

ADVANCED CLOUDS, AEROSOLS AND WATER VAPOUR PRODUCTS FOR SENTINEL-3/OLCI

Requirements Baseline Document

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Table of Content

1	INTRODUCTION	6
1.1	PURPOSE	6
1.2	STRUCTURE OF THE DOCUMENT	6
1.3	SATELLITE INSTRUMENTS	6
1.3.1	<i>MERIS and OLCI</i>	6
1.3.2	<i>MODIS</i>	7
1.3.3	<i>PARASOL / POLDER</i>	9
2	WATER VAPOUR	9
2.1	RELEVANCE OF WATER VAPOUR MEASUREMENTS AND THEIR STATUS	10
2.2	REQUIREMENTS ANALYSIS	11
2.3	BASELINE REQUIREMENTS FOR WATER VAPOUR PRODUCTS	12
2.4	SPECIFIC PROPERTIES TO DEFINE WATER VAPOUR ALGORITHM	13
2.5	SUMMARY	16
3	CLOUD-TOP AND SURFACE PRESSURE	17
3.1	RELEVANCE OF CLOUD TOP AND SURFACE MEASUREMENTS AND THEIR STATUS	17
3.2	REQUIREMENT ANALYSIS	18
3.3	BASELINE REQUIREMENTS FOR CLOUD-TOP AND SURFACE PRESSURE PRODUCTS	19
3.4	SPECIFIC PROPERTIES TO DEFINE THE CLOUD-TOP AND SURFACE PRESSURE ALGORITHM	19
3.5	SUMMARY	19
4	AEROSOL AND SURFACE PROPERTIES	19
4.1	RELEVANCE OF AEROSOL MEASUREMENTS AND THEIR STATUS	19
4.2	REQUIREMENT ANALYSIS	21
4.3	BASELINE REQUIREMENTS FOR AEROSOL AND SURFACE PRODUCTS	21
4.4	SPECIFIC PROPERTIES TO DEFINE THE GRASP ALGORITHM	22
4.5	SUMMARY	22
5	DATA PROCESSING	24
5.1	WATER VAPOUR PRODUCTS	24
5.2	CLOUD PRODUCTS	24
5.3	AEROSOL AND SURFACE PRODUCTS	24
5.4	SUMMARY	24
6	CONCLUSIONS AND OUTLOOK	25
7	REFERENCES	25

Acronyms and Abbreviations

AATSR	Advanced Along Track Scanning Radiometer
AERONET	AERosol RObotic NETwork
AOD	Aerosol Optical Depth
ANN	Artificial neural network
ATBD	Algorithm Theoretical Basis Document
BC	Brockmann Consult
BEAM	Basic Envisat Tool for AATSR & MERIS (http://envisat.esa.int/services/beam/)
CNES	Centre National d'Etudes Spatiales
CTP	Cloud-top pressure
DJF	Design justification file
DPM	Detailed Processing Model
DQWG	Data quality working group
DUE	ESA Data User Element programme (http://due.esrin.esa.int/)
ECSS	European Co-operation for Space Standardisation (documents available at ESTEC at the Requirements and Standards Division)
Envisat	ESA satellite (see http://envisat.esa.int/)
EO	Earth Observation
ESA	European Space Agency (http://www.esa.it/export/esaCP/index.html)
ESTEC	European Space Research and Technology Centre
ESRIN	European Space Research Institute (http://www.esa.it/export/esaCP/index)
FUB	Freie Universität Berlin
FoV	Field of View
GCOS	Global Climate Observing System
GEWEX	Global Energy and Water Exchanges Project
GPS	Global Positioning System
GUAN	GCOS Upper Air Network
GVaP	GEWEX Global Water Vapor Project
HITRAN	High-resolution transmission molecular absorption database
HOAPS	Hamburg Ocean Atmosphere Parameters and Fluxes from Satellite
ICAP	International Cooperative for Aerosol Prediction (ICAP)
IODD	Input Output Data Definition Doc.

ISCCP	GEWEX International Satellite Cloud Climatology Project
L1/L2	Level 1 / Level 2
LBL	Line-by-line
LUT	Look-up table
MERIS	Medium Resolution Imaging Spectrometer Instrument (http://envisat.esa.int/)
MODIS	Moderate Resolution Imaging Spectroradiometer (on board the NASA EOS-Aqua satellite)
MOMO	Matrix Operator Modell
MSG	METEOSAT Second Generation
MWR	Microwave Radiometer
NASA	National Aeronautics and Space Administration
OE	Optimal estimation
OLCI	Ocean and Land Colour Instrument on board Sentinel-3
PARASOL	Polarization & Anisotropy of Reflectances for Atmospheric Sciences mission
PDF	Portable Document Format
POLDER	Polarization and Directionality of the Earth's Reflectances
PVR	Product Validation and evolution Report
QA4EO	Quality Assurance framework for Earth Observation
RB	Requirements baseline
RTC / RTM	Radiative Transfer Code / Model
RR	Reduced Resolution
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
SEOM	ESA Scientific Exploitation of Operational Missions Element programme (http://seom.esa.int/)
SOS	Successive Order of Scattering
SoW	Statement of Work
TCWV	Total Column Water Vapour
TOA	Top of atmosphere
VISAT	Visualisation and analysis tool

References

Applicable Documents

[AD-1]	ESRIN Statement of Work. GMES-GSEG-EOPG-SW-13-0047, iss. 1 rev0, dated 14.01.2014
[AD-2]	QA4EO documentation (http://www.qa4eo.org)
[AD-3]	NetCDF Climate and Forecast (CF) Metadata Convention (http://cf-pcmdi.llnl.gov/)

Reference Documents

[R-1]	MERIS Cloud-Top Pressure Algorithm Theoretical Basis Document - ATBD 2.3 (https://earth.esa.int/instruments/meris/atbd/atbd_2.3.pdf)
[R-2]	Bevan, S.L., et al. (2012). A global dataset of atmospheric aerosol optical depth and surface reflectance from AATSR. <i>Remote Sens. of Environment</i> , 116, 119-210.
[R-3]	DUE GlobVapour - Algorithm Theoretical Basis Document L2 MERIS, Version 3.0 (http://www.globvapour.info/download/GlobVapour_D16_ATBD_L2_MERIS_v3.0.pdf)
[R-4]	O. Dubovik et al. (2011). Statistically optimized inversion algorithm for enhanced retrieval of aerosol properties. <i>Atmos. Meas. Tech.</i> , 4, 975-1018.
[R-5]	DUE GlobVapour – Product Validation Report, Cross-Comparison, Version 1.1 (http://www.globvapour.info/download/GlobVapour_D19_PVR_CrossComp_V1.1.pdf)
[R-6]	Hollmann et al. (2013) The ESA Climate Change Initiative: Satellite Data Records for Essential Climate Variables ESA Climate Change Initiative. <i>Bull. Amer. Meteor. Soc.</i> , 94, 1541-1552.

1 Introduction

1.1 Purpose

The SEOM S3 'advanced Clouds, Aerosols and Water vapour products for Sentinel-3/OLCI' CAWA project aims to the development and improvement of advanced atmospheric retrieval algorithms for the Envisat/MERIS and Sentinel-3/OLCI mission. A sensor comprehensive and consistent 1D-Var water vapour algorithm will be developed and applied to the MERIS, MODIS and upcoming OLCI measurements. An innovative and consistent cloud top pressure 1D-Var procedure will be defined for MERIS and all three OLCI O2 A-band channels, which will significantly improve the retrieval accuracy. The challenging and innovative GRASP algorithm for the retrieval of aerosols and surface properties has already shown its advantage in comparison to conventional aerosol retrieval methods. All three algorithms will be further improved, applied to the complete MERIS dataset, to a four months MODIS global time series and six months of OLCI data. We expect to create improved consistent datasets of water vapour, cloud properties, namely cloud top pressure, and aerosol and surface pressure. The intention of the CAWA team is to establish new and improved procedures to estimate atmospheric properties, which also improve the retrieval of land and ocean properties.

