transparent.

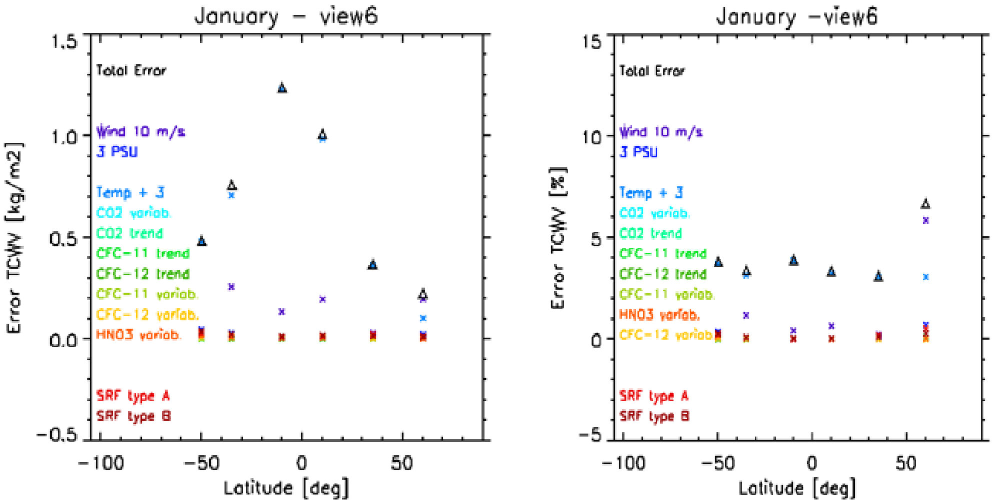


***Figure 2**: Type B errors in absolute (left) and percentage (right) values for January in the along track position. See text for details.*

Results for each error source are interpolated on 180 Latitudes, 12 months and 11 Tie points and stored into an IDL structure. This structure is, then, read by the retrieval code. The off-line interpolation on this finer grid speeds up the computing time during the retrieval.

The structure contains both the total error and the single error components and can be updated adding other error sources if needed. We recall here that the retrieval is independent from the errors, thus they can be calculated separately (e.g. if a new source of error needs to be included the errors evaluation can be modified without changing the TCWV results).

Total errors plus the ten single error components are stored into a structure named “SLSTR_ERR.sav”. The errors are stored into an array with dimensions [11, 181, 12, 13], that are the number of angles, the latitudes, months and error type.

4.3 Algorithm Inputs

4.3.1 Primary Sensor Data

The primary input data for the SLSTR-AIRWAVE algorithm is SLSTR Level-1B data from which the SLSTR radiances are derived. The SLSTR TCWV production package includes a function which computes the spectral radiance from the reported brightness temperature. In particular, the following input files are ingested:

- the latitude/longitude of the detector FOV centre on the Earth's surface (nadir and oblique views): geodetic_in.nc, geodetic_io.nc
- the gridded pixel brightness temperature for 11 and 12 μm channels, named S8 and S9 (1km TIR grid, nadir and oblique views): S8_BT_in.nc, S8_BT_io.nc, S9_BT_in.nc, S9_BT_io.nc

- the quality indicators on brightness temperature for 11 and 12 µm channels (i.e. black body noise equivalent brightness temperature, nadir and oblique views): S8_quality_in.nc, S8_quality_io.nc, S9_quality_in.nc, S9_quality_io.nc
- the flag masks (nadir and oblique views), including the cloud mask: flags_in.nc, flags_io.nc

4.3.2 Ancillary Data

There are some ancillary data (namely, the static data) that are required for theSLSTR TCWV production. As reported in equation (16) of Castelli et. al, 2019 [RD.2], the AIRWAVEv2 solution formula requires pre-computed parameters, for both the 11 and 12 µm channels and for both for nadir and oblique views:

- the coefficients Δσ, Δρ, and G
- the CO_2 optical depths
- the water surface emissivities

The code requires also λ1 and λ2, the central frequency values respectively in the 11 and 12 µm channels.

In AIRWAVEv2, the retrieval parameters are estimated not only according to the instrument type but also accounting for possible latitudinal and seasonal variations. This means that several RTM runs have been performed in order to compute all the required quantities in the defined scenarios.

