DUE GLOBVAPOUR

Technical Specification Document

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Project Coordinator: Marc Schröder
Deutscher Wetterdienst
marc.schroeder@dwd.de

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1. Introduction

1.1 Purpose

This document represents the technical response to the ESA DUE GlobVapour Requirements Baseline [AD-5] and will provide a technical description for the ESA DUE GlobVapour product portfolio as well as the proposed methodological approaches to be implemented and validated in the project. This includes a description of:

- The technical specifications for the products in terms of spatial and temporal sampling, temporal and geographic coverage, and accuracy.
- The input data sources and the output data description.
- The proposed preliminary methodological approaches to implement the products.
- The proposed validation approaches and the required data.

1.2 Definitions, acronyms and abbreviations

AATSR	Advanced Along Track Scanning Radiometer
AMF	Air Mass Factor
ATSR	Along-Track Scanning Radiometer
DOAS	Differential Optical Absorption Spectroscopy
GDP	GOME Data Processor
GOME/GOME-2	Global Ozone Monitoring Experiment
MERIS	Medium Resolution Imaging Spectrometer
MOMO	Matrix Operator MOdel
RTM	Radiative Transfer Model
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SSM/I	Special Sensor Microwave/Imager
TCWV	Total Column of Water Vapour

UKMO	United Kingdom Meteorological Office
UPAS	Universal Processor for UV/VIS Atmospheric Spectrometers

1.3 Applicable Documents

[AD-1] ESRIN Statement of Work. EOEP-DUEP-EOPS-SW-09-0003, issue 1 revision 1, dated 13 May 2009.

[AD-2] European Cooperation for Space Standardization: Space Engineering Software; ECSS-E-ST-40C, Part 1B, 6 March 2009; available from http://www.ecss.nl.

[AD-3] DUE GLOBVAPOUR Proposal, issue 1 revision 3, dated 9 July 2009.

[AD-4] DUE GLOBVAPOUR Clarification Note, issue 1, revision 1, dated 29 October 2009.

[AD-5] GlobVapour: Requirements Baseline Document, issue 1, revision 0, 05 March 2010

1.4 Reference Documents

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1.5 Structure of the document

Section 1 is the Introduction. It explains the purpose of the report and it's structure, it also lists relevant documents as well as definitions, acronyms and abbreviations.

Section 2 provides the technical specifications of the total column water vapour products derived from GOME/SCIAMACHY/GOME2 (subsection 2.1), from SSM/I-MERIS (subsection 2.2), and from ATSR/AATSR (subsection 2.3).

Section 3 provides the technical specifications of the water vapour profile product derived from IASI and SEVIRI.

Finally, section 4 gives the conclusions.

2. Total column water vapour specifications

2.1 GOME/SCIAMACHY/GOME2

2.1.1 Overview

The GOME/SCIAMACHY/GOME-2 family of instruments are nadir-looking spectrometers operating in the UV/VIS/near-IR wavelength region (SCIAMACHY has more extended capabilities as well, which are not considered here). For the retrieval of H_2O, we will use a spectral window around the H_2O absorption lines near 630 nm. The retrieval can be employed both over ocean and over land surfaces. The properties of the various instruments are summarised in Table 2-1.

Global total column water vapour from GOME/SCIAMACHY/GOME-2 is mature enough to be used as climate data series, as demonstrated in a number of publications. However, the absolute accuracy estimate on the water vapour columns needs further investigation. Validation studies using an earlier version of the retrieval algorithm show acceptable bias against the SSM/I instruments.

The GlobVapour Total Column of Water Vapour (TCWV) product from the GOME/SCIAMACHY/ GOME-2 family of instruments will be based on the GDP 4.4 algorithm, as currently being used in the O3M-SAF for the generation of H_2O total column from GOME-2. The GDP algorithm has two major steps: the Differential Optical Absorption Spectroscopy (DOAS) least-squares fitting for the trace gas slant column, followed by the computation of a suitable Air Mass Factor (AMF) to make the conversion to the vertical column density. The AMF algorithm used here is optimised for generating self-consistent long-term climatological data, by minimising external inputs. The algorithm is not tuned to achieve maximum accuracy for each individual measurement (see also Section 2.1.4). Time series of TCWV will be derived for each instrument. These datasets will be harmonised, with the very stable long-term record of the GOME data as reference. The delivered GlobVapour data set will cover the period 1995-2008.

