

Comparison of the AMTROC 1D-VAR wet tropospheric correction (WTC) against Sentinel-3 standard WTC products. See section 5.6 in the AMTROC Validation Report for further details.

Source: AMTROC Validation Report.




*EUMETSAT contract
EUM/CO/19/4600002223/EO*

*Altimeter 1D-VAR
Tropospheric Correction
(AMTROC)*

**Algorithm
theoretical basis
document
for
AMTROC products**

(Deliverable D-7)

Berlin, 31. March 2020

Altimeter 1D-VAR Tropospheric Correction			
Algorithm Theoretical Basis Document			




Document control sheet	
Project	Altimeter 1D-VAR Tropospheric Correction (AMTROC)
Client	EUMETSAT Eumetsat-Allee 1 64295 Darmstadt, Germany http://www.eumetsat.int 
Main contractor	Informus GmbH Brehmestr. 50 13187 Berlin, Germany http://www.informus.de 
Other project partners	Fluctus SAS 54, Promenade des Lices 81800 Rabastens, France http://satobsfluctus.eu/ 
Title	Algorithm theoretical basis document for AMTROC products
Status	Released
Authors	Ralf Bennartz (VU), Frank Fell (INF), Bruno Picard (FLU)
Distribution	AMTROC consortium, EUMETSAT
Version control	2019-11-26 V0.9, final draft 2020-03-30 V1.0, initial version 2020-03-31 V1.1, added Ku-band attenuation

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1 Introduction

1.1 Context

The EUMETSAT-funded activity “*Altimeter 1D-VAR Tropospheric Correction*” (AMTROC) aims at implementing a robust operational method to correct sea surface height (SSH) retrievals from Sentinel-3 altimeter observations for the effects of atmospheric moisture, a process often termed as “*Wet Tropospheric Correction*” (WTC).

To this aim, each satellite of the Sentinel-3 series carries a dedicated instrument, the Microwave Radiometer (MWR), to determine total column water vapour (TCWV) and liquid water path (LWP), concomitantly to the altimeter observations, both day and night under cloudy and clear sky conditions. These observations are then further processed to provide precise information on the WTC for the area observed by the altimeter.

1.2 Purpose of the document

This Algorithm Technical Basis Document (ATBD) describes the theoretical basis of Total Column Water Vapour (TCWV), Cloud Liquid Water Path (LWP), and Wet Tropospheric Correction (WTC) retrieval from observations of the Microwave Radiometer (MWR) instruments flown on-board the Sentinel-3 series of satellites. The method presented herein can in principle be applied to any downward looking microwave radiometer observing at frequencies of 23.8 and 36.5 GHz.




While the AMTROC retrieval presented herein builds on results obtained from an earlier ESA-funded study targeting the MWR time series from the ENVISAT, ERS-1, and ERS-2 platforms [*EMIR-ATBD*], it is based on a completely fresh implementation using updated radiative transfer models and retrieval packages, as well as other improvements.

The structure of this ATBD follows in principle the lay-out suggested in the “Generic Statement of Work for Level 2 Product Evolution/Development Studies” [*AD-AMTROC-GSOW*], with the exception that aspects related to “Performance estimates” and “Validation” are covered in the separate AMTROC Validation Report [*AD-AMTROC-VALREP*] to avoid redundancies and to keep the ATBD contents focused on the theoretical basis of the implemented retrieval scheme. Consequently, all results that are specific to the particular Sentinel-3A dataset investigated under AMTROC are discussed in [*AD-AMTROC-VALREP*].

1.3 Acronyms and abbreviations

Acronym	Description
1D-VAR	One-dimensional Variational Data Assimilation
AltiKa	Ka-Band Altimeter
AMSU	Advanced Microwave Sounding Unit
AMTROC	Altimeter 1D-VAR Tropospheric Correction
ATBD	Algorithm technical basis document
CDR	Climate data record
CM SAF	Satellite Application Facility on Climate Monitoring
CNES	Centre National d’Études Spatiales

Acronym	Description
DUE	Data User Element
ECMWF	European Centre for Medium-Range Weather Forecasts
EMiR	ERS/Envisat MWR Recalibration and Water Vapour FDR Generation
Envisat	Environmental Satellite
ERA-5	ECMWF Reanalysis 5th Generation
ERS	European Remote Sensing satellite
ESA	European Space Agency
EUMETSAT	European Organization for the Exploitation of Meteorological Satellites
FASTEM	Fast Microwave Emissivity Model
FDR	Fundamental data record
GEWEX	Global Energy and Water Cycle Experiment
GMES	Global Monitoring for Environment and Security
GSOw	Generic Statement of Work
GTOPO30	Global DEM with a grid spacing of 30 arc seconds by USGS
G-VAP	GEWEX Water Vapor Assessment
ISRO	Indian Space Research Organisation
JASON	Joint Altimetry Satellite Oceanography Network
L1	Level-1 processing
LWP	Liquid water path
MWR	Microwave Radiometer
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
NWP	Numerical weather prediction
RTM	Radiative transfer model
RTTOV	Radiative Transfer for TOVS
RMS	Rot mean square
S-3	Sentinel-3
SAF	Satellite Application Facility
SARAL	Satellite with Argos and AltiKa
SOW	Statement of Work
SRAL	SAR Radar Altimeter
SSH	Sea surface height
SSM/I	Special Sensor Microwave/Imager
SSMIS	Special Sensor Microwave Imager/Sounder
SST	Sea surface temperature
SWS	Surface wind speed
TOA	Top of atmosphere
TOPEX	Topography Experiment
TCWV	Total column water vapour
USGS	United States Geological Survey
WTC	Wet tropospheric correction
WVP	Water vapour path

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1.4 Applicable documents

[AD-S3-SRD] GMES Sentinel-3 System Requirements, Document S3-RS-ESA-SY-0010, Issue 4.0, 13. November 2009.

[AD-AMTROC-SSOW] EUMETSAT, 2018: Statement of Work for Altimeter 1-D VAR Tropospheric Correction, Document EUM/RSP/SOW/18/1001261, Issue v1, 18 June 2018.

[AD-AMTROC-GSOW] EUMETSAT, 2018: Generic Statement of Work for Level 2 Product Evolution/Development Studies, Document EUM/TSS/SOW/18/1018464, Issue v1A, 4. September 2018.

[AD-AMTROC-SUG] AMTROC Software User Guide, Version 1.0, April 2020.

[AD-AMTROC-VALREP] AMTROC Product Validation and Evolution Report, Version 1.0, 33 pp., 27. March 2020.

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2 Product overview

2.1 Product description

Table 1 lists the geophysical parameters derived from observations of the MWR instrument flown onboard the Sentinel-3 series of satellites in the frame of the AMTROC project, together with their main characteristics. A number of ancillary and quality assurance parameters are provided as well, see Table 6 for details.

Table 1: Geophysical parameters derived from observations of the MWR instrument flown onboard the Sentinel-3 series of satellites in the frame of the AMTROC project. Since MWR is a nadir-viewing instrument, a temporal resolution cannot be specified at Level-2.

AMTROC parameter	Spatial resolution	Temporal resolution	Remark
Total column water vapor (TCWV)	Ca. 20 km	n/a	Nadir viewing instrument
Liquid water path (LWP)	Ca. 20 km	n/a	See above
Wet tropospheric correction (WTC)	Ca. 20 km	n/a	See above

2.2 Product requirements

The GMES Sentinel-3 System Requirements [AD-S3-SRD] has defined the requirements for the Sentinel-3 altimeter observations over ocean as detailed in Table 2. The overall objective is a measurement of the altimeter range with an error below 3 cm as per requirement RA-PE-400 a. Considering the likely contribution from the other error sources, this requires the determination of the WTC with an accuracy of 1.4 cm.