The defined scenarios foresee six latitude bands (polar, mid-latitude, equatorial for both North and South hemispheres), four seasons and eleven tie points (every 90 across-track positions, for more details, see Table 4). The different latitude bands and seasons are characterized by different inputs to the RTM.

A-track position	0	90	180	270	360	450	540	630	720	810	900
NADIR [deg]	32.56	26.79	20.81	14.72	9.11	6.16	9.16	14.78	20.89	26.86	31.89
OBLIQUE [deg]	55	55	55	55	55	55	55	55	55	55	55

Table 4*: value of the satellite zenith angle in function of the across-track position (nadir and oblique views).*

As can be seen from Table 4, with respect to ATRS where Nadir and Forward view were present, for SLSTR we have Nadir and Oblique view. The oblique view is acquired looking backward. We investigated if this choice can have an impact on our simulations and then on the calculation of the retrieval coefficients. Since thermal radiation is isotropic, the only thing that can have a directional effect is the Solar radiation. In this spectral region the solar contribution is extremely low. However, we tested the impact on the measured BT the presence of the solar radiation simulating day/night radiances with the DISORT solver and a solar radiance spectrum. As expected, the difference on the simulated radiances reaches a maximum value of 0.08nW/(cm^{-1}.m^2.sr) over the measured 9800 nW/(cm^{-1}.m^2.sr)(0.0004 K or 0.0008%) on the S8 Oblique channel. The maximum variation for the different SZA is 0.0002 K on the S8 Oblique View. Since the S8 noise is about 0.015 K, about 40 times higher than these values, we can assess that the difference on the radiances due to measuring backward or forward in both day/night scenarios is negligible.

As stated above, the RTM needs atmospheric and surface profiles to produce the coefficients used for TCWV AIRWAVE retrieval. For ATSR we used the IG2 [RD.22] climatology for atmospheric profiles and ECMWF values for SSTs. The IG2 dataset was developed for MIPAS and thus was suitable to represent the average atmospheric state during the (A)ATSR missions. For SLSTR we decide to use the same IG2 dataset for retrieval parameters calculations.

However, in order to evaluate if improvements are possible, we produce a second set of retrieval coefficients changing the atmospheric dataset. We use pressure, temperature, ozone, water vapour and sea surface temperature from the ECMWF ERA-Interim monthly means of daily means at 3x3 deg grid products. The values are averaged within the considered latitude band and within the time interval related to the season and using the available full years 2015, 2016, 2017 and 2018. The ECMWF products are used from the surface up to 42 km, above the profiles are set to climatological IG2 data [RD.22]. The climatological products are also used for the other species present in the considered spectral intervals. However, the IG2 profiles are available only within the time range 2002-2012, therefore, for the species having significant trends (CO_2, CFC-11, CFC-12), the profiles are extrapolated to the year 2018. The errors caused by trends in the interfering atmospheric constituents, considered for the whole (A)ATSR1/2 mission (about 20 years), are of minor entity. More details can be found in the appendix of [RD.2].

This second set of retrieval parameters will be evaluated also in the light of the results of the validation.