Table 2-1: Satellite instrument properties.

Parameter	GOME	SCIAMACHY	GOME-2
Data Availability	06/1995 – today (1)	07/2002 - today	03/2007 - today
Spectral resolution at 630 nm	0.35 nm	0.4 nm	0.5 nm
Ground Pixel size	320 x 40 km^2	60 x 30 km^2	40 x 80 km^2
Swath Width	960 km	960 km	1920 km
Equator crossing local time	10:30 a.m.	10:00 a.m.	9:30 a.m.
Global Coverage	3 days (1)	6 days	almost daily

(1) no global coverage since June 2003

Table 2-2: Technical Specifications for the GlobVapour GOME/SCIAMACHY/GOME2 TCWV product.

ID	Name	Acronym	Input satellite data	Dissemination			Spatial		Temporal	
				type (NRT/ off-line)	Means	Format	coverage	resolution	coverage	resolution
GVAP-GSG	GlobVapour GOME/SCIAMACHY /GOME2 Total columnar water vapour (kg m^{-2})	WV_GOME_TYPE	GOME, SCIAMACHY, GOME-2	Offline	ftp or web	netCDF CF standard	Global	(0.5°)^2	1996-2008	weekly, monthly

Accuracy		Verification method	Applications and users
Bias (kg m^{-2})	RMSE (kg m^{-2})		
2	3	ground based measurements, Inter-satellite comparison	NMHSs, climate research

Table 2-4 shows the technical specifications of the final GlobVapour GOME/SCIAMACHY/GOME2 TCWV product. The numbers for the estimated accuracy for the GOME family TCWV product can be found in O3MSAF-ATBD (2010). The Bias is based on a comparison of GOME/ERS-2 with SSM/I, showing differences within 20% (Slijkhuis, 2008). The RMSE is taken from the error in "clear sky" air mass factors (AMF) in O3MSAF-ATBD (2010), which is based on an upper limit theoretical estimate of the "scene noise" introduced by the simplifying assumptions in the AMF calculation.

2.1.2 Description of methodology

As basis of the processing we will use Level 1b data for GOME and SCIAMACHY, and Level 2 Total H_2O from the O3M-SAF for GOME-2. Total H_2O from GOME and SCIAMACHY is then derived using the GDP 4.4 algorithm in DLR's UPAS processing environment. Cloud information (fractional cover, cloud-top height and cloud-top albedo) for GOME and SCIAMACHY will also be derived from this system, using the Optical Cloud Recognition Algorithm (OCRA) and the Retrieval Of Cloud Information by Neural Networks (ROCINN) algorithm (Loyola et al., 2007). As the same algorithms are used in the O3M-SAF for processing GOME-2 data, this ensures consistent H_2O and cloud information from all three instruments.

Various input parameters to the DOAS algorithm for GOME and SCIAMACHY will be adjusted, e.g. cross-sections (dependent on instrument resolution) or instrument correction factors (e.g. for residual polarisation). Also details of the AMF calculation will be reviewed, e.g. saturation correction or pixel size.

The harmonisation of the TCWV time series from the various instruments is done following the method described in Loyola (2009) for the harmonisation of Ozone time series. The single GOME, SCIAMACHY, and GOME-2 ozone total column measurements are averaged to monthly means for each instrument using a grid of 0.5° x 0.5°. The satellite measurements are projected onto this regular grid using the Lambert Azimuthal equal-area projection. A daily composite is then created from forward scan measurements only (the backward scan measurements cover the same area as the forward scans, but with bigger ground pixel size). Measurements with cloud cover above a certain threshold will not be considered.