Table 2: Altimeter range estimation error breakdown [AD-S3-SRD].

S3-A error budget, phase E1	
Noise source	Requirements
Instrument range noise / altimeter noise	1.3 cm
Ionosphere	0.7 cm
Sea state bias	2.0 cm
Dry troposphere	0.7 cm
Wet troposphere	1.4 cm
Altimeter range RSS	2.94 cm

The study-specific Statement of Work (SOW) to AMTROC [AD-AMTROC-SSOW] lists several further requirements with direct impact on the scientific approach to be chosen when deriving the target parameters. These requirements are listed in Table 3 below where it is also stated if and/or how these requirements are met and where further information can be found in the present document.

Table 3: Scientific requirements on the AMTROC geophysical parameters as stated in the Statement of Work. Here, R-n refers to requirements from the Generic SOW for Level 2 Product Evolution/Development Studies [AD-AMTROC-GSOW], while REQ-n designates requirements specified in the AMTROC-specific SOW [AD-AMTROC-SSOW].

REQ-ID	Shortened description from SOWs	Do we comply?	Section
REQ-1	Apply novel developments in WV 1D-VAR retrievals	Yes	4.1
REQ-2	Improvements: 1D-VAR retrieval, bias reduction, uncertainty, quality flag, ancillary data	Yes	4.1-4.4
REQ-3	Start retrievals with MWR Level-1B calibrated and geolocated brightness temperatures (MW_1_MWR)	Yes	4.2
R-7	Uncertainty issues shall be specifically addressed for each product.	Yes	4.3.2.3, 4.5
R-8	Uncertainty characterisation for each product shall follow the approach outlined by QA4E0.	Yes	4.3.2.2
R-9	New products shall be accompanied with per-pixel uncertainties.	Yes	4.5
R-11	Algorithms shall be suitable for integration into EUMETSAT's Offline environment.	Yes	4.7.3




2.3 Scientific state-of-the-art

Altimetry missions are key to progress in oceanography. The sun-synchronous, high inclination observations taken between 1991 and 2012 by the radar altimeters and microwave radiometers on-board the ERS-1, ERS-2, and Envisat satellites are at the core of any global altimetry Climate Data Record (CDR), complementing the mid-inclination, drifting TOPEX/Jason time series (see Table 4).

Table 4: List of current and past radar altimeter missions with Sentinel-3 MWR-like instruments. Sun-synchronous high inclination orbits are marked light orange. Drifting mid-inclination orbits are marked light blue.

Mission	Start	End	Orbit	Operator
Sentinel-3A	02-2016	operational	10:00 sun-sync., desc.	EUMETSAT/ESA
Sentinel-3B	04-2018	operational	10:00 sun-sync., desc.	EUMETSAT/ESA
ERS-1	07-1991(*)	06-1996(*)	10:00 sun-sync., desc.	ESA
ERS-2	04-1995(*)	07-2011(*)	10:30 sun-sync., desc.	ESA
ENVISAT	03-2002(*)	04-2012(*)	10:30 sun-sync., desc.	ESA
SARAL/AltiKa	06-2013	operational	6:00 sun-sync., ascend.	CNES/ISRO
TOPEX/Poseidon	08-1992	09-2005	66° inclination, drifting	NASA/CNES
Jason-1	12-2001	06-2013	66° inclination, drifting	NASA/CNES/ EUMETSAT/NOAA
Jason-2	07-2008	operational	66° inclination, drifting	NASA/CNES/ EUMETSAT/NOAA
Jason-3	02-2016	operational	66° inclination, drifting	NASA/CNES/ EUMETSAT/NOAA

(*): Refers to actual instrument lifetime

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After an observation gap of ca. four years, sun-synchronous observations are being continued since February 2016 through the SRAL / MWR pair of instruments flown on-board the Sentinel-3A (S3-A) satellite, which in April 2018 has been complemented by the identically equipped Sentinel-3B (S3-B). S3-A, S3-B, and the future S3-C will provide critical radar altimeter and MWR coverage at a 10:00 local time sun-synchronous high inclination orbit for the next ten or more years.

During the meanwhile 28+ years of combined radar altimeter and microwave radiometer observations, improvements in instrument data processing as well as orbit and geophysical corrections allowed reaching an accuracy/sensitivity of 1 cm on observations of the instantaneous sea surface height (SSH) and demonstrated the capability to observe a 3 mm/year sea level rise [Ablain et al., 2009].

A major source of uncertainty for radar altimetry is the wet tropospheric correction (WTC) accounting for the reduction of the speed of light in the atmosphere due to the highly variable presence of water vapour. To provide the observations required for the WTC is the primary role of the nadir looking Microwave Radiometer (MWR) embedded into the altimetry missions on board Sentinel-3. In this context, requirements on accuracy, sensitivity, and long term stability of the atmospheric water vapour observations are particularly strong since altimetry missions require a precision better than 1.4 cm in WTC (RMS) [see Table 2], and a temporal stability better than 0.3 mm/year [Ablain et al., 2009].

Note in this context that a (TCWV content of 1 kg/m² is equivalent to a WTC of about 6 mm.

TCWV is also highly important climate variable in its own right. The atmospheric water vapour feedback is believed to be the strongest feedback mechanism in climate change, approximately doubling the direct warming impact of increased CO₂ forcing [Cess et al., 1990; Forster et al., 2007]. Various groups have reported trends in the amount of columnar water vapour. In particular, over the oceans, a strong trend in TCWV has been observed [Trenberth et al., 2005]. TCWV also appears to be a key factor regulating tropical precipitation [Bretherton et al., 2004].

The importance of water vapour in the climate system is recognized by the Global Energy and Water Cycle Experiment (GEWEX), which is currently performing an assessment of long-term water vapour products, the GEWEX Water Vapour Assessment (G-VAP, see [Schroeder et al., 2019]).

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3 Satellite instrument description

3.1 Assessment of instrument benefit and capabilities with respect to the product

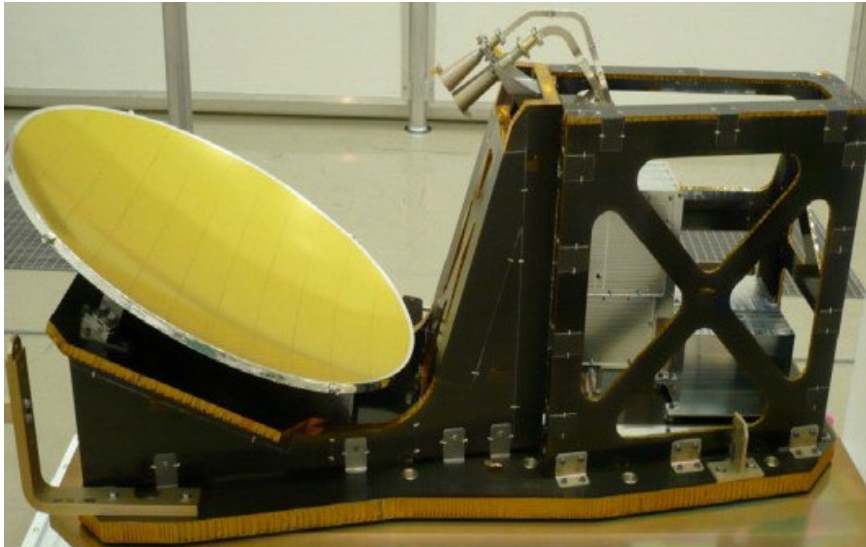


Figure 1: MWR instrument onboard Sentinel-3. Source:

<https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-3-altimetry/instrument/mwr>.