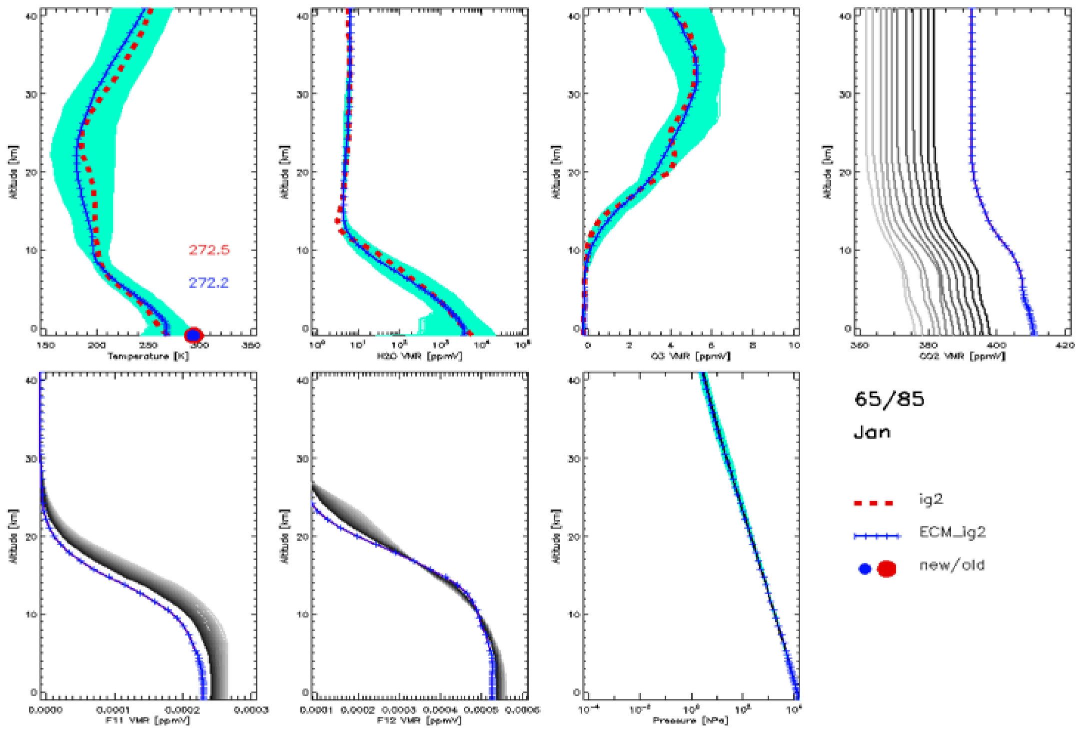


Figure 3: *Temperature, H_2O, O_3, CO_2, CFCs, and pressure as a function of altitude for January in the 65-85N latitude band. Red profiles from IG2, blue from ECMWF. See text for details.*

The surface emissivity is an essential input for AIRWAVE retrieval. For SLSTR, as well as for ATSR, it was taken from the University of Edinburgh database [RD.23]. This dataset contains emissivities tabulated as a function of wavenumber (600–3350 cm^{-1} or 3–16.7 µm), viewing angle (0 – 85 deg), temperature (270 – 310 K), and wind speed (0 – 25 m s^{-1} at 12.5 µm) for sea water (35 PSU). The nadir and oblique viewing angles of the instruments have been defined at 11 tie points of the SLSTR swath (pixels associated with specific points equally spaced across a single image or instrument scan). For each tie point, we then used the corresponding viewing angles to extract the correct emissivity values, with fixed wind speed (3 m s^{-1}). The errors associated possibly to wind speed variations with respect to the reference case are described in detail in the appendix of [RD.2].

The choice of this dataset for SLSTR retrieval was performed after a scientific review of the available emissivity dataset. The review also focused on emissivity datasets also for fresh water in addition to sea water. The JCSDA Infrared Sea Surface Emissivity Model is instrument oriented, and it is not clear if it has an angular dependence, but it considers fixed salinity. The RTTOV V12 emissivity model accounts for salinity. However, the salinity dependence it is not used in the IR. For ocean, previous IREM model (v11) parameterizes the emissivity from satellite viewing angle, while the new IREMIS model uses the zenith angle, 10 m wind speed, and skin temperature for emissivity parameterization. No salinity dependence is considered. The University of Edinburgh has also a version of the emissivity dataset with the same characteristic for pure water. For this reason it is the most suitable dataset for our purposes. A mixed salinity, if needed, can be obtained from the interpolation of the two datasets. In order to understand if such an interpolation is needed we analyse ocean salinity climatology and seasonality [RD.24].