This document compiles the baseline requirements for different applications for the atmospheric and surface products developed in CAWA from literature analysis and algorithm needs. This will be the basis to derive the Technical Specifications of the CAWA products and to assess how well the products produced in the CAWA project meet these requirements. The algorithms are described in some details to address the specific needs of mathematical treatment, instrumental constrains and required input data.

1.2 Structure of the document

This document address the baseline requirements for the different applications, this includes a short description of the used satellite instruments and a detailed analysis of:

- Water vapour (Chapter 2)
- Cloud top and surface pressure (Chapter 3)
- Aerosol and surface properties (Chapter 4)
- Product generation (Chapter 5).

1.3 Satellite instruments

The measurements of the satellite sensors MERIS, OLCI, MODIS and POLDER, used in this study, are described in following with respect to their characteristics and specific differences. Here the observation geometry as well as the spectral and spatial resolutions of the instruments are important, especially when used as demonstrator of Sentinel-3 mission.

1.3.1 MERIS and OLCI

The key mission objective for the Sentinel-3 OLCI instrument is the continuity of the ENVISAT MERIS instrument capability. The primary mission of OLCI is the observation of the spectral distribution of upwelling radiance just above the sea surface (the water-leaving radiance) that is then used to estimate a number of geophysical parameters through the application of specific bio-optical algorithms. Atmospheric correction for ocean colour data is challenging (International Ocean Colour Coordinating Group - IOCCG, 2010) as only about 4% of the radiation measured by a satellite instrument originates from the water surface and sensors require high signal to noise ratio (SNR), particularly for the 'blue' bands (Donlon et al, 2012). This requires an accurate retrieval and description of the atmospheric state with respect to scattering and absorption processes. This points

to the secondary objective, the detection of atmospheric properties, which include cloud detection (pixel classification) and aerosol detection, which is important not only for atmospheric correction but also for the monitoring of air-pollution.

The S-3 OLCI instrument is based on the opto-mechanical and imaging design of ENVISAT MERIS (see Table 1). The instrument is a quasi-autonomous, self contained, visible push-broom imaging spectrometer and incorporates the following significant improvements when compared to MERIS:

- An increase in the number of spectral bands (from 15 to 21),
- Improved SNR and a 14-bit analogue to digital converter,
- Improved long-term radiometric stability,
- Mitigation of sun-glint contamination by tilting cameras in westerly direction by 12.6° ,
- Complete coverage over both land and ocean at 300 m Full-Resolution (FR),
- Improved instrument characterization including stray light, camera overlap, and calibration diffusers.

The cameras are arranged to slightly overlap with each other to cover a wide 68.5° across-track field of view as shown in Figure 1. The OLCI swath is not centred at nadir (as in the MERIS design) but is tilted 12.6° westwards to mitigate the negative impact of sun-glint contamination that affects almost half of the MERIS observations at sub-tropical latitudes.

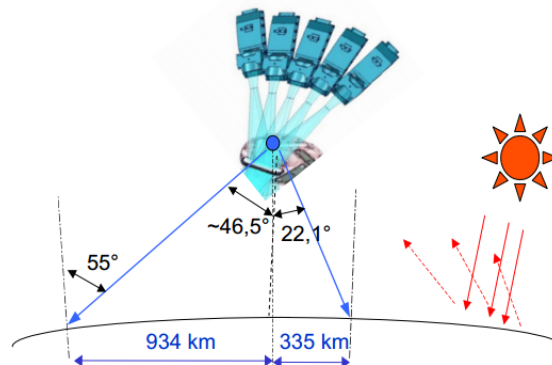


Figure 1: OLCI features a tilted field of view to avoid sun-glint

OLCI bands are optimised to measure ocean colour over the open ocean and coastal zones. A new channel at $1.02 \mu\text{m}$ has been included to improve atmospheric and aerosol correction capabilities, additional channels in the O2A spectral region are included for improved cloud top pressure (height) and water vapour retrieval, and a channel at 673 nm has been added for improved chlorophyll fluorescence measurement. In principle, the OLCI programmable acquisition design allows spectral bands to be redefined in both location and width during commissioning of the instrument after which time they will be fixed for the mission duration.

1.3.2 MODIS

The MODIS instrument provides high radiometric sensitivity (12 bit) in 36 spectral bands ranging in wavelength from $0.4 \mu\text{m}$ to $14.4 \mu\text{m}$. The responses are custom tailored to the individual needs of the user community and provide exceptionally low out-of-band response. Two bands are imaged at a nominal resolution of 250 m at nadir, with five bands at 500 m, and the remaining 29 bands at 1 km. A ± 55 -degree scanning pattern at the EOS orbit of 705 km achieves a 2,330-km swath and provides global coverage every one to two days. For more details of the MODIS instrument and its applications see <http://modis.gsfc.nasa.gov/about/design.php>. The MODIS instrument is flying on board the Terra (10:30 equator crossing time) and on board Aqua (13:30 equator crossing time). The later is also part of the A-train.

OLCI Band	Center [nm]	Width [nm]
Oa1	400	15
Oa2	412,5	10
Oa3	442,5	10
Oa4	490	10
Oa5	510	10
Oa6	560	10
Oa7	620	10
Oa8	665	10
Oa9	673,75	7,5
Oa10	681,25	7,5
Oa11	708,75	10
Oa12	753,75	7,5
Oa13	761,25	2,5
Oa14	764,375	3,75
Oa15	767,5	2,5
Oa16	778,75	15
Oa17	865	20
Oa18	885	10
Oa19	900	10
Oa20	940	20
Oa21	1020	40

MERIS Band	Center [nm]	Width [nm]
Me1	412,5	10
Me2	442,5	10
Me3	490	10
Me4	510	10
Me5	560	10
Me6	620	50
Me7	670	15
Me8	681,25	10
Me9	708,75	10
Me10	753,75	10
Me11	761,25	3,75
Me12	778,75	15
Me13	865	10
Me14	885	10
Me15	900	10

Table 1: The spectral bands of OLCI and MODIS.

MODIS Band	Center [nm]	Width [nm]
Md1	645	50
Md2	858,5	35
Md3	469	20
Md4	555	20
Md5	1240	20
Md6	1640	24
Md7	2130	50
Md8	412,5	15
Md9	443	10
Md10	488	10
Md11	531	10
Md12	551	10
Md13	667	10
Md14	678	10
Md15	748	10
Md16	869,5	15
Md17	905	30
Md18	936	10
Md19	940	50

Table 2: The spectral bands of MODIS within the solar spectral domain, the spatial resolution is 250 m for Md1-Md2, 500m for Md3-Md7 and 1000m for Md8-Md19.

Given the wide swath of the MODIS instrument, which stretches over 2330 km, the tilted swath of OLCI can be simulated. This will provide an accurate assessment whether any problems with the surface elevation are to be expected and whether an orthorectification would be required. Reducing the swath will also improve the coverage characteristics, including the revisit rates, yet not fully given the different orbital heights of 814.5 km and 705 km for Sentinel-3 and EOS-Aqua respectively. In terms of the spatial resolution, only the OLCI Reduced Resolution products can be generated. MODIS only offers a 250 m resolution for the first two bands, Md1 and Md2. (Md3-Md7 features 500 m, while the remaining ones feature 1000 m).