The MWR instrument on board the Sentinel-3 series of satellites is a dual-channel nadir-pointing Dicke-type radiometer operating at frequencies of 23.8 and 36.5 GHz¹ (see Figure 1), allowing for the simultaneous retrieval of TCWV and LWP as outlined in Section 4.

The main purpose of the MWR instrument is to provide the information required for tropospheric path correction of the radar altimeter signal, which is influenced both by the integrated atmospheric water vapour content and by cloud liquid water. As shown in [AD-AMTROC-VALREP], MWR retrievals of TCWV are of high accuracy and available day and night under most atmospheric conditions, except for heavy precipitation.

While MWR-based Level-2 products are primarily applied to providing support information to concomitantly acquired altimeter data, averaging over space and time provides Level-3 products of high interest for e.g. climatological purposes, most notably TCWV [Schroeder et al., 2019].

¹ <https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-3-altimetry/instrument/mwr>

4 Algorithm description

4.1 Processing outline

The AMTROC TCWV retrieval is based on a 1D-VAR scheme initially developed at ECMWF by *Phalippou [1996]* with a focus on microwave observations from SSMIS and AMSU. It was later extended by *Deblonde and English [2001]* towards a stand-alone scheme applicable to SSM/I, SSMIS, and AMSU. In the context of the ESA DUE GlobVapour project [*GlobVapour, 2012*], the TCWV retrieval scheme has been adapted to the CMSAF SSM/I Fundamental Data Record (FDR), and later on by *Bennartz et al. [2017]* to MWR observations in the context of the EMiR study.

Over the past years, significant progress has been made by the NWP SAF in upgrading both the 1D-VAR and the RTTOV software packages. The retrieval methodology used for the earlier EMiR study could not reasonably be transferred to AMTROC and required a full re-implementation using the latest versions of 1D-VAR and RTTOV. Within the AMTROC project, this scheme has been further improved to derive TCWV from brightness temperatures specifically from the MWR sensor family on-board the S-3 series of satellites over the ice-free ocean.

The best estimate of the atmospheric state, characterised through atmospheric temperature and moisture profiles as well as surface temperature and wind speed, is determined by an iterative procedure to match simulated satellite radiances with the corresponding measurements within their respective uncertainties. The scheme follows optimal estimation theory considering the uncertainties in the required meteorological background information, forward modelling (radiative transfer simulations), and satellite observations. This methodology enables the provision of retrieval uncertainties that are mathematically consistent with the uncertainties of the input brightness temperatures and background fields and consistent among the retrieved variables.

4.2 Algorithm input

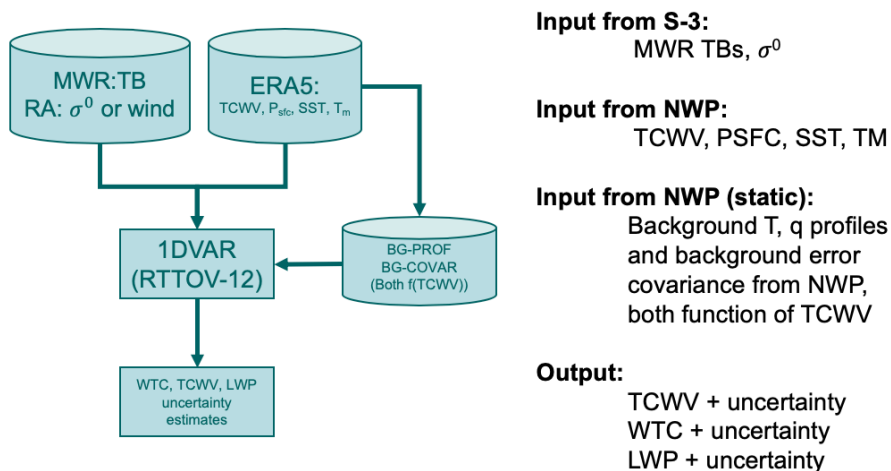


Figure 2: Flow chart of the AMTROC processor. The different input sources and the output are listed on the right. All profile and background error covariance information are obtained from static climatologies.

Main input to the AMTROC retrieval are calibrated and geolocated observations of the MWR brightness temperatures (TBs) at 23.8 GHz and 36.5 GHz as well as information on the surface roughness σ from concomitant radar altimeter observations.

The AMTROC scheme additionally requires collocated TCWV, sea surface temperature (SST), and surface wind speed fields as *a priori* (background) but, differing from the earlier EMIR retrieval, uses climatological fields for the first guess information and background vertical profiles. This change makes the algorithm faster and more flexible, eliminates the need for time-intensive collocation of three-dimensional temperature and water vapor profiles, and does not adversely impact the accuracy of the retrieval. Figure 2 shows a simplified sketch of the AMTROC processing flow. Detailed considerations on the various input data are provided further below in Section 4.3.

4.3 Theoretical description of TCWV and LWP retrieval

4.3.1 Physical description

Passive microwave imagers have a long history for the retrieval of total column water vapour by measuring radiation close to the 22.231 GHz water vapour absorption line. Figure 3 shows the atmospheric zenith transmittance in the microwave region for different humidity levels and absorbing/emitting species. In the left panel, the sensitivity of microwave measurements to the total columnar water vapour is apparent both in the line centres, such as the absorption line centred around 22.231 GHz, as well as in the continuum between the individual absorption/emission lines. The right panel shows the transmittance in the same spectral range, indicating the individual contributions to the transmittance by water vapour, oxygen, and cloud liquid water.

Clouds are semi-transparent throughout the microwave region and their transmittance does not exhibit line structures. It is possible to distinguish the signals due to water vapour and clouds by using channels at different water vapour optical depths, such as the Sentinel-3 MWR channels at 23.8 GHz and 36.5 GHz. Passive microwave measurements can therefore be used for the retrieval of water vapour under all-sky conditions except for heavily precipitating situations.

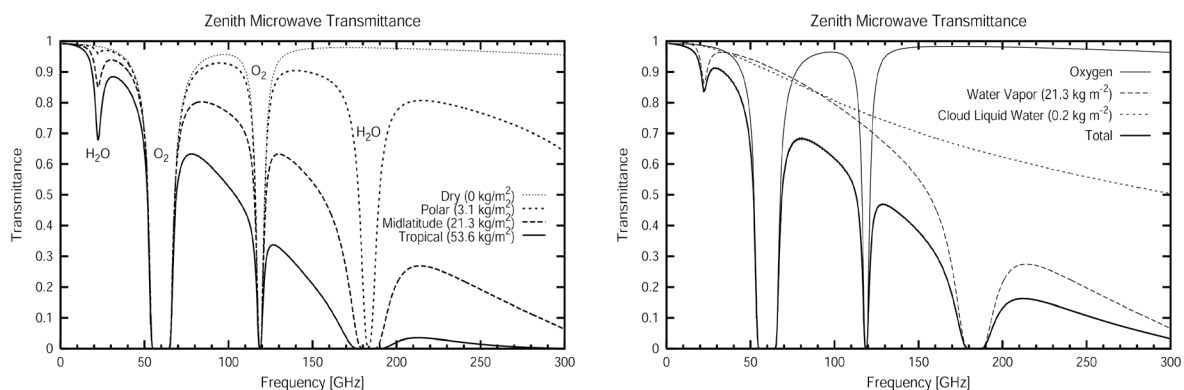


Figure 3: Zenith transmittance in the microwave spectral domain at different humidity levels (left) and for different absorbers / emitters (right) [Petty, 2006].