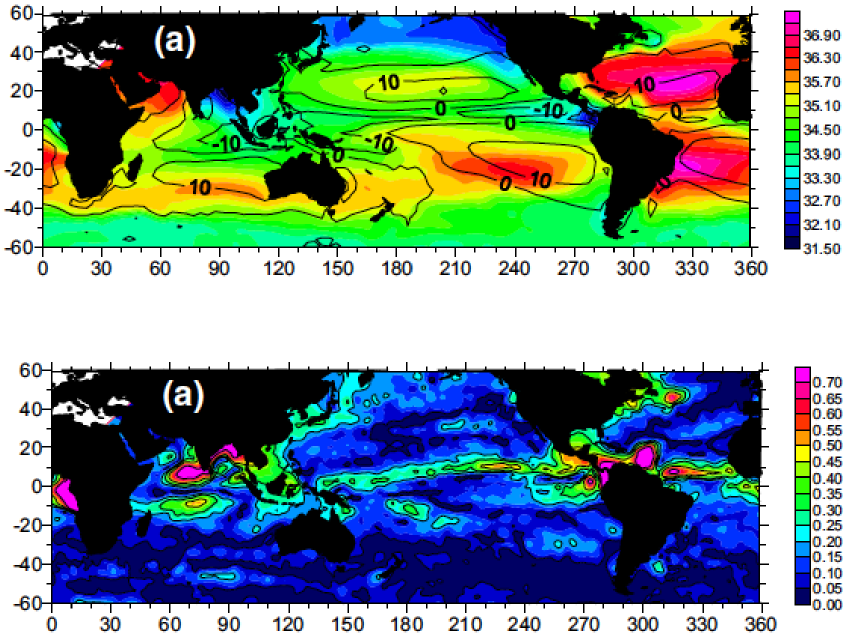


Figure 4: *SSS climatology (top) and seasonality (bottom) 2004-2014 from "Chen et al., 2018, Climatology and seasonality of upper ocean salinity: a three dimensional view from argo floats."*

As can be noticed from Fig.4, globally ocean SSS varies from 31.5 to 37 PSU, Annual variations are really small and a value of 35 PSU is representative of average ocean conditions (STD about 3 PSU). Regarding lakes, not only fresh water but also Mixed and Saline Lakes are present. Lakes are generally located at Mid-latitude and there are large salinity variations from lakes from 0 to 400 PSU (with some seasonality). Due to these variations the effect of salinity on emissivity has been evaluated against the effects of SST and wind for ATSR-type instruments. As can be seen from Fig.5, the major impact is due to angular variations, then SST variations, salinity (minor) while wind has almost negligible effects. To fully quantify the effects on simulated BTs and retrieval we simulate AATSR BTs for 6 latitude bands in summer at 11 and 12 micron using emissivity for pure water with the RTM.

Then we calculate the differences between pure water and sea water BTs: we find out that the difference is positive in the 11 band and negative in the 12 micron band, that differences are lower, or of the order of the noise at Mid-latitude and in Tropical regions, higher in Polar regions where however few lakes are present. The impact of retrieving TCWV from simulated BTs with sea and pure water emissivities and performing the retrieval using sea emissivity has practically no effect in Tropics, (globally 0.02 kg/m^2 bias) small effect of the order of the wind effect estimated for AIRWAVEv2 in worst cases.

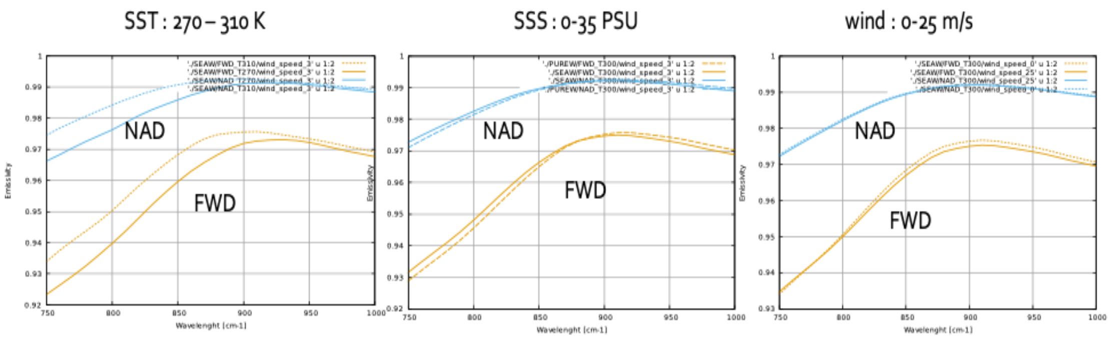


***Figure 5**: impact of SSTs (left), salinity (centre) and wind (right variations) on emissivity for Nadir and Oblique view as a function of wavenumber.*