1.3.3 PARASOL / POLDER

The Parasol payload consists of a digital camera with a 274 x 242-pixel CCD detector array, wide-field telecentric optics and a rotating filter wheel, enabling measurements at different wavelengths and in several polarization directions. This instrument configuration acquires a sequence of images every 20 seconds and the instrument views ground targets from different angles. The Parasol mission, operated from 2004 to 2013 as part of NASA's A-train, relies on the former POLDER missions, which instruments had been operated from the Japanese satellites ADEOS I and II. Compared to POLDER, the telecentric optics array has been turned 90 degrees to favour multidirectional viewing over daily global coverage. A channel at 1020 nm has been added to conduct observations for comparison with data acquired by the Lidar on Calipso, which is also within the A-train. Both, Parasol and Calipso, are in a privileged flight constellation for validation studies of GRASP.

2 Water Vapour

The absorption of electromagnetic radiation by water vapour, occurring at characteristic wavelengths throughout the solar and terrestrial spectrum, is related to the excitation of various combinations of the three fundamental vibrational modes of the water molecule. Measurements of the reflected sun light within the resulting absorption bands enable a determination of the total columnar water vapour (hereafter referred to as TCWV), provided that ground-reflected direct solar radiation is available, precluding night-time observations and clouds.

The motivation to establish a method to observe TCWV with satellite measurements in the $\rho\sigma\tau$ -H₂O absorption band is based on the issue, that TCWV estimates in the thermal infrared and microwave are accurate above oceans, but suffer above land surface with variable and high surface emissivity. MERIS and MODIS, missions offer measurements in the $\rho\sigma\tau$ -H₂O absorption band with one channel for MERIS and three for MODIS.

The TCWV algorithms have been undergone drastic changes and improvements during the beginning of the MERIS mission. Validation exercises with different ground based data sets have demonstrated the already achieved quality of the MERIS TCWV product, but also provoked modifications and improvements of the TCWV algorithm. The actual 1D-var MERIS TCWV algorithm considers surface elevation and temperature effects and estimates a pixel-by-pixel uncertainty (Lindstrot et al., 2011). Although the validation of this algorithm has been very successful, a definite wet bias between 5% and 10% is obvious for all different validation test datasets. Those findings provoke room for speculation, that either radiometric calibration (stray-light correction) or spectroscopic line parameter inaccuracies could be responsible for the wet-bias.

Analysis of the MODIS TCWV product and its validation point to higher uncertainties of the derived product than found for MERIS (Albert et al., 2005). There are still a potential for evolutions and improvements of the TCWV algorithms for both, MODIS and MERIS (Diedrich et al., 2013).

When combining MERIS and MODIS TCWV dataset to accomplish an ECV dataset, a consistent retrieval procedure has to be established. This is also required for the upcoming OCLI, which will be launched in 2015 on board Sentinel-3. The proposed procedure has to account for the different specifics of the satellite sensors, while taken all relevant channels of the different sensors, which enhance the retrieval of TCWV.

The following sections are partly taken from the Globvapour documents [R-3] and [R-5] as long as relevant to CAWA and no updates have been published.

2.1 Relevance of water vapour measurements and their status

Water vapour is a key climate variable. In the lower troposphere, condensation of water vapour into precipitation provides latent heating, which dominates the structure of tropospheric diabatic heating (Trenberth and Stepaniak, 2003a,b). Water vapour is also the most important gaseous source of infrared opacity in the atmosphere, accounting for about 60% of the natural greenhouse effect for clear skies (Kiehl and Trenberth, 1997), and provides the largest positive feedback in model projections of climate change (Held and Soden, 2000).

In the stratosphere, there are potentially important radiative impacts due to anthropogenic sources of water vapour, such as from methane oxidation. In the troposphere, the radiative forcing due to direct anthropogenic sources of water vapour (mainly from irrigation) is negligible. Rather, it is the response of tropospheric water vapour to warming itself – the water vapour feedback – that matters for climate change. In GCMs, water vapour alone provides the largest positive radiative feedback, it roughly doubles the warming in response to forcing (such as from greenhouse gas increases). There are also possible stratospheric water vapour feedback effects due to tropical tropopause temperature changes and/or changes in deep convection.

The radiative effect of absorption by water vapour is roughly proportional to the logarithm of its concentration, so it is the fractional change in water vapour concentration, not the absolute change that governs its strength as a feedback mechanism. Randall et al. (2007) stated in the IPCC Fourth Assessment Report that calculations with GCMs suggest that water vapour remains at an approximately constant fraction of its saturated value (close to unchanged relative humidity (RH)) under global-scale warming. Under such a response, for uniform warming, the largest fractional change in water vapour, and thus the largest contribution to the feedback, occurs in the upper troposphere. In addition, GCMs find enhanced warming in the tropical upper troposphere, due to changes in the lapse rate. This further enhances moisture changes in this region, but also introduces a partially offsetting radiative response from the temperature increase, and the net effect of the combined water vapour/lapse rate feedback is to amplify the warming in response to forcing by around 50%. The close link between these processes means that water vapour and lapse rate feedbacks are commonly considered together. The strength of the combined feedback is found to be robust across GCMs, despite significant inter-model differences, for example, in the mean climatology of water vapour.

For NWP models the water vapour information is assimilated directly from the satellite radiances (infrared and microwave) in channels affected by water vapour absorption. This is achieved by 4D variational analysis utilising a fast radiative transfer model as the observation operator. Currently infrared radiances from IASI, AIRS, HIRS, SEVIRI, GOES-Imager and MTSAT-Imager and microwave radiances from AMSU-A, AMSU-B, MHS, SSM/I, SSMI(S) and AMSR-E are all used in global NWP centres to complement the radiosonde measurements network. GPS total zenith delay is also used to define the total column water vapour at GPS sites and the MERIS total column water vapour is beginning to be used over land during the day. The impact of the water vapour measurements improves the water vapour analyses but it has been harder to demonstrate improvements to the forecasts by improving the water vapour field especially for low level water vapour analysis changes. This is because the models are often tuned to their own water vapour climatology and modifying the low level water vapour can often lead to changes in the model spin up which have detrimental effects on the forecasts.

The global network of radiosonde measurements provides the longest record of water vapour measurements in the atmosphere, dating back to the mid-1940s. However, early radiosonde sensors suffered from significant measurement biases, particularly for the upper troposphere, and changes in instrumentation with time often lead to artificial discontinuities in the data record (e.g., see Elliott et al., 2002). Consequently, most of the analysis of radiosonde humidity has focused on trends for altitudes below 500 hPa and is restricted to those stations and periods for which stable instrumentation and reliable moisture soundings are available.

Satellite observations provide near-global coverage and thus represent an important source of information over the oceans, and over land where radiosonde observations are scarce, and in the upper troposphere and stratosphere, where radiosonde sensors are unable to measure or at best unreliable.

An area of concern for infrared based products is that they cannot infer the tropospheric water vapour in cloudy areas whereas the microwave products can. Various studies (e.g. Mieruch et al., 2010 and Xavier et al., 2010) have shown this can lead to a dry bias for the infrared products. All satellite measurements of lower tropospheric water vapour over land are challenging but developments using products based on visible and near infrared radiance are showing new insights into the heterogeneous spatial water vapour distribution above land surface.