The time series from GOME have showed that the retrieval using the DOAS method provides a very stable long-term ozone record (against ground-based instruments), despite a strong instrument throughput degradation in the UV. On the other hand, the time series from SCIAMACHY were found to be less stable (Loyola, 2009). For GOME-2, the time series is too short to make any conclusions. Since there is no reason to expect that the GOME instrument stability in the H_2O retrieval window is worse than in the ozone retrieval window, we will use GOME as reference for the long-term time series of GlobVapour TCWV too. For the periods (and, after June 2003, the geographical regions) of overlap, TCWV from the other instruments will be adjusted to the GOME series and adjustment parameters will be interpolated for non-overlapping periods as necessary. In the course of the GlobVapour project, it will be assessed if other adjustment parameters than time are necessary, e.g. dependence on total column itself (saturation effects) or dependence on scan angle.

2.1.3 Validation approach and required data

An independent geophysical validation of the GOME-2 H_2O product, using ground-based data from the global radiosonde network, will be performed by the O3M-SAF. In the framework of the GlobVapour project, we will make inter-comparisons between the TCWV from GOME/SCIAMACHY/GOME-2 and other satellite instruments. Measurements from SSM/I will be the main source of validation data. However, using SSM/I the TCWV can only be validated above oceans. For land surfaces a comparison to MERIS will be made.

The validation will address known or suspected issues with the retrieval scheme, such as dependence on surface albedo, or dependence on scan angle.

Data requirements are as follows. GOME and SCIAMACHY input products will be provided by DLR. In the same way the GOME-2 operational products will be provided by DLR on behalf of EUMETSAT O3M-SAF. For SSM/I and MERIS we require global data from the F13, F14 instruments, for the years 2007 and 2008. For SSM/I we also require global data for several months in earlier years from 1995 onwards (for validation of GOME, SCIAMACHY) from the F13, F14 and F15 instruments.

2.1.4 Assumptions and limitations

The TCWV from instruments operating in the visible/near-infrared wavelength region is by principle limited to clear sky conditions (see also Section 3.1.4). Especially in the case of GOME, with its big pixel size, the number of truly cloud-free pixels is very small, and a limited amount of cloud contamination may have to be accepted. Furthermore, there is an issue with cloud detection above snow/ice surfaces. The validation will have to address these points.

The calculation of slant columns of water vapour, as derived by the DOAS method, is free from a priori assumptions on the state of the atmosphere. However, to convert measured slant columns to vertical columns (by means of AMF), a certain amount of a priori information is needed. The baseline of the current algorithm is to use as little external information as possible. The atmospheric profile of H_2O, which is an important parameter in the AMF calculation, is assumed the same everywhere on Earth. The influence of variable aerosol loading is neglected. Only the surface albedo for each pixel is taken from a (seasonally dependent) database. These assumptions will inevitably cause higher errors in TCWV for each individual measurement, but provide on climatologically relevant time scales a result which is independent of external input.

Another limitation is that this level 2 water vapour products will only be generated under (almost) clear sky conditions. The filling of cloud gaps is an unresolved issue. Studies on the so called clear sky bias exist and indicate that cloudy areas should not be filled with values from neighbouring clear sky pixels.

2.1.5 Compliance with requirements baseline

In Table 2-3 differences between the Requirements Baseline and the Technical Specifications for the combined SSM/I+MERIS TCWV product are summarized.

As outlined above, the algorithm is tuned for long-term self-consistency, not for maximum accuracy on each individual measurement. The accuracy requirement of the TCWV may not be achieved when comparing to other data (ground-based, SSM/I or other instruments). However, it is expected that the requirement can be met, if it is interpreted as a self-consistency figure within the dataset itself. This is with exception for small water vapour columns, where percent accuracy is not a realistic parameter, as explained more in detail in Section 3.1.5.

Table 2-3: Compliance matrix between Requirements Baseline (RB) and Technical Specifications (TS). Columns are present only, if differences between RB and TS occur (order of values from RB: goal, breakthrough, threshold).