To validate our choice, we analyse the results of the AIRWAVEv2 validation using the ARSA database and considering only lakes. In this way we can evaluate if the sea emissivity coefficients produce a bias on freshwater and extremely saline lakes. The outcome of the validation shows that for freshwater lakes no significant bias (STD larger than bias) is found and possibly there are some LSWT effects in some lakes. For saline lakes a small bias is found: AIRWAVEv2 tends to slightly overestimate the ARSA TCWV values, however only few lakes are saline and they are a very small part of the lakes and ocean global dataset, as can be seen from Fig. 6. Furthermore, salinity varies a lot among them and varies in time.

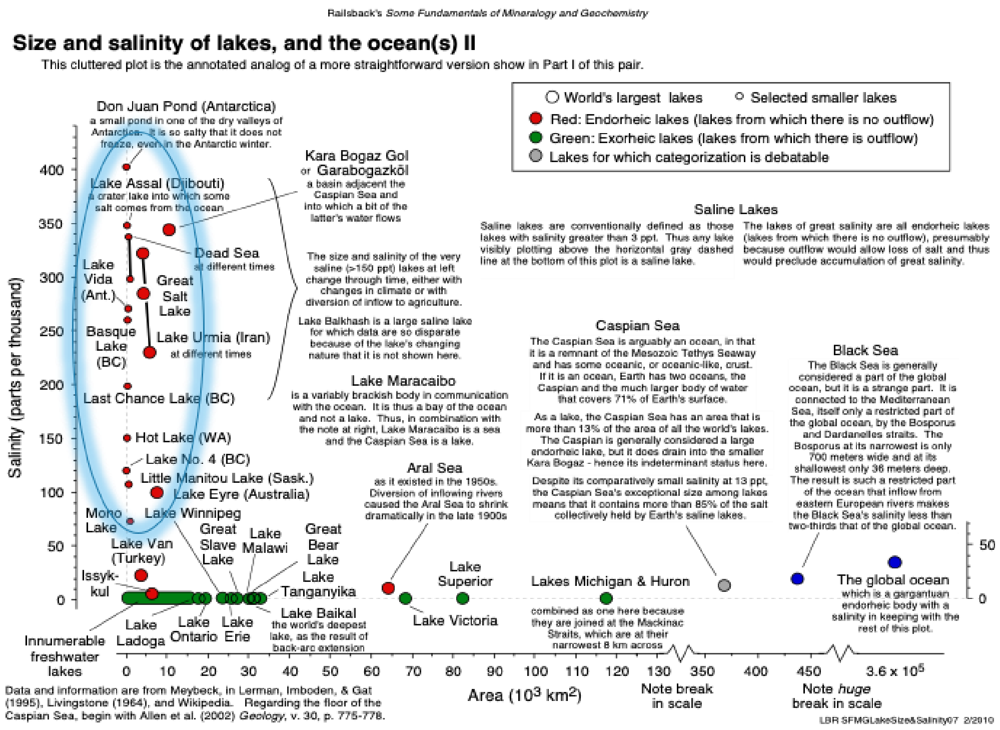


***Figure 6**: Size and salinity of lakes as a function of dimensions.*

Following these considerations, as stated above, we adopt the same strategy used for ATSR for Emissivity dataset selection: Emissivity is extracted from Edinburgh database for sea water at 35 PSU, accounting for angular variations and seasons (SST). Salinity and wind effects, that are minor, are kept as constant and error contribution is evaluated. The same emissivity at 35 PSU is used also for inland waters since the impact of using seawater emissivity retrieval parameters on fresh inland water is minor (from simulations and validation of AATSR). The impact is possibly higher on salty lakes. However, since these are only few and small lakes and with different and not constant salinity, these can be considered as particular cases (that cannot be handled in the generic retrieval approach).

4.3.2.1 Calculation of retrieval parameters

Using the selected Ancillary data, we computed the SLSTR retrieval parameters using the RTM code already used in [RD.2] for (A)ATSR retrieval parameters calculations. We performed the RTM simulations for 11 viewing angles for Nadir view and 11 for Oblique view covering, at steps of 90 pixels, the range from 0 to 900 pixels in the across track direction. Each angle has a specific value which has been derived from the information contained in the Level 1b SLST files (Table 4).