2.2 Requirements analysis

The requirements for water vapour profiles for global NWP and climate modelling were collated starting with the Global Climate Observing System (GCOS) (for climate) and WMO (for NWP) user requirements as a baseline (both on WMO UR, 2010). The consolidated set of user requirements includes horizontal and vertical resolution, temporal sampling, and accuracy of the TCWV product. In addition the dissemination timeliness requirements were defined. Other requirements on long-term stability are of high importance for climate monitoring applications. Within the GCOS framework a list of Essential Climate Variables (ECVs) were defined. Among atmospheric ECVs total column water vapour as well as tropospheric and lower stratospheric water vapour profiles are recommended for priority analysis. It is stated in GCOS (2006) taking into account Ohring et al. (2005) that in-situ and satellite observations are vital to achieve an integrated observing system for ECVs in general and more specific, that water vapour observations will largely depend upon satellite observations. The Global Satellite-based Inter-Calibration System, GSICS will also help to improve the calibration of the satellite sensors. It is emphasised in all user requirement documents that the validation of the satellite products is of utmost importance.

GCOS have postulated their requirements for satellite observations suitable for climate variability and trend analysis. WMO also published user requirements for surface-based, airborne and space-based observations for other applications such as global and regional numerical weather prediction (NWP), see WMO UR (2010), SoG (2008) and its former version ReqObs (2001). Three-dimensional humidity fields are key model variables for which observations are needed. The horizontal resolution and coverage are major advantages of satellite observations. The vertical resolution of recent spaceborne instruments on polar-orbiting satellites can be considered as acceptable. The temporal resolution of geostationary satellites not only allows analysis of diurnal cycles but also increases the number of clear sky observations. The availability of total column water vapour from MERIS and MODIS over land is also important. It is indicated in ReqObs (2001) that disadvantages through lack of accuracy might be more than overcome through advantages in coverage and spatial resolution. This is even more valid with the launch of Sentinel-3a/b, EUMETSAT EPS-SG and MTG.

During the ESA DUE GlobVapour project user consultation meeting a Requirements Baseline for water vapour climatology and its use in climate model validation was discussed. Representatives from space agencies, experts in the field of satellite remote sensing and climate analysis, and potential users of water vapour products from satellite observations, mainly regional and global scale climate modellers, expressed their interest in total column water vapour (at a small/fine grid size) and considered profile information, even if limited in temporal and spatial resolution, useful. In general, the meeting resulted in requirements similar to those stated in GCOS, 2006 (see UWR, 2009 for a meeting summary).

Finally, EUMETSAT (2000) and EUMETSAT (2004) provide information on requirements of end-users for the EPS and MSG programs, respectively. These documents have been established by representatives nominated by the national meteorological services of EUMETSAT bodies and is

reviewed by the EUMETSAT Scientific and Technical Group.

The requirements of the CAWA products are mainly oriented at WMO UR (2010), UWR (2009), and WACMOS RB (2009). Temporal and spatial resolution and coverage are oriented at known characteristics of the satellites observations used as input for the CAWA products, in compliance with EUMETSAT (2000), EUMETSAT (2004) and UWR (2009), and are given on the basis of those input observations which allow the highest resolution or largest coverage.

It is likely that climate modellers prefer to use single sensor products instead of merged products. The modellers need well-defined error characteristics, which are known for single sensor products.

2.3 Baseline requirements for water vapour products

On the basis of the requirements analysis in section 2.2, the Requirements Baseline was developed for the CAWA water vapour products and is summarized in Table 3, which provides an overview of the requirements from different centres being active in diverse application areas. These requirements are to a large extent taken from WMO and GCOS tables (WMO UR, 2010). A significant benefit for the users can probably not be gained when the product quality falls below the “threshold” value. The “goal” requirement is the value at which it is anticipated that no further improvements for the user’s application can be expected. The “breakthrough” requirement always lies between “threshold” and “goal” requirement and can be interpreted as value at which user requirements can be met in the most cost-effective way (WMO UR, 2010). Accuracy is given as root mean square error (RMSE). The values given in Table 3 are taking into account known observational satellite characteristics. Therefore, threshold, breakthrough and goal values are given for accuracy.

Table 3: User requirements for water vapour profiles (Break: Breakthrough, Thresh: Threshold, AOPC: Atmospheric Observation Panel for Climate)

Application area	Horizontal [km]			Observing cycle [h]			Accuracy [%]		
	Goal	Break	Thresh	Goal	Break	Thresh	Goal	Break	Thresh
Aeronautical meteorology	50	63	100	1	1.5	3	5	6.3	10
Atmospheric chemistry	50	100	500	6	14	72	5	8	20
Global NWP	15	50	250	1	6	12	2	5	10
Nowcasting	5	17	200	0.25	0.4	1	5	8	20
Regional NWP	10	20	100	0.5	1.5	12	5	8	20
Synoptic meteorology	20	40	200	3	5	12	5	8	20
Climate research	50	60	100	3	5	12	5	8	20
AOPC*	10	15	25	3	4	6	2	4	15
Regional climate monitoring	1	7	50	1	3	12	5	8	20

Concerning the temporal coverage a reliable trend analysis might be feasible when the dataset exceeds a length of 20 years. Certainly, longer time series are preferred but a length of 20 years is considered as a reasonable length to start with. Global coverage is a common requirement from GCOS and users. It was also stated that reduced accuracies could be accepted as long as the accuracy is known.

A summary of the requirements from the various applications areas is listed in Table 1. The application areas were global and regional NWP, AOPC (to cover reanalyses and climate applications), regional climate modelling, and now-casting.

The Requirements Baseline for the CAWA total column water vapour product G_{Vap}-TCWV is summarized in Table 3. The summary utilises the requirements for all applications in the climate sector rather than NWP or now-casting applications.

The requirement on stability is 1% or 0.4 kg.m⁻² a decade in order to be able to infer trends in total column water vapour.

2.4 Specific properties to define water vapour algorithm

The near-infrared total column water vapour (TCWV) retrieval over cloud-free water and land surfaces is based on differential absorption using satellite measurements between 890 and 1000 nm and requires measurements in at least one absorption channel and another in the close by spectral region with less or no absorption (window channel). There are MERIS, MODIS and PARASOL, which already provide those measurements. In the next future there will be METimage, ENMAP, Meteosat Third Generation (MTG) and the Ocean and Land Colour Instrument (OLCI), which all have even improved capacities to measure TCWV. To use all this measurement in weather forecast assimilation or in climate datasets a consistent retrieval procedure has to be established.

In the framework of the CAWA project we propose to develop a consistent retrieval procedure for MERIS, MODIS and OLCI TCWV retrievals. We also address the detected bias problem in the MERIS TCWV retrievals.

In the following we sketch the principles of the proposed TCWV procedure, which can be classified as a 1D-Var approach, and we discuss the input data and assumptions. The forward operator is expressed as look up tables (LUT), which have been calculated by means of radiative transfer simulations taken into account various atmospheric conditions.

First, gaseous absorption will be treated according an advanced k-distribution routine from Doppler et al. (2013) for different standard temperature profiles and calculated from the HITRAN 2012 database (Rothmann et al., 2012). Following a sensitivity study, the standard McClatchey (1972) atmospheric profiles seem to be sufficient to cover the global variability (Lindstrot et al, 2013), however within CAWA we further look into the effects of varying temperature profiles.

The later TCWV algorithm chooses a temperature profile depending on the surface temperature, which is taken from reanalysis data such as ERA interim or actual ECMWF analysis.

The impact of multiple scattering and absorption processes due to molecules and mainly due to aerosols are estimated by means of the radiative transfer code MOMO (Hollstein and Fischer, 2012). Different surface reflectance values, aerosol optical thickness (AOT) and the water vapour amounts are considered covering the natural variability of those properties.

The TOA-radiance in the sensor-specific absorption channel is modelled by:

1. The transmittance for a given water vapour amount and observation geometry
2. A scattering correction, depending on the observation geometry, surface reflectance, aerosol optical thickness (AOT) and the water vapour amount.