ID	**Accuracy**			**Temporal coverage**			
Reference	**Bias (kg m^{-2})**	**RMSE (kg m^{-2})**		**coverage**		**resolution**	
	TS	TS	RB	TS	RB	TS	RB
GVAP-GSG	2	3	1, 2, 5	1996-2008	>20 years	Weekly, monthly	Daily, monthly

2.2 SSM/I/MWR – MERIS

2.2.1 Overview

This TCWV product will be based on firstly, over-ocean passive microwave retrieval using SSM/I measurements, and secondly, over-land VIS/NIR retrieval using MERIS measurements. Both retrieval methods are based on the variational approach applied in one dimension (one atmospheric column). Background information will be provided by ECMWF's ERA-Interim reanalysis/forecast data. Since the MERIS algorithm relies on measured reflected sun light, the same sensor merged product will only be produced over land and during day time. The full diurnal variability will therefore not be reflected in the final product. The 1D-Var approach and the utilized background data in both retrievals support a high-quality combined TCWV product on global scale including well estimated measures of uncertainties.

The proposed SSM/I 1D-Var retrieval will be adapted to allow an application to MWR observations. However, the MWR TCWV product is considered as not suitable to build up a global climate series because of its limited spatial sampling. There is no additional information compared to SSM/I or other potential instruments as AMSR-E etc. expected.

The final quality of the combined product will depend on the accuracies of the individual algorithms as well as on the performed same sensor merging approach. Possible biases need to be assessed and removed before merging and combination. Particularly coastal regions will be challenging during the combination process. However, since the measurements of both instruments include strong water vapour signal the final product will generally be of high quality.

To align the MERIS TCWV retrieval with the SSM/I results we will perform a bias assessment in which the MERIS algorithm will be applied to cases of sea surfaces with sun glint conditions. The comparison to collocated SSM/I retrieval results will reveal possible systematic biases of the MERIS scheme. These results will guide a corresponding bias correction.

Table 2-4 shows the technical specifications of the final GlobVapour SSM/I-MERIS TCWV product. Note that a significant reduction in quality above coastal areas is expected. The quality of MERIS over mountainous and/or ice-covered areas is unknown and potentially reduced, mainly caused by problematic cloud detection.

Table 2-4: Technical Specifications for the GlobVapour SSM/I-MERIS TCWV product. Quality above coastal areas will be significantly lower.

ID	Name	Acronym	Input satellite data	Dissemination			Spatial		Temporal	
				type (NRT/ off-line)	Means	Format	coverage	resolution	coverage	resolution
GVAP-SMT	GlobVapour SSM/I-MERIS Total columnar water vapour (kg m^{-2})	WV_SSMI_MERIS	SSM/I (ocean), MERIS (land)	Offline http://www.geo.uu.nl/jcu/vbergen/vulkanisme_1.pdfline	ftp or web	netCDF CF standard	Global, ice-free	ocean: $(0.5°)^2$ land: $(0.05°)^2$	ocean: Jan 1996 - Dec 2002 (SSM/I) land/ocean: Jan 2003 - Dec 2008 (MERIS, SSM/I)	daily, monthly

Accuracy		Verification method	Applications and users
Bias (kg m^{-2})	RMSE (kg m^{-2})		
ocean: 1.0 land: 1.0	ocean: 3.0 land: 3.0	ground based measurements, Inter-satellite comparison	NMHSs, climate research

2.2.2 Description of methodology

2.2.2.1 SSM/I/ MWR

SSM/I Level 1C data, including a homogenisation with respect to F11 (Fennig, 2001), will be utilized in the applied 1D-Var. The core of the 1D-Var scheme is based on developments at ECMWF by Phalippou (1996), which was further extended to be a stand-alone scheme applicable to SSM/I. The reader is referred to Deblonde (2001) and NWP-SAF User's Guide (2001) for further details about the developments and utilization of the scheme. The 1D-Var is using all 7 SSM/I channels, spectrally located at 19.35 GHz (horizontal (H) and vertical (V)), 22.235 GHz (V), 37.0 GHz (H and V), and 85.5 GHz. Each channel is weighted differentially by the specified corresponding observation error and internally in the 1D-Var according to the contained information content. Output of the 1D-Var are vertical profiles of water vapour defined on a discrete vertical grid, which is then integrated to the finale TCWV value.

The 1D-Var is only applied in non-precipitating scenes which will be filtered using a preceding SSM/I rain flag module. Furthermore, the algorithm is only applied to footprints completely filled with ocean surfaces. Land and