However, due to the high and highly variable emissivity of land surfaces, this technique can only be applied over the oceans. The microwave emissivity of the ocean surface is a function of temperature,

salinity and surface roughness, but is generally small, providing a good background for water vapour retrievals.

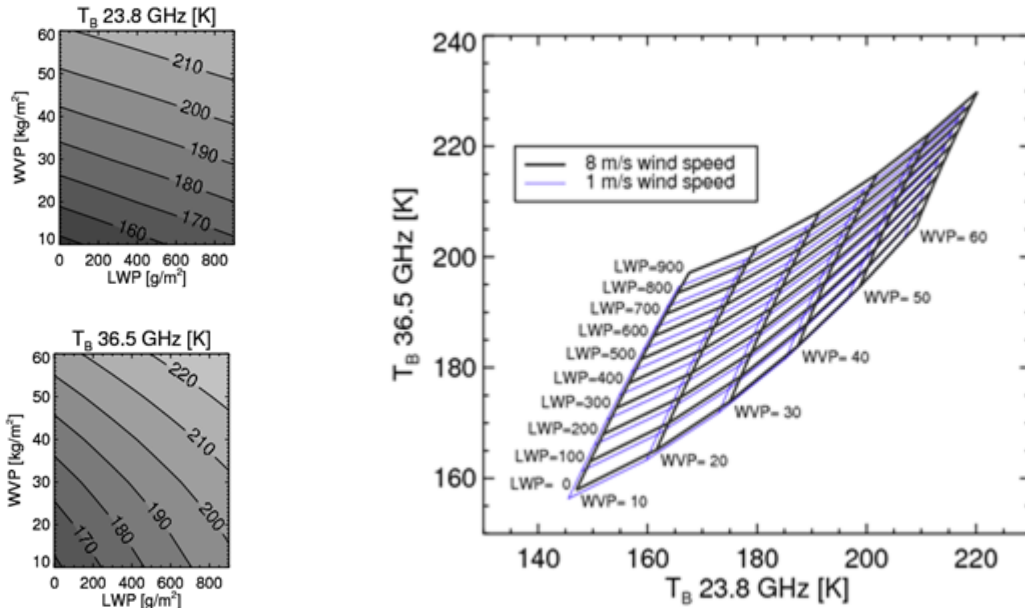


Figure 4: Relationship between MWR-observed brightness temperatures, LWP and WVP (=TCWV), assuming a surface wind speed of 8 m/s. The left two panels show brightness temperatures as function of LWP and WVP. The right panel shows the inverse problem, *i.e.* LWP and WVP as function of the two observed brightness temperatures. To illustrate the effect of surface wind speed, a second grid (blue) is overlain, calculated for a wind speed of 1 m/s.

Figure 4 shows contour lines of equal brightness temperature in both MWR channels as a function of liquid water path and TCWV, termed water vapour path (WVP) in the figure. In both channels, the measured brightness temperature is a function of water vapour as well as liquid water, but with differing sensitivities to the two parameters. This is reflected in the right plot, showing contour lines of equal amounts of TCWV and liquid water, with the x- and y-axis representing the brightness temperatures at 23.8 GHz and 36.5 GHz, respectively. The influence of the sea surface roughness (using the surface wind speed as a proxy) is shown as well to indicate the impact of the resulting sea surface emissivity on the top-of-atmosphere (TOA) brightness temperature.

4.3.2 Mathematical description

4.3.2.1 Radiative transfer

The following section about radiative transfer was adopted from the Climate Monitoring Satellite Application Facility's (CMSAF) ATBD on water vapour products [CMSAF, 2009], which builds on the same underlying software package for water vapour retrievals as used herein [Deblonde, 2001].

The radiative transfer is approximated by Equation (1):

$$I_v = \varepsilon_v B_v(T_s) \tau_v^* + \int_{p_s}^0 B_v(T) \frac{\partial \tau_v}{\partial p} dp + R_v \tau_v^* \int_0^{p_s} B_v(T) \frac{\partial \tau_v}{\partial p} dp \quad (1)$$

where ν is frequency, T is temperature, T_s is surface temperature, ϵ_ν is surface emissivity, R_ν is surface reflectivity, B_ν is the Planck function, p is pressure, p_s is surface pressure, τ_ν is transmission and τ_ν^* is total atmospheric transmission. The three right-hand terms describe the following processes:

- The first (left-most) term describes surface emission at temperature T_s and emissivity ϵ_ν , transmitted through the atmosphere with transmissivity τ_ν^* .
- The second term describes the upwelling radiation emitted in the atmosphere integrated from the surface to the top (in pressure coordinates). The emission $B_\nu(T)$ is weighted by the vertical derivative of transmission as function of atmospheric pressure.
- The third term describes the downwelling atmospheric radiation reflected at the surface with reflectivity R_ν and transmitted through the atmosphere with the total transmissivity τ_ν^* . Note that over a rough ocean surface, $R_\nu \neq 1 - \epsilon_\nu$, because of the effect of the slope variability of the ocean surface facets. For the particular treatment and it's evolution within RTTOV, see e.g. *Bormann et al. [2012]*.

The solution of the radiative transfer equation in the microwave part of the spectrum requires a description of the transmission of the atmosphere and the quantification of the surface emission. As e.g. shown in Figure 5, water vapour and oxygen are the relevant absorbers within the spectral range of MWR observations. In the radiative transfer model RTTOV used for AMTROC, gaseous absorption coefficients are calculated using a combination of different gas absorption models and spectroscopic database. For details, see *Saunders et al. [2008]*.

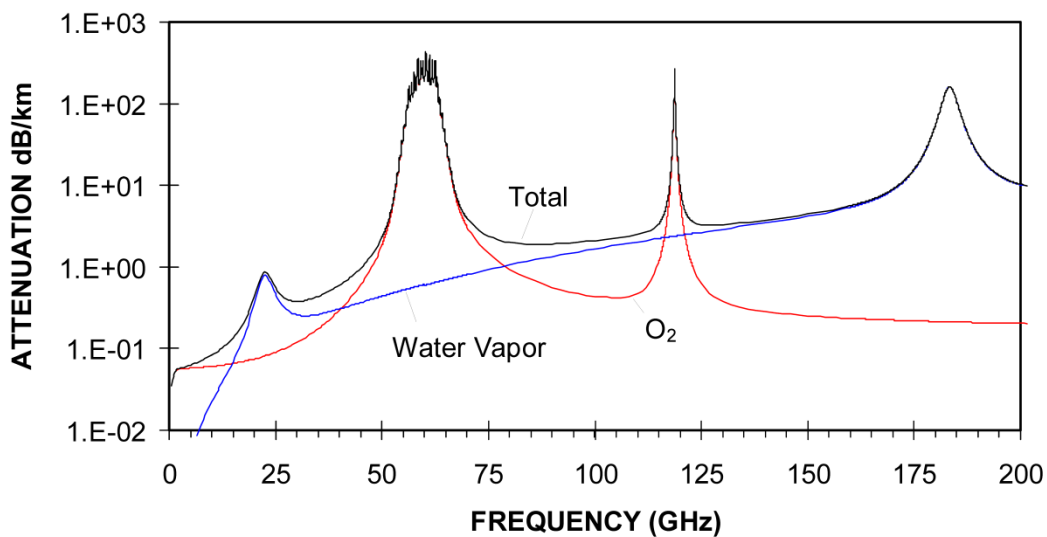


Figure 5: Microwave attenuation of water vapour and oxygen [Liebe, 1985].