The TCWV is derived by matching the modelled and measured radiances using an optimal estimation approach (Rogers, 2000). Estimates of AOT from the satellite observations themselves, and the surface temperature from ERA interim are beneficial. Uncertainty estimates are provided by taking into account all relevant sources of error such as sensor noise, and errors of forward modelling parameters such as AOT, aerosol vertical distribution, surface reflectance, surface elevation and temperature. All those data could be provided with sufficient accuracy.

The formulation of a universal forward operator consists of two elements: First, the calculation of the transmittance T_{noscat} and secondly the calculation of a scattering factor f . T_{noscat} , which is the pure absorption part of the simulated transmittance, is derived from pre-calculated absorption coefficients using an advanced k-distribution method (Doppler et al, 2013). The coefficients are calculated for a different TCWV amounts (WV_0) and atmospheric conditions. In order to obtain the absorption coefficient of a definite WV-channel, which covers a large number of spectral absorption

lines, the quasi-monochromatic intervals are sorted with respect to their optical thickness (absorption). Afterwards they are combined to a significantly lower number of pseudo-spectral intervals. The optical depths in each pseudo-spectral interval i for TCWV value of WV^* are then obtained from multiplying the stored coefficients accordingly:

$$\tau_i^* = \tau_i \frac{WV^*}{WV_0}$$

This is performed for every vertical layer j of the preconditioned TCWV-profile. Subsequently, for every pseudo-spectral interval the transmittance is derived from the sum of the optical depth for all layers along the line of sight. The total transmittance is the sum over all pseudo spectral intervals multiplied with the associated weights w_i and the air-mass factor amf accordingly:

$$T = \sum_{i=1}^{\#intervals} w_i * \exp\left(- \sum_{j=1}^{\#layers} \tau_{ij} * amf\right)$$

The optical depth values τ_{ij} and the corresponding weights w_i are stored in lookup tables for different pressure levels and atmospheric profiles, which are so far defined according to six standard profiles namely tropical, mid-latitude summer, mid-latitude winter, subarctic summer, subarctic winter and US standard (McClatchey et al., 1972). These model atmospheres have been widely used in the atmospheric research community and provide standard vertical profiles of pressure, temperature, and water vapour. The transmittance is calculated for the four look-up table grid points closest to the actual surface pressure and temperature of the considered scene, hereby assuming that the surface temperature is highly correlated with the lower part of the actual vertical temperature profile. The surface pressure is derived from converting land elevation to pressure, using the GTOPO30 digital elevation model (US Geological Survey, 1996), while the surface temperature is extracted from NWP reanalysis data (ERA interim 2m-temperature). The final transmittance of the channel is then calculated as a weighted average among those four parameters, with the weights determined by the distances to the closest grid points of temperature and pressure.

Radiative transfer simulations are performed to determine the scattering correction factor f , which is needed to obtain the total atmospheric transmittance in the spectral domain of the water vapour absorption channel including scattering on air molecules and aerosol particles. T^* is defined as:

$$T^* = L_{sim} / L_{sim}^0$$

Where L_{sim} is the total TOA-radiance and L_{sim}^0 is the TOA-radiance presuming a TCWV value of 0 mm. The simulations are performed by MOMO, calculating radiances for different viewing geometries, AOTs, surface reflectances and TCWV values and stored in LUTs. The US-standard temperature and water vapour profile is preconditioned here. The scattering properties of the aerosols are calculated using a Mie code. For the standard simulations an aerosol layer of 1500 m height with an exponential decrease of the volume-mixing ratio to the ground is assumed. The aerosol type is set based on whether the surface is land or ocean. For land surfaces a continental mixture is assumed, for ocean regions a maritime aerosol mixing is presumed (Hess et al., 1998).

The surface albedo in the absorption channels is estimated by the surface albedos in the two neighbouring window channels and either inter- or extrapolated, depending on the position of the channels. The surface albedo of the window channel is extracted for a given viewing geometry, AOT and the TOA-radiance from a LUT-approach.

Once the TCWV iteration procedure has converged the retrieval uncertainty is calculated, taking into

account direct measurement errors, that is instrumental noise, as well as the uncertainties of all those parameters that are not part of the state vector but fixed a priori. Those are the surface albedo and its spectral dependency, the temperature profile, the surface pressure, the aerosol optical thickness and the aerosol height. The uncertainty introduced by those modelling parameters b_i is determined by converting the individual error contributions into the measurement space via the 'modelling parameter' Jacobian K_b and adding them to the measurement error covariance matrix S_e :

$$S_y = S_e + K_b^T S_b K_b$$

The resulting error covariance matrix S_y , due to all measurement and model parameter uncertainties, is converted into parameter space using the Jacobian K , that is the partial derivative of the radiance L with respect to TCWV at the retrieved state. As a result we get \hat{S} , the error covariance of the retrieved state, which is directly used to define the measurement uncertainty:

$$\hat{S}^{-1} = K^T S_y^{-1} K$$

In particular, the uncertainties of the individual parameters are estimated as follows.

A validation of the MERIS 1D-Var algorithm against ARM-site MWR and GPS-based TCWV retrievals indicate, that the MERIS retrieval has a wet-bias between 5% and 10% as ready discussed above (see Figure 1). Further investigations point to bias-correction by the use of ARM-site MWR measurements. A consistent bias correction is proposed for all satellite sensors in the framework of the CAWA project. The TCWV retrievals will thoroughly validated by comparing them to ground-based reference data over land and satellite-borne microwave wave radiometer data over ocean.

Above land surfaces: Ground-based ARM Southern Great Plains (SGP), Tropical Western Pacific (TWP) and North Slope of Alaska (NSA) microwave radiometer (MWR) data will used. The MWR instruments are microwave radiometers designed to measure the radiation emitted by atmospheric water vapour and liquid water at frequencies of 23.8 GHz and 31.4 GHz (Turner et al., 2007). Since there is no uncertainty introduced by the background emission of the cold space, ground-based microwave data is considered as one of the most accurate methods for the determination of the water vapour column amount. The measurement uncertainty is expected to be in the range of 0.3 mm (Turner et al., 2003). For the comparison, the cloud-free and valid pixels were averaged within 10 km \times 10 km around the ARM sites (see Figure 10, left panel). The MWR measurements, provided minute-by-minute, will averaged in a ± 15 min time frame around the satellite overpass. This averaging has to be performed in order to minimize disturbing effects such as undetected clouds, inaccurate geo-location and the different observing geometries. From MERIS heritage we expect a mean absolute deviation below 1kg/m² and a root mean square deviation below 1.5 kg/m².

Further we will use a global GNSS (Global Navigation Satellite Systems) based dataset of TCWV (Wang 2007) using three different resources: the International Service (IGS), U.S. SuomiNet (UCAR/COSMIC) products and Japanese GEONET data. The measurement of the temperature- and humidity dependent zenith path delay (ZTD) allows the retrieval of TCWV. For detailed description of the analysis method and the data-set see (Wang et al., 2007). The uncertainty of this data is not precisely stated by the author but Gendt et al. (2004) provides an accuracy of 1-2 mm. The third source of validation data over land will be a global data-set of TCWV derived from GCOS Upper Air Network (GUAN) radiosondes, distributed via the GTS network and extracted from the DWD archive for the period 2003-2005. As radiosondes do not measure the whole vertical column at once, the accumulated TCWV has a relatively high uncertainty which can range between 1 and 10 % (Turner et al. (2003) Miloshevich et al. (2004)). In order to account for the displacement of the radiosonde during its ascent, only cases with a time difference of maximum two hours between radiosonde and the satellite measurement will be considered.