The calculation of retrieval parameters is a time-consuming procedure. In particular, the simulation of the high spectral resolution spectra through the use of the RTM is the most time-demanding step. The computation of the retrieval coefficients, consisting of a set of 1584 parameters (6 coefficients × 6 latitude bands × 4 seasons × 11 tie points), is therefore performed off-line. The final step of the procedure involves the convolution of the simulated BTs with the corresponding SLSTR filter functions of the 11 and 12 µm channels.

The computed retrieval parameters are stored into an IDL structure called “udt_coeff_slstr.sav”, which is read by the AIRWAVE retrieval code.

4.4 Algorithm Output (Product Specification Document - D8 of SoW)

The L2 algorithm output is produced using netCDF4 format.

The output file (named ‘tcwv.nc’) is created inside a directory following the file naming convention of SLSTR products (https://earth.esa.int/documents/247904/1964331/Sentinel-3_PDGS_File_Naming_Convention)

MMM_SL_L_TTTTTT_yyyymmddThhmmss_YYYYMMDDTHHMMSS_YYYYMMDDTHHMMSS_[instance ID]_GGG_[class ID].SEN3

The table below shows only the “naming elements” of the L2 product name which are modified with respect to the original L1B product name:

NAMING ELEMENT	*SIZE IN CHAR.*	*DESCRIPTION*
L	1	**Processing level** Consists of 1 digit or 1 underscore "_" if processing level is not applicable. This field can indicate the instrument data product processing stage or the processing level of applicability for the auxiliary data. "**2**" for Level-2
TTTTTT	6	**Data Type ID** Consists of 6 characters, either uppercase letters or digits or underscores "_". first 3 characters "**TCW**" for Total Column Water Vapour (TCWV) derived with the AIRWAVE algorithm
YYYYMMDDTHHMMSS	15	**Creation Date** Consists of 15 characters, either uppercase letters or digits and is applicable both to the Instrument Data Products and the Auxiliary Data format: 8 char., all digits, for the date: "YYYYMMDD", year, month, day 1 uppercase T: "T" 6 char., all digits, for the time: "HHMMSS", hour, minutes, seconds

The AIRWAVE-SLSTR L2 output file reports the following variables:

Name	Long Name
tcwv.nc	SLSTR-AIRWAVE Level 2 WATER Product, Integrated Water Vapour Data Set
flg	SLSTR-AIRWAVE Level 2 masks
lat	Latitude of detector FOV centre on the earth surface
lon	Longitude of detector FOV centre on the earth surface
tcwv	Integrated water vapour column above the current pixel
tcwv_tpA	Type A error estimate for integrated water vapour column above the current pixel
tcwv_tpB	Type B error estimate for integrated water vapour column above the current pixel

The variables are stored as UBYTE (flg, tcwv_tpA, tcwv_tpB), as SHORT (tcwv) and LONG (lat, lon). If "*scale_factor*" and "*add_offset*" attributes are present and different from zero, the data should be multiplied by the "scale_factor" value and should be offset using the "add_offset" number.

To limit the amount of disk storage, the compression of the single variables (GZIP option) has been adopted.

The output file also contains a series of global attributes (most extracted from the manifest file) as additional information. Hereafter, an example is reported:

```
// global attributes:
:absolute_orbit = "4880";
:cycle = "13";
:collection = "003";
:contact = "------";
:creation_time = "2019-10-24T12:38:21Z";
:duration = "179";
:ground_direction = "descending";
:netCDF_version = "4";
:platform = "Sentinel-3A";
:product_name = "S3A_SL_2_TCW____20170124T000144_20170124T000444_20191024T123821_0179_013_287______LR1_R_NT_003.SEN3";
:product_L1BT = "S3A_SL_1_RBT____20170124T000144_20170124T000444_20181004T071422_0179_013_287______LR1_R_NT_003.SEN3";
:relative_orbit = "287";
:relative_pass = "574";
:references = "------";
:start_time = "2017-01-24T00:01:43.837391Z";
:stop_time = "2017-01-24T00:04:43.837391Z";
:title = "SLSTR-AIRWAVE Level 2 WATER Product, Integrated Water Vapour Data Set";
```

4.5 Performance Estimates

4.5.1 Test Data Description

Considering that EUMETSAT does not provide problematic Level 1 data, we decided to use the validation dataset as a test dataset. During the processing of the validation dataset, we will report to the agency every unexpected stop, fault or anomaly.