Hydrometeors do also affect atmospheric transmission by scattering. As this process is not covered by the radiative transfer model (RTM) applied for the retrieval of TCWV, heavy precipitation events have to be filtered out prior to the application of the algorithm or be identified as low-quality and removed afterwards by applying constraints on the retrieved chi-squared error. The latter method is used within AMTROC.

4.3.2.2 General overview on 1D-VAR

The 1D-VAR retrieval used herein optimally combines an iterative approach to calculate the best estimate of TCWV and LWP, given the observed brightness temperatures and other information, which we specify and discuss below. Speaking in generic terms, 1D-VAR finds an optimal solution for a vector of variables, \mathbf{x} , termed the ‘state vector’, given the observations, \mathbf{y} , and a set of other parameters that describe (among other things) the prior knowledge of the state of the parameters before the observations are incorporated. This prior knowledge is broadly termed the “background knowledge” or *a priori* knowledge [Rodgers, 2000].

One of the advantages of the 1D-VAR approach is that it explicitly distinguishes different types of other input data, depending on their role in the retrieval process. This sets 1D-VAR approaches apart from other methods such as statistical inversion methods and provides better control over how input is handled and more insights into the behaviour of the system and its uncertainty characteristics. In this context, four different types of input can be distinguished as outlined in Table 5. This is in line with the Quality Assurance Framework for Earth Observation (QA4EO) which requires that the result of any retrieval process must have associated with it a quality indicator derived from a quantitative assessment of uncertainty.

Table 5: The different types of variables used in 1D-VAR and their realization within AMTROC. For more details, see Section 4.3.2.6.

Type of variable	Symbol	Principal function	AMTROC 1D-VAR realisation	Remarks
Observations and observation error covariance matrix	\mathbf{y} , ($E+F$)	Observations \mathbf{y} and their error characteristics ($E+F$). E : instrumental error F : representativeness error	MWR TBs	The importance of the observations versus the background is determined by the magnitude of the observation error covariance matrix compared to the magnitude of the background error covariance matrix.
Parameter vector	\mathbf{b}	Provide additional parameters, needed in the forward model, but not retrieved.	SST, U10M, TM, PSFC	The 1D-VAR retrieval will depend on those parameters.
Background profiles and background error covariance matrix	\mathbf{x}_b , \mathbf{B}	Describes the best estimate of the state to be retrieved, before observations are included (\mathbf{x}_b) and its error covariance (\mathbf{B}).	Parameterized as a function of an initial guess for TCWV	The degree to which the result of the 1D-VAR depends on the background information, depends on the information content of the observations.
First guess	\mathbf{x}_0	Gives the starting point of the iterative 1D-VAR process.	Parameterized as a function of an initial guess for TCWV	In a well-posed 1D-VAR, the result is independent of the first guess.

In the context of AMTROC, it is particularly important to understand the relevance and relative importance of \mathbf{b} , \mathbf{x}_o , \mathbf{x}_b , and \mathbf{B} . In order to arrive at such understanding, we first introduce the iterative approach that is followed in the 1D-VAR retrieval. We will then discuss the impact of various input parameters in Section 4.3.2.6.

4.3.2.3 The MWR 1D-VAR retrieval scheme

[This section follows the NWP SAF User Guide [Deblonde, 2001]]

The MWR 1D-VAR solves for atmospheric temperature T , atmospheric water vapour Q , oceanic surface wind speed (SWS) and liquid water path (LWP). The scheme requires atmospheric input profiles (background profiles) that are spatially and temporally collocated with the satellite observations and returns solution for T and Q profiles as well as LWP that optimally fit both observations and background profiles. The optimal fit is determined by the relative weight of the background error covariances and the observation errors. The forward model applied is RTTOV 12.3² (as opposed to RTTOV 6.7 for the earlier EMiR project). The FASt Emissivity ocean model (FASTEM) Version 6.0 [Deblonde and English, 2001; English and Hewison, 1998] is used to provide the ocean surface emissivity required as input to RTTOV. The 1D-VAR used herein is version NWP SAF 1D-VAR Version 1.1.1 from June 2018³. A variational retrieval is applied whereas *a priori* or background information of the atmosphere and surface \mathbf{x}_b , and the measurements \mathbf{y} (observed brightness temperatures) are combined in a statistically optimal way (with a Bayesian analysis) to estimate the most probable atmospheric state \mathbf{x} . The approach is common to a number of areas where non-linear inverse problems are encountered and has been described in detail by various authors [Rodgers, 1976; Tarantola and Valette, 1982; Lorenc, 1986]. Gaussian error distributions are assumed and, consequently, obtaining the most probable state is equivalent to minimising a cost function $J(\mathbf{x})$ also referred to as penalty function. Following the notation of Ide et al. [1997], $J(\mathbf{x})$ may be written as:

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + \frac{1}{2}[\mathbf{y} - \mathbf{H}(\mathbf{x}, \mathbf{b})]^T (\mathbf{E} + \mathbf{F})^{-1}[\mathbf{y} - \mathbf{H}(\mathbf{x}, \mathbf{b})] + J_s \quad (2)$$

where \mathbf{B} , \mathbf{E} , and \mathbf{F} represent background, instrumental, and representativeness (including errors of the forward model) error covariance matrices. J_s is a cubic function that limits the super-saturation and acts as a weak constraint [Phalippou, 1996]:

$$J_s = a (\mathbf{x} - \mathbf{x}_s)^3 \quad (3)$$

where \mathbf{x}_s is the value of the control variable at saturation, $\mathbf{H}(\mathbf{x}, \mathbf{b})$ is the forward operator that maps the control vector \mathbf{x} into measurement space. Here, $\mathbf{H}(\mathbf{x}, \mathbf{b})$ is represented by the radiative transfer model RTTOV 12.3 further described in above Section 4.3.2.1. The superscripts T and $^{-1}$ denote matrix transpose and inverse respectively.

² <https://www.nwpsaf.eu/site/software/rttov/rttov-v12/>

³ <https://www.nwpsaf.eu/site/software/1d-var/>

One of the major advantages of 1D-VAR over other retrieval schemes lies in the explicit separation of the formal parameters \mathbf{x} and \mathbf{b} in the forward operator $\mathbf{H}(\mathbf{x}, \mathbf{b})$. The parameter \mathbf{x} describes the state vector, i.e. the set of variables to be retrieved. The vector \mathbf{b} , termed "parameter vector" in Rodgers [2000], describes other parameters that are also needed in the forward model but not retrieved.