Above ocean surfaces: Over ocean the TCWV will be compared to TCWV from MWR on Envisat. The MWR radiometer has the main objective to measure the atmospheric humidity as supplementary

information for tropospheric path correction of the radar altimeter signal, which is influenced both by the integrated atmospheric water vapour content and by liquid water. It will measure brightness temperature at 23.8 GHz and 36.5 GHz covering a bandwidth of 200 MHz in each channel. The lower frequency channel is mostly sensitive to atmospheric water vapour and the higher frequency channel to cloud liquid water. The MWR will have a 20 km × 20 km footprint at nadir, so only the central part of the swath can be compared to MWR data. Properly calibrated MWR can deliver TCWV with accuracy better than 1kg/m². The NIR water vapour retrieval needs reflective ground targets, thus as long as sun glint is apparent we expect accuracies in the same order of magnitude as over land. Outside the glint we anticipate accuracy better than 10kg/m² (depending on the absolute amount of TCWV).

The validation will follow the guidelines as recommended by GEOSS's *Quality Assurance for Earth Observation*, (QA4EO).

2.5 Summary

This document summarises the Requirements Baseline for ESA's CAWA project. On the basis of an extensive requirement analysis and taking into account requirements published in the literature or on documented by the relevant agencies and international organisations, spatial and temporal resolution and coverage as well as accuracy requirements have been defined for the products total column water vapour.

CAWA focuses on the development and improvement of an advanced water vapour retrieval algorithm for the Envisat/MERIS and Sentinel-3/OLCI mission. We have discussed the requirements of TCWV product addressing NMP and climate research issues as well as the requirements for an advanced and sensor independent algorithm. This is essential to generate long-term data records on TCWV from different satellite sensors (here: MERIS, MODIS, OLCI) and to take advantage of the improved observing capacities of OLCI.

3 Cloud-top and surface pressure

ISCCP (2013) reports, that a small decline in total cloud cover of about 0.4% per decade have been extracted from a global analysis of surface observations spanning the period 1971–2009 (Eastman and Warren, 2012). Changes in upper-level cloud cover and total cloud cover over particular areas of the tropical Indo-Pacific Ocean have been found consistent with island precipitation and SST variability (Deser et al., 2010). Compared to surface observations long-term cloud observations from satellites provide a much better spatial and temporal coverage. An assessment of long-term variations in global-mean cloud amount from nine different satellite data sets by Stubenrauch et al. (2013) show differences between the data sets which are comparable in magnitude to the inter-annual variability (2.5 to 3.5%). The inconsistencies result from differences in sampling and changes in instrument calibration, which limits the accuracy of the extraction of global-scale cloud cover trends (ISCCP, 2013). Satellite observations of the dominating low-level marine clouds suggest no long-term trends in cloud liquid water path or optical properties (O'Dell et al., 2008; Rausch et al., 2010). ISCCP (2013) summarises that surface-based observations show region- and height-specific variations and trends in cloudiness but there remains substantial ambiguity regarding global-scale cloud variations and trends, especially from satellite observations.

3.1 Relevance of cloud top and surface measurements and their status

Since the height of clouds affects the Earth radiation budget and is of interest in weather forecasts and climate studies cloud-top pressure is a meteorological standard product of satellite observations. There are several techniques to infer cloud top pressure from space borne measurements, such as based on the *brightness temperature* in which the cloud top pressure is estimated from the temperature profile and the cloud radiance in an infrared-window channel, on the *CO₂-slicing*, using radiance measurements along the edge of the CO₂ absorption band at 14 μm (Menzel et al. 1983), on *stereoscopic* measurements, or on active *lidar* measurements (Boers et al. 1988). All the different methods have advantages and disadvantages, whereby the measuring constraints and conditions have an impact on precision and accuracy of the estimated cloud top pressure (Preusker et al. 2005).

The use of backscattered sunlight at wavelengths within the oxygen A-band has been proposed already in 1961 by Yamamoto and Wark. The initial cloud top pressure retrievals were mostly too high because the former investigations by Saily et al. (1965) or Wu (1985) neglected or treated not adequately the absorption by oxygen within the clouds. Subsequent attempts to model the absorption processes into the clouds failed because of insufficient modelling of the scattering and absorption of oxygen. Fischer et al. (1991) investigated the impact of cloud optical thickness and the vertical profile of liquid water on the O₂ A-band based cloud top pressure retrieval. To account for the penetration of photons into the clouds at least a reference channel and measurements within the O₂ A-band are required. The fundament of this approach is the adequate description of the absorption process of oxygen and the interaction of scattering due to cloud droplets.

The retrieval of cloud properties from MERIS is focused on the cloud amount, cloud top pressure and to some extent to cloud optical thickness. MERIS provides no observation beyond 1 μm , which excludes observation of cloud liquid or ice water or cloud top temperatures. The only benefit of MERIS for cloud observation is the O₂ A-band channel, which have been used to derive cloud top pressure. MERIS observes boundary layer clouds with high accuracy, but fail when optically thin cloud layers are on top (Lindstrot et al., 2006). Lindstrot et al. (2010) studied two multilayer clouds by the combination of MERIS and AATSR observations and found that both, the O₂ A-band and the thermal infrared measurements, contribute to a more accurate cloud top pressure retrieval for vertically structured clouds. Those findings motivated Carbajal-Henken et al. (2012) to develop a 1D-Var approach for a cloud properties retrieval. When the vertical cloud profile, as measured by Cloudsat is taken into the retrieval of the MERIS cloud top pressure the agreement is surprisingly good with the

active radar measurements. Within the thin upper layers the photons penetrate quite deeply in the cloud and miss to detect the cloud top. The O2 A-band of MERIS is not sensitive enough to detect clouds with optically thickness less than 0.5. The upper layer clouds in the tropics and mid-latitudes consist usually of optically thin clouds, which require additional spectral measurements in the O2 A-band for their detection.

The main problem in the cloud top pressure retrieval using the O2 A-band is the photon penetration into the clouds as already discussed in Fischer and Grassl (1990) and Preusker and Lindstrot (2010). The fact that MERIS has only one O2 A-band channel limits the potential to get direct information on the vertical cloud structure. A significant improvement in the cloud-top pressure is expected by the use of the OLCI three O2 A-band channels (Kollewe and Fischer, 1994; Hollstein and Fischer, 2014).

Beyond the MEIRS O2 A-band implementation, measurements within the O2 A-band has been realised for GOME and Sciamachy as well as for POLDER/Parasol. The GOME/Sciamachy instruments provide high spectral resolution (ca. 0.3 nm) measurements, but with a coarse spatial resolution of more than 60 km. Those measurements are used to identify cloud pixels and to correct for cloud effects to a certain extent, but are only of limited gain for cloud studies. POLDER/PARASOL covers the O2 A-band with 2 channels with different spectral resolution 10nm and 40 nm. The lower spectral resolution is less sensitive to the oxygen absorption and the coarse spatial resolution of more than 7 km often does not resolve the cloud structures.

3.2 Requirement analysis

The actual challenge for the cloud top pressure algorithm is to account for the high-level thin cloud layers and vertical structure of the cloud optical thickness (Carbajal-Henken et al., 2014). This might be tackled by the introduction of cloud types, which are related to distinct cloud profiles. First attempts in using ISSP cloud types lead to an improved cloud top detection. This has to be studied in further details and will surely lead to an advanced single sensor MERIS cloud top pressure retrieval.

We expect that the new MERIS CTP product will benefit from the introduction of cloud-types with more realistic cloud optical thickness profiles and an uncertainty estimate.

The challenge for the next generation O2 A-band based CTP retrieval is the efficient use of the three OLCI O2 A-band channels to account more realistically for the penetration depth of the photon into the clouds.