According to EUMETSAT, the validation dataset will contain SLSTR Sentinel - 3A Level 1 data of January, April, July and October 2018. Besides, in order to exploit the tandem phase, it will include also the Sentinel - 3B Level 1 data of July 2018.

4.5.2 Sensor Effects

We account for the sensor effects in the following points during the retrieval:

1) the retrieval parameters are calculated by convolving the simulated spectra with the SRF (different SRF for SLSTR A and B);

2) the retrieval parameters are calculated for eleven couples of viewing angle to map the whole range of the across track swath (same angles for SLSTR A and B);

3) the emissivities accounts for channels positions and viewing angles;

4) the frequencies used into Eq. 3 are the ones for SLSTR A and B;

Despite the fact we account for sensor effects some unknown sensor effects may be possible.

4.5.3 Retrieval Errors

Retrieval errors have been described in Section 4.3.3. An example of retrieval errors for the 2nd July 2018 is given in figures 7 and 8. In Fig. 7 we report the values of Type A and Type B components separately and in absolute values, while in Fig.8 we show the total error in percentage values. As can be noticed from the right panel of the figure the values reach more than 30% in polar regions while it is of the order of 8-15 % in tropical regions.

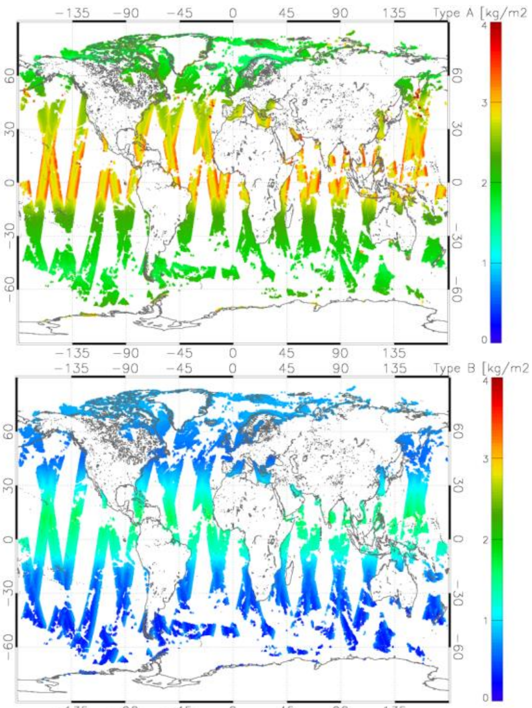


Figure 7: *Example of Type A (left) and Type B (right) errors for 2nd July 2018.*