In our case, the state vector \mathbf{x} consists of temperature (at 43 fixed RTTOV standard pressure levels), the natural logarithm of specific humidity (defined for the lowest 19 of those pressure levels) and the oceanic surface wind speed. Optionally, the liquid water path (LWP) defined below can also be added to the control vector (done within the AMTROC context):

$$LWP = \frac{1}{g} \int_0^{P_s} q_L(P) dP, \quad (4)$$

where g is the gravitational acceleration at the Earth's surface, P_s is the surface pressure and q_L is the cloud liquid water content (kg kg^{-1}). If LWP is not chosen as a control variable, then one solves for the natural logarithm of total water content. The total water content is defined as follows:

$$q_{total}(P) = q(P) + q_L(P), \quad (5)$$

where q is the specific humidity (kg kg^{-1}). In general, the minimum of the cost function is found by the iterative solution of Newtonian iteration approach:

$$\mathbf{J}''(\mathbf{x}_n)(\mathbf{x}_{n+1} - \mathbf{x}_n) = -\mathbf{J}'(\mathbf{x}_n), \quad (6)$$

and

$$\mathbf{J}'(\mathbf{x}_n) \rightarrow 0, \quad (7)$$

where \mathbf{x}_n and \mathbf{x}_{n+1} are the n -th and $(n+1)$ -th approximation of \mathbf{x} , \mathbf{J}' and \mathbf{J}'' are the first and second derivatives of the cost function with respect to \mathbf{x} . These are given by:

$$\mathbf{J}'(\mathbf{x}_n) = \mathbf{B}^{-1}(\mathbf{x}_n - \mathbf{x}^b) - \mathbf{H}'(\mathbf{x}_n, \mathbf{b})^T (\mathbf{E} + \mathbf{F})^{-1} (\mathbf{y} - \mathbf{H}(\mathbf{x}_n, \mathbf{b})), \quad (8)$$

Where $\mathbf{H}'(\mathbf{x}_n, \mathbf{b})$ is the Jacobian matrix and contains the partial derivatives of $\mathbf{H}(\mathbf{x}, \mathbf{b})$ with respect to \mathbf{x} . In the linear limit,

$$\mathbf{J}''(\mathbf{x}_n) = \mathbf{B}^{-1} + \mathbf{H}'(\mathbf{x}_n, \mathbf{b})^T (\mathbf{E} + \mathbf{F})^{-1} \mathbf{H}'(\mathbf{x}_n, \mathbf{b}) = \mathbf{A}^{-1} \quad (9)$$

where \mathbf{A} is the error covariance matrix of the solution if $\mathbf{H}(\mathbf{x}, \mathbf{b})$ is linear. $\mathbf{J}''(\mathbf{x}_n)$ is also referred to as the Hessian of the cost function. \mathbf{A} is also called the analysis error covariance matrix. In this document, \mathbf{A} will be referred to as the theoretical error.

4.3.2.4 Accounting for clouds

To properly account for the absorption of cloud particles in the retrieval system, LWP is included in the state vector. Thus, the control vector consists of the profile of natural logarithm of specific humidity ($\ln q$), the oceanic surface wind speed (SWS) and LWP:

$$\mathbf{x} = \{\ln q, SWS, LWP\}.$$

During the minimisation process of Eq. (2), LWP is allowed to vary while the cloud structure $S(P)$ is maintained fixed. The cloud structure $S(P)$ is defined as follows:

$$S(P) = q_L(P) / LWP, \quad (10)$$

with $q_L(P)$ as the profile of cloud liquid water.

If there is a cloud in the background profile, then $S(P)$ is given by:

$$S(P) = q_{LB}(P) / LWP_B, \quad (11)$$

where $q_{LB}(p)$ is the background profile of cloud liquid water content and LWP_B is the liquid water path of the background profile.

If there is no cloud in the background profile, then a non-zero cloud structure is generated where the relative humidity of the background profile exceeds a pre-set threshold value (e.g. 80%). If there is still no cloud, then a non-zero cloud structure is assigned to the lowest levels of the profile. In all cases, the first guess LWP is set to 0.1 kg m^{-2} . The inclusion of the LWP in the state vector allows the retrieval to converge and retrieve meaningful water vapour values in the presence of clouds and it allows for the retrieval of LWP itself.

4.3.2.5 Minimization technique

The Levenberg-Marquardt method was implemented for the minimisation as described in *Press et al. [1989]* (see page 523). The control vector is iteratively changed towards the most likely solution where the control vector fits best both the background information and the MWR observations, under consideration of the corresponding background and observation errors. The iteration is stopped after the gradient of the cost function fulfils a minimum condition.

4.3.2.6 Principal impact of various input parameters on retrieval

4.3.2.6.1 Observation vector \mathbf{y} and observation error covariance ($\mathbf{E}+\mathbf{F}$)

In AMTROC, the observation vector \mathbf{y} consists of the two MWR brightness temperatures at 23 GHz and 36 GHz. Their associated observation error covariance matrix ($\mathbf{E}+\mathbf{F}$) is a 2-by-2 matrix with zero off-diagonal elements and the diagonal elements representing instrument noise plus forward modelling errors as outlined above. The retrieval problem in the context of the MWR is well-defined as the information content of the MWR brightness temperatures with respect to LWP and WVP is very high. Therefore, the retrieved state will be largely, almost entirely, independent from the background as shown in *Bennartz et al., [2017]*. This is a desirable feature for any retrieval as the information content for the retrieved TCWV comes nearly entirely from the observations. Caveats to this statement concern the parameter vector \mathbf{b} , as discussed next.

4.3.2.6.2 Parameter vector \mathbf{b}

As outlined above, the parameter vector \mathbf{b} denotes further input into the forward model that is not retrieved. In our implementation, this parameter vector consists of four scalars, that are needed in the forward model, namely sea surface temperature, surface wind speed, surface pressure, and the atmospheric mean water-vapour weighted temperature T_m (see Section 4.4.2.3). T_m is only used in the WTC diagnostics and not in the 1D-VAR itself but can nevertheless be interpreted as a parameter vector element in that it directly affects the ultimate retrieval but is not itself retrieved.

It is important to understand the critical nature of the parameter vector \mathbf{b} as it will have direct influence on the retrieval via its impact on the forward model. In particular for parameters in \mathbf{b} that

vary on fast time scales or short temporal scales, such as T_m , or U10m, or PSFC it is important to provide as accurate as possible values that are temporally and spatially coincident with the observations [AD-AMTROC-VALREP].

In the AMTROC processing, we recommend using coincident NWP model estimates for SST and PSFC and using wind speed estimates from the radar altimeter where available; otherwise, one can resort back to wind speed estimates from NWP with little degradation in accuracy, as shown in the validation report.

Critically, \mathbf{b} behaves differently from the background information discussed next in that it does affect the retrieval potentially strongly and poor choices of \mathbf{b} will degrade the retrieval more so than do poor choices of the background.

In particular, the use of climatological values is discouraged, because these will likely lead to correlated errors in the retrieval, if the observed weather situation is different from the situation assumed in the climatology.

4.3.2.6.3 Background profile \mathbf{x}_b and background error covariances \mathbf{b}

1D-VAR expects background temperature and humidity profiles, which are also used as first guess in the 1D-VAR retrievals. For the purpose of the AMTROC 1D-VAR, we have implemented a climatological first guess that depends on an initial guess derived from TCWV which can either be obtained from collocated NWP observations or e.g. from an initial statistical retrieval of TCWV from the observed brightness temperatures. Background error covariances are equally derived based on tabulated climatological values.

This approach provides several advantages over the approach initially taken in the ESA precursor retrieval (EMiR). Firstly, by allowing for a climatological first guess of temperature and humidity profiles, 1D-VAR computation time is significantly reduced. Only very few scalar parameters are now needed from temporally and spatially collocated NWP. Secondly, by implementing a background error covariance that is consistent with the background profiles used in the 1D-VAR retrieval, we improve on an issue in the precursor implementation where just one globally fixed background error covariance was used which was independent of the actual background temperature and moisture profiles.