Hollstein and Fischer (2014) studied the potential of O2 A-band measurements by means of an independent information analysis. They simulated the potential OLCI channels around the O2 A-band by measurements of the TANSO-Fourier-Transform-Spectrometer on board the Japanese GOSAT satellite, which provides radiances with spectral resolutions of 0.01 nm. The reflected nadir radiances are taken along a polar orbit. The spectrally high-resolution data were binned to build individual OLCI channels, whereby the reference channels are assumed to be free of atmospheric absorption features with a reduced response function. Two years of observations were used to invest the information content of potential OLCI O2 A-band measurements above clouds. The reconstruction of the full TFS observed spectra could be achieved with 3 independent pieces for the northern and southern hemispheric clouds. Above the tropics the complex cloud systems effect more independent information, expressed in a reduced signal-to-noise ratio where already 3 pieces are sufficient to construct the full observed spectra. Following these results we expect a significant increase in the accuracy of OLCI cloud-top pressure product, when the retrieval algorithm is able to account for the radiation transfer processes within the oxygen absorption of a cloudy atmosphere.

Since the absorption line parameters are sensitive to pressure and temperature, the vertical structure of the atmosphere has to sufficiently be resolved with respect to pressure and temperature. The temperature profile might be taken from ERA-interm or ECMWF reanalysis.

In summary of this investigation we conclude, that OLCI's O2 A-band channels carry three independent pieces of information, which can be detected with the sensors SNR characteristic. The

measurements carry a fourth piece of independent information, which might be more complicated to retrieve, since the variations caused by it are beyond a signal to noise level of 500.

3.3 Baseline requirements for cloud-top and surface pressure products

The baseline requirements of for cloud-top and surface pressure products are driven by needs in climate studies as well as in weather prediction. Following the user consultancy (EUMETSAT, 20xx) it can be stated that the cloud-top pressure has to be estimated within 30 hPA

With respect to algorithm development, the most important parts in a radiative transfer code, suitable to simulate the radiative transfer processes in the O₂ A-band, are the description of the interaction of scattering and absorption processes, the adequate formulation of the gaseous absorption in the vertical structure of the atmosphere, and the incorporation of the instrumental constraints. This points to a critical review of the commonly used HITRAN data-base, even though it has undergone several revisions including the oxygen line by line parameters during the last decade. To address the vertical structure of the atmosphere more correctly than before, recent improvements in the formulation of the atmospheric transmission have been considered to overcome significant uncertainties in the estimation of the absorption coefficients (Bennartz and Fischer, 2001; Doppler et al., 2013). The radiative transfer model MOMO, based on a matrix operator method, has been designed for a complete cloudy and cloud-free atmosphere-ocean system including rough water surfaces (Fell and Fischer, 2001) and has been extended to simulate the complete Stokes vector (Hollstein and Fischer, 2011).

3.4 Specific properties to define the cloud-top and surface pressure algorithm

In comparison to the MERIS ground-segment CTP algorithm, the proposed CAWA CTP algorithm will be based on a 1D-Var approach and will be extended by the three OLCI O₂ A-band channels. We expect that the new MERIS CTP product will benefit from the introduction of cloud-types with more realistic cloud optical thickness profiles and an uncertainty estimate.

3.5 Summary

4 Aerosol and surface properties

4.1 Relevance of aerosol measurements and their status

The MERIS mission has been focused on the retrieval of surface properties and thus the retrieval of aerosols are a by-product of the atmospheric correction above oceans (Antione and Morel, 1999). Above land surfaces a dark dense vegetation approach is used to derive aerosol properties. Several algorithms were developed for aerosol optical thickness retrieval from MERIS including: - MERIS ESA standard algorithms by Santer et al. (1999) and Ramon and Santer (2001), - MERIS ALAMO (Aerosol Load and Altitude from MERIS over Ocean) algorithm by de Leeuw et al. (2013) and MERIS BAER (Bremen AERosol Retrieval) algorithm by von Hoyningen-Huene et al. (2003-2006). All these

algorithms use look-up-tables, obtained from radiative transfer calculations using predefined limited set of the aerosol model with given phase functions and single scattering albedo. Validation exercises showed rather high level of uncertainties in the retrieval and a need for improvements especially above land surfaces (see Leeuw et al., 2013 and Bréon et al. 2011). Recently, in frame of ESA CCI (Climate Change Initiative) “aerosol” project, some efforts have been undertaken for standardizing and improving the aerosol retrieval from satellite observations. Significant part of the efforts was devoted to refining and harmonizing the aerosol models used in the retrieval look-up-tables (Holzer-Popp et al, 2013). For example, updated desert dust model included realistic spectrally dependent absorption with phase function calculated using spheroidal model accounted for the non-spherical shape of the dust particles. As a result, the algorithm performance was improved especially over ocean. Nonetheless, the analysis showed that the accuracy of MERIS retrieval was notably lower than for the retrieval from other sensors, especially over land surfaces. This probably relates to fundamentally limited information content in the one viewing observations of MERIS. Kokhanovsky et al. (2010) demonstrated that such observations might not be sufficient for unique determination of the aerosol properties that leads to a very strong dependence of the retrieval from the made assumptions. Therefore additional efforts are need to be undertaken for enhancing the retrieval strategy and improving MERIS retrievals.

The aerosol retrieval algorithm, described by Dubovik et al. (2011) and recently called GRASP (Generalized Retrieval of Aerosol and Surface Properties), is planned to be employed in this study for deriving aerosol properties from MERIS and OLCI data. The retrieval strategy used in GRASP is significantly different to previous approaches.

First, in a contrast with most of conventional algorithms, GRASP uses some a priori assumptions on the expected smoothness of the retrieved functions that help to constrain the solution but generally introduce much less biases in the retrievals compared to direct fixing/assuming some of retrieved parameters. Specifically, similarly to the original AERONET retrieval algorithm (Dubovik and King, 2000) GRASP as it is applied to satellite observations uses several sets of a priori constraints to limit retrieved variability of the most of characteristics derived for each single pixel as described in Table X (see Dubovik et al. 2011). Second, Dubovik et al. (2011) have suggested using an additional second constraining factor by conducting so called multi-pixel retrieval. In this multi-pixel retrieval strategy the aerosol retrieval is performed for a group of pixels simultaneously. The multi-pixel retrieval regime takes an advantage from known limitations on spatial and temporal variability in both aerosol and surfaces properties. The pixel-to-pixel or day-to-day variations of the retrieved parameters are enforced to be smooth by an appropriate set of a priori constraints. This new concept is expected to provide a higher consistency for aerosol retrievals from satellites by enriching the retrieval over each single by co-incident aerosol information from neighbouring pixels, as well, from the information about surface reflectance (over land) obtained in preceding and consequent observation over the same pixels. Figure 6 illustrates the multi-pixel retrieval approach.

The multi-pixel retrieval strategy allows implementing fundamentally different retrievals compare to conventional satellite retrieval approaches for instruments like MERIS and OLCI. Indeed, the achievement of complete and accurate aerosol retrieval from MERIS is not evident because of the limited information content of the observation. Indeed, MERIS aerosol retrieval relies on one view observation at selected 7 wavelengths (0.41, 0.43, 0.49, 0.51, 0.56, 0.67 and 0.87 μm). This number of observations over each observed pixel is not sufficient for deriving all atmosphere/surface parameters affecting the observation, because the measured characteristics are formed by a larger number of natural factors. For example, in order to model the atmospheric radiances observed by MERIS with reasonable accuracy one need to use a radiative transfer model dependent on, at least $N_{\text{par}}=42$ including 6 characterizing aerosol size distributions, 14 values for spectrally dependent complex refractive index (7 for real part and 7 for imaginary), fraction of spherical particles and 21 values for spectrally dependent parameters of surface reflectance: 7 spectral values for each of 3 parameters driving a BRDF model.