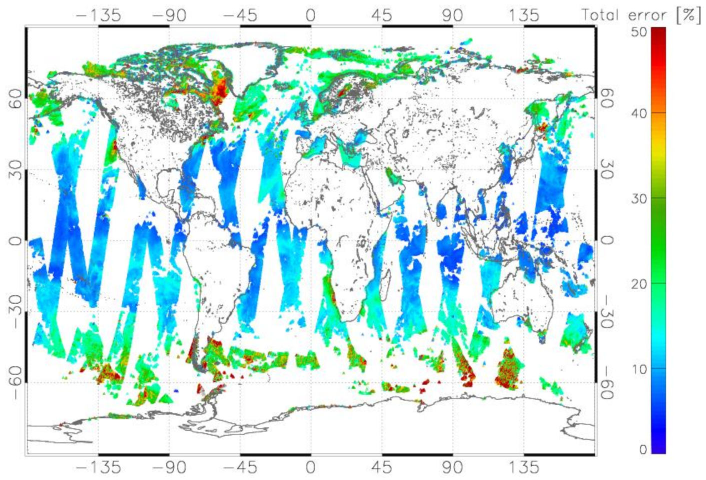
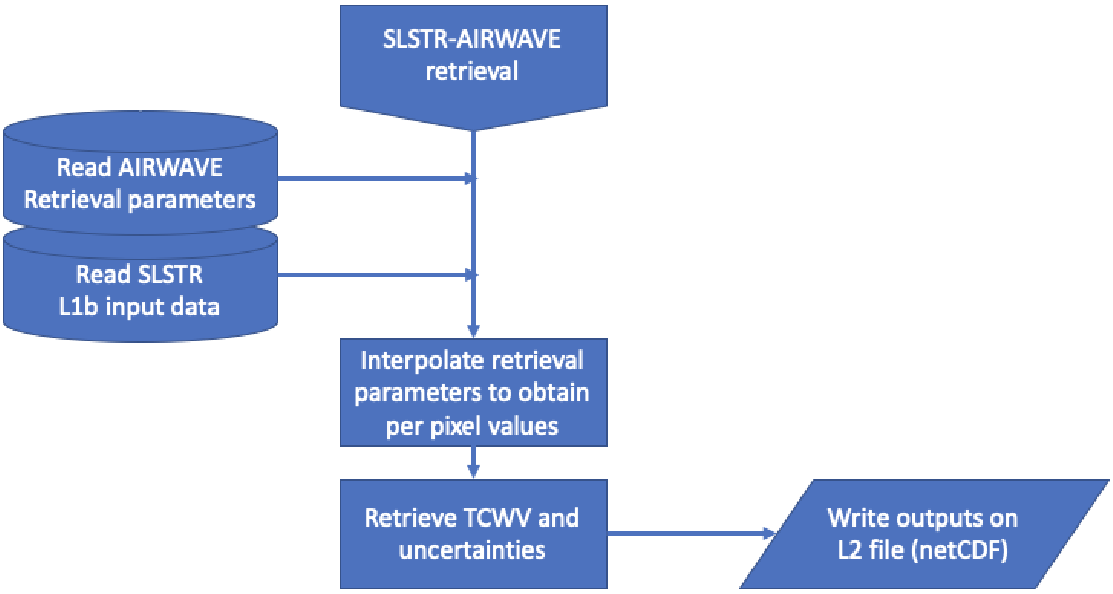


Figure 8: *Example of TOTAL percentage errors for 2nd July 2018.*

4.6 Practical Considerations

4.6.1 High-Level Description of the Prototyped Software

The AIRWAVE-SLSTR data processing is illustrated by the following flowchart:



The overall procedure can be divided mainly in the following blocks:

• *Extract and ingest input parameters and auxiliary information*

The code reads:

- the configuration file containing all the information required to run the code (e.g. input and output paths, ...)
- all the required input data from L1 SLSTR netCDF input files (NADIR/OBLIQUE views)
- Latitude / longitude coordinate.
- The gridded pixel brightness temperature for 11 and 12 µm channels.
- Flags: land, cloud (standard or Bayesian).
- retrieval parameters lookup tables (pre-computed).
- noise equivalent brightness temperature at the scene radiance on the Level-1 image per pixel for 11 and 12 µm channels. It is derived using the "Sentinel-3 SLSTR Uncertainties in Level-1 Products Algorithm python tool" developed by RAL, in order to compute type A errors.
- type B error estimation lookup tables (to save time, already interpolated on a fine grid).
- auxiliary information contained in the "manifest" xml file (e.g. L1 product name, start/stop time, nadir/oblique track offsets, ...).
-

• *Perform basic Quality Check of SLSTR Level 1B calibrated top-of-the- atmosphere brightness temperature.*

All the pixels having positive BT and that are not over land are processed. The code interpolate the retrieval parameters and compute the TCWV and TCWV Type A error.

• *Run the AIRWAVE Block.*

• *Write the L2 output data in the defined file format.*

netCDF-4 file format is used to store L2 output, containing:

- TCWV
- TCWV Type A error
- TCWV Type B error
- Level 2 masks
- Latitude/longitude

To limit the amount of disk storage, we foresee both the compression of the single variables (GZIP option) and, when possible, their conversion to data types which requires less storage on disk.

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