In the context of earlier studies [Bennartz et al., 2017], we have already investigated the impact of different first guess/background profiles on the retrieved WTC and TCWV and have shown that it is to a large extent independent of the exact choice of the background. In the framework of the current study, we have assessed this issue again and come to the same conclusion, as documented in the accompanying validation report [AD-AMTROC-VALREP].

4.3.2.6.4 First guess

In the RTTOV 1D-VAR, the first guess \mathbf{x}_o is set to be equal to the background \mathbf{x}_b . This is a convenient choice [Rodgers, 2000] and has no impact on the retrieval accuracy as the retrieved state is independent on the first guess.

4.4 Theoretical description of WTC retrieval

4.4.1 Physical description

[The text in this subsection is based on material available from <http://www.altimetry.info/>]

Altimetry satellites basically determine the distance from the satellite to a target surface by measuring the satellite-to-surface round-trip time of a radar pulse. The principle is that the altimeter emits a radar wave and analyses the return signal that bounces back from the surface. Sea surface height (SSH) is then the difference between the satellite's altitude (*i.e.* the height above the chosen reference ellipsoid) and the satellite-to-surface range, inferred from the time it takes for the signal to make the round trip (see Figure 6). Besides surface height, by looking at the return signal's amplitude and waveform, one can also measure wave height and wind speed over the oceans, and more generally, backscatter coefficient and surface roughness for most surfaces from which the radar signal is reflected.

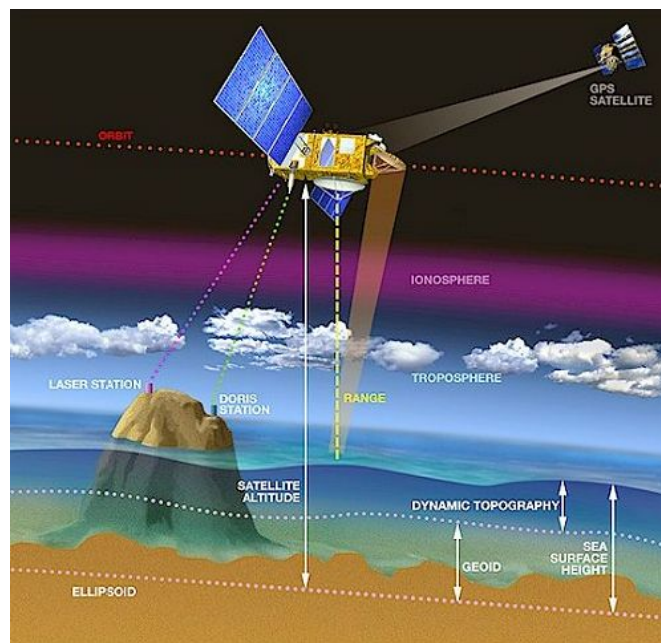


Figure 6: Principle of altimetry measurements.

Source: <http://www.aviso.altimetry.fr/en/techniques/altimetry/principle/basic-principle.html>.

To obtain measurements accurate to within a few centimetres over a range of several hundred kilometres requires an extremely precise knowledge of the satellite's orbital position. Therefore, several location systems are typically carried on board altimetry satellites. Any interference on the radar signal itself also needs to be taken into account. Water vapour and electrons in the atmosphere, sea state and a range of other parameters affect the velocity of the radar beam, thus distorting range measurements. One can correct for these interference effects on the altimeter signal by measuring them with supporting instruments, or by modelling them.

The tropospheric path delay has the largest impact on altimeter measurements, requiring corrections of up to ca. 2.5 m. More than 80% of the tropospheric path delay correction relates to the dry

atmosphere while up to 20% is due to atmosphere moisture. However, atmospheric moisture is highly variable and may therefore cause significant errors in the retrieved SSH.

The wet troposphere correction (WTC) is the correction for the path delay in the radar return signal due to atmospheric moisture. Over the ocean, it is usually derived from microwave radiometer observations taken concomitantly to the actual altimeter observations. Over land surfaces, the wet tropospheric correction is usually derived from atmospheric models.

4.4.2 Mathematical description

4.4.2.1 General overview

The radar altimeter path delay Δz along a path H is directly related to the real part of the refractive index of moist air n :

$$\Delta z = \int_0^H (n - 1) dz. \quad (12)$$

Expressing this in terms of refractivity N , with N in ppm being:

$$N = 10^6 (n - 1), \quad (13)$$

we get:

$$\Delta z = 10^{-6} \int_0^H N dz. \quad (14)$$

Assuming H is the satellite altitude, nadir view, T_v to be the virtual temperature, and using hydrostatic equilibrium we get:

$$\Delta z = 10^{-6} \frac{R_{AIR}}{g} \int_0^{P_{SFC}} N \frac{T_v}{P} dp. \quad (15)$$

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The refractivity N can be parameterized following references cited in *Mangum [2009]*:

$$\begin{aligned}
 N &= a_d \frac{p_d}{T} + a_w \frac{e}{T} + b_w \frac{e}{T^2} \\
 a_d &= 0.776890 \frac{\text{ppm} \cdot \text{K}}{\text{Pa}} \\
 a_w &= 0.712952 \frac{\text{ppm} \cdot \text{K}}{\text{Pa}} \\
 b_w &= 3754.63 \frac{\text{ppm} \cdot \text{K}^2}{\text{Pa}}
 \end{aligned} \tag{16}$$

The variable p is the total pressure and p_d represents the pressure of dry air, where the total pressure $p = e + p_d$, with e being the water vapour partial pressure. With these definitions we can write the total path delay Δz as:

$$\Delta z = 10^{-6} \frac{R_{AIR}}{g} \left[\int_0^{p_{SFC}} a_d \frac{p_d}{T} \frac{T_v}{p} dp + \int_0^{p_{SFC}} a_w \frac{e}{T} \frac{T_v}{p} dp + \int_0^{p_{SFC}} b_w \frac{e}{T^2} \frac{T_v}{p} dp \right]. \tag{17}$$

The first term in the brackets in Equation (17) can be split as follows:

$$\int_0^{p_{SFC}} \frac{p - e}{T} \frac{T_v}{p} dp = \int_0^{p_{SFC}} \frac{p}{T} \frac{T_v}{p} dp - \int_0^{p_{SFC}} \frac{e}{T} \frac{T_v}{p} dp, \tag{18}$$

so that Equation (17) can be expanded to become:

$$\Delta z = \underbrace{10^{-6} \frac{R_{AIR}}{g} \int_0^{p_{SFC}} a_d \frac{p}{T} \frac{T_v}{p} dp}_{\text{Dry tropospheric delay}} + \underbrace{10^{-6} \frac{R_{AIR}}{g} \left[\int_0^{p_{SFC}} (a_w - a_d) \frac{e}{T} \frac{T_v}{p} dp + \int_0^{p_{SFC}} b_w \frac{e}{T^2} \frac{T_v}{p} dp \right]}_{\text{Wet tropospheric delay}}. \tag{19}$$

Note that $T_v / T \approx 1$.

4.4.2.2 Dry delay

Integrating the dry tropospheric part of Equation (19) yields:

$$\Delta z_d = 10^{-6} \cdot \frac{R_{AIR}}{g} \cdot a_d \cdot P_{SFC} \quad (20)$$

The dry delay is in the order of 2.3 m for a straight vertical path through the atmosphere whereas the wet tropospheric delay is only on the order of 0.4-0.5 m at maximum. However, the dry delay can be accurately calculated from the generally well known and smooth atmospheric pressure fields while the wet delay is highly variable in space and time (and is therefore the more critical component).