4.2 Requirement analysis

In 2011 the Global Climate Observing System (GCOS) released a new revision of the aerosol requirements analysis (GCOS -154, 2011 update). These requirements are specified for four variables: aerosol optical depth (AOD), single scattering albedo (SSA), aerosol layer height, and aerosol extinction profile. They are tabulated under the headings horizontal, vertical and temporal resolution, accuracy and stability (see Table 4) (GCOS-154, 2011 update).

Table 4: GCOS requirements for aerosol

Variable	Horizontal resolution	Accuracy
AOD	5-10 km	Max (0.03; 10%)
SSA	5-10 km	0.03
Aerosol layer height	5-10 km	1 km
Aerosol extinction coefficient (profile)	200-500 km	10%

Due to limitation of information contents, some of GCOS requirements cannot be fulfilled from the single view instruments like MERIS, AATSR, MODIS (L. A. Remer et al., JAS 205, L. A. Remer et al., AMT 2013 ; de Leeuw, G et al., RSE, 2013). In particular, sensitivity of passive remote sensing instruments to aerosol profile is very low, and information content from single viewing limits the possibilities of accurate AOD and SSA retrieval.

Within CCI aerosol project through interaction with AEROCOM (aerosol modelling), the Climate Model user Group (CMUG) of the CCI program and the Copernicus atmosphere service ECMWF / MACC-II (data assimilation) there were formulated aerosol requirements for MERIS and AATSR instruments (Aerosol_cci URD, 2012). In these requirements GCOS variables of interest extended to multi-spectral aerosol total AOD, AOD fine and coarse mode, Angstrom coefficient. CCI aerosol AOD requirements are less strict than GCOS requirements but more related to possibility of AOD retrieval from MERIS and AATSR instruments. According to these requirements, at superpixel level of 10x10 km² required RMS of AOD is 0.05 or 20%. Despite a big progress achieved in AATSR and MERIS algorithm improvement within CCI aerosol projects, the general formulated AOD requirements as well as Angstrom coefficient and SSA retrieval are still an issue (Aerosol_cci, final report, 2014). That is especially the case for very small and big (bigger than 2) values of AOD and over the bright surfaces.

Accurate separation of surface and atmosphere signals is the crucial requirement of any algorithms of aerosol retrieval. Surface characterization in most of algorithm relies on number of a priori assumptions regarding surface reflection. For example, some of them can be applied for dark surfaces, other take into account some surface reflection particularities: empirical relationship between the albedo retrieved at the 2100 nm band (where the aerosol contribution is small) and the albedo at other wavelengths (MODIS retrievals (Remer et al. 2005)); the ratio of the reflectances measured in the forward and nadir views (AATSR retrievals (de Leeuw, G et al., 2013)); slight spectral dependences of surface polarized reflectance (PARASOL operational algorithm over land (Deuzé et al. 2001)). Nevertheless, limited information about surface reflection represents one of the largest error sources for aerosol retrieval.

4.3 Baseline requirements for aerosol and surface products

GRASP is designed to retrieve aerosol properties simultaneously with the parameters of underlying surface. In order to achieve reliable retrieval from PARASOL observations even over very reflective desert

surfaces, the algorithm was designed as simultaneous inversion of a large group of pixels within one or several images. Such, multi-pixel retrieval regime takes advantage from known limitations on spatial and temporal variability in both aerosol and surface properties. Specifically the variations of the retrieved parameters horizontally from pixel-to-pixel and/or temporary from day-to-day are enforced to be smooth by additional appropriately set a priori constraints. This concept provides satellite retrieval of high consistency.

The baseline aerosol requirements within the CAWA is highly accurate multi-spectral AOD and Angstrom exponent retrieval over different kind of surfaces regardless their reflectivity properties (bright or dark, land or ocean). CAWA requirements on AOD accuracy are based on CCI aerosol requirements (0.05 or 20% RMS of AOD).

Surface reflection in GRASP is described with BRDF allowing the determination of different kinds of surface albedo (Directional Hemispherical reflectance (DHR), Bi-Hemispherical Reflectance (BHR)) and other related characteristics (for example, Normalized Difference Vegetation Index (NDVI)). Surface characterisation in the same 10x10 km² scale as aerosol characterisation is one of the baseline requirements of CAWA project.

4.4 Specific properties to define the GRASP algorithm

In the framework of the CAWA project we adapt GRASP algorithm for the purposes for MERIS, MODIS and OLCI TCWV aerosol/surface retrievals. Initially GRASP was developed for the retrieval from POLDER like instruments. Because of multi-spectral, multi-angle, multi-polarization POLDER measurements, its information content for aerosol/surface retrieval is much higher than that of MERIS, MODIS and OLCI TCWV. Some adaptation of GRASP for MERIS, MODIS and OLCI TCWV retrieval is required.

Although, information content in single view satellite observation is limited, it is expected that new improved aerosol and surface product will developed using GRASP that has special convenient and original features:

- *First of all* the above mentioned multi-pixel approach should significantly help to achieve robust separation of aerosol and surface contribution into satellite observations over land surfaces.
- *Second*, the GRASP has unique flexibility in changing assumptions on aerosol and surface reluctance models in the retrieval. This should allow achieving high optimization of many aspect of GRASP retrieval including retrieval completeness (set of the retrieved parameters), accuracy and speed of calculations.

Third, the GRASP structure is developed with the idea of convenient implementation diverse synergy retrieval. Therefore, in case if some severe information content limitation will be identified regarding retrieval of certain parameter, there is always a possibility to employ some synergy solutions in order to overcome the limitations.

4.5 Summary

According to extensive requirement analysis, CAWA focuses on robust and accurate aerosol/surface retrieval with GRASP applied to Envisat/MERIS and Sentinel-3/OLCI mission. Long-term data records of multi-spectral aerosol AOD and surface albedo from different satellite sensors (MERIS, MODIS, OLCI) are expected to be provided within the project with accuracy satisfying the necessary requirements of the community. Moreover, the accuracy and the scope of aerosol and surface products to be provided within CAWA project are likely to exceed most of available products obtained from satellite observation of similar type.

5 Data Processing

We will use the Calvalus Cluster at BC for production of the MERIS data for TCWV and CTP and the Cluster at Catalyst for the production of for AER products. The full mission RR archive is available on both clusters and the full mission FR archive is also available at the Calvalus Cluster and will be used for the FR case studies. In case that one of the processing centers has problem with the production of the RR data, the other is available as back-up.

The MODIS data are a comparably small data set that will be downloaded from NASAs archives and used by both partners.

The availability of OLCI data is not 100% ensured yet. BC is contributing to the German National Ground Centre (COPACI) and expects that access to the S3 data will be through COPACI. BC plans to systematically ingest globally the S3 data from COPACI into its Calvalus System for its services. Fallback solution of BC's plan is to access the ESA Data Hub due to its involvement in the ESA CCI projects and ingest from there. The COPACI solution might also offer the possibility to host users processing and BC might use this for deploying the CAWA processors at COPACI. In any case, BC ensures to collect maintain an archive of 6 months of OLCI data for use in the CAWA project. As a back-up solution, Catalyst is similarly engaged in the Austrian collaborative ground segment.

The overall estimated processing time is a couple of weeks for all products. A precise estimation will be made when the prototypes are available.

5.1 Water vapour products

All

5.2 Cloud products

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5.3 Aerosol and surface products

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5.4 Summary

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6 Conclusions and outlook

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7 References

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