4.4.2.3 Wet delay

Integrating the wet tropospheric terms in Equation (19) yields:

$$\Delta z_w = 10^{-6} \frac{R_{AIR}}{g} \left[\int_0^{P_{SFC}} (a_w - a_d) \frac{e}{T} \frac{T_v}{p} dp + \int_0^{P_{SFC}} b_w \frac{e}{T^2} \frac{T_v}{p} dp \right] \quad (21)$$

The specific humidity r is defined as:

$$r = \frac{R_{H2O}}{R_{AIR}} \frac{e}{p} \quad (22)$$

Replacing e/p accordingly with r into Equation (21) yields:

$$\Delta z_w = 10^{-6} \frac{R_{H2O}}{g} \left[(a_w - a_d) \int_0^{P_{SFC}} r dp + b_w \int_0^{P_{SFC}} \frac{r}{T} dp \right] \quad (23)$$

The total column water vapour ($TCWV$) is defined as:

$$TCWV = \frac{1}{g} \int_0^{P_{SFC}} r dp \quad (24)$$

We further define a "water-vapour-averaged mean inverse atmospheric temperature", T_m :

$$T_m = \left(\int_0^{p_{SFC}} \frac{r}{T} dp / TCWV \right)^{-1} \quad (25)$$

With these two quantities, Equation (23) becomes:

$$\Delta z_w = 10^{-6} R_{H_2O} \left((a_w - a_d) + \frac{b_w}{T_m} \right) \cdot TCWV = \left(A + \frac{B}{T_m} \right) \cdot TCWV \quad (26)$$

$$A = 10^{-6} \cdot R_{H_2O} \cdot (a_w - a_d) = -2.95077 \cdot 10^{-5} \quad [m / (kg / m^2)]$$

$$B = 10^{-6} \cdot R_{H_2O} \cdot b_w = 1.73276 \quad [m / (K \cdot kg / m^2)]$$

The wet tropospheric delay is in the order of 0.4-0.5 m for high atmospheric water vapour content. The wet tropospheric delay reported in the AMTROC output-files is calculated using Equation (26) with T_m being calculated from ERA reanalysis via Equation (25).

4.4.2.4 Ku-band attenuation

Once WTC is derived, Ku-band attenuation by water vapor is also calculated from retrieved TCWV using *Lillibridge et al. [2014]* and also reported in the output files.

4.5 Algorithm output

The revised AMTROC 1D-VAR retrieval output dataset is summarized in Table 6. The individual data files contain TCWV retrievals, the background equivalent, and the corresponding retrieval error.

Table 6: Contents of AMTROC 1D-VAR retrieval Level-2 NetCDF files.

Variable	Name	Units	Description
Time	time	days	Days since 1950-01-01 00:00:00.0
Latitude	lat	degrees N	Geographical latitude (WGS 1984), North positive
Longitude	lon	degrees E	Geographical longitude (WGS 1984), Range 0°-360°, East: 90°
Prior for total column water vapour	TCWV_PRIOR	kg/m ²	<i>A priori</i> value used for TCWV in RTTOV retrieval
Total column water vapour	TCWV	kg/m ²	Instantaneous retrieved value
Uncertainty of TCWV	TCWV_UNC	kg/m ²	<i>A posteriori</i> uncertainty of instantaneous retrieved value
Liquid water path	LWP	kg/m ²	Instantaneous retrieved value
Uncertainty of LWP	LWP_UNC	kg/m ²	<i>A posteriori</i> uncertainty of instantaneous retrieved value

Variable	Name	Units	Description
Wet tropospheric correction	WTC	m	Instantaneous retrieved value
Uncertainty of WTC	WTC_UNC	m	<i>A posteriori</i> uncertainty of instantaneous retrieved value
Attenuation at Ku-band	ATT_KU	dB	Ku-band attenuation calculated from retrieved TCW using <i>Lillibridge et al. [2014]</i>
Cost function	cost	unitless	1D-VAR retrieval cost function
Retrieval quality flag	flag	unitless	<ul style="list-style-type: none"> – 1: Retrieval performed – 98: Retrieved values out of range – 99: No retrieval (above sea ice or land, or missing TB)

4.6 Performance estimates

The performance of the AMTROC retrieval is investigated in detail in the AMTROC Validation Report *[AD-AMTROC-VALREP]*.

4.7 Practical considerations

4.7.1 High-level description of the prototyped software

We present a scheme to retrieve TCWV and subsequently WTC over the ice-free oceans from Sentinel-3 MWR satellite observations. The derived TCWV is an optimal estimate considering the provided background information and the satellite measurements with their associated errors. The derived TCWV values are provided at Level-2 satellite swath resolution and are estimated to be of high standard with respect to the measurements provided.

The AMTROC retrieval scheme developed for the MWRs onboard the Sentinel-3 series of satellites is built on the software packages RTTOV 12.3 and 1D-VAR 1.1.1 from NWP SAF as discussed above.

The AMTROC scheme provides python interfaces to those programmes together with climatological auxiliary data (background profiles and background error covariance) that have been derived to be consistent with the retrieval application here.

Implementation details are given in the Software User Guide (SUG) *[AD-AMTROC-SUG]*.

4.7.2 Numerical computation considerations

No specific comments.

4.7.3 Programming and procedural considerations

The AMTROC interface is programmed in the programming language python as per EUMETSAT's instructions. The underlying NWP SAF 1D-VAR and RTTOV software packages are programmed in Fortran 90.

4.7.4 Quality assessment and diagnostics

The algorithm is only applied to MWR footprints completely filled by open ocean surfaces. Land and ice surfaces are not processed due to difficulties in the provision of reliable surface emissivity values.

A quality flag exists in the AMTROC 1D-VAR output, adopting the values shown in Table 7. The pixel-based quality check is applied within the 1D-VAR. The valid range for TCWV is set from 0.1 to 90 kg/m².

Table 7: Quality flags of the AMTROC MWR 1D-VAR output.

Flag value	Meaning
0	Data not in valid range
1	Good value
2	Data not taken over ocean or brightness temperature is not correct
99	Default

4.7.5 Exception handling

No specific comments.

4.8 Validation

The performance of the AMTROC retrieval is investigated in detail in the AMTROC Validation Report [AD-AMTROC-VALREP].

5 Assumptions and Limitations

5.1 Performance Assumptions

AMTROC Level-2 data products are affected by a number of assumptions and limitations.

Since MWR is nadir looking only, it does not provide any polarization information. Compared to other microwave sensors, its spectral range is also limited to frequencies below 37 GHz. Therefore, identifying and screening observations affected by frozen hydrometeor scattering will not be possible. Thus, in cases of moderate to heavy frozen hydrometeor load, such as in deep convective cores, retrieval results will likely be degraded. Here we employ a screening based on the final value of the cost function which has proven efficient in eliminating outliers.

The algorithm relies on accurate information about surface wind speed, surface pressure, sea surface temperature, and T_m , which are taken from the radar altimeter (wind speed) and NWP data (all other parameters). It is thus not entirely independent on auxiliary information.



The exact uncertainties in the forward modelling process are not entirely known. Only an estimation can be given which is included in the observation error covariance matrix. The observation error covariance matrix contains only values at the diagonal elements. Off-diagonal elements are currently set to zero.

5.2 Potential Improvements

A number of recommendations towards further improving the AMTROC products have been made as a result of the validation activities. Please consult the AMTROC Validation Report [AD-AMTROC-VALREP] for further details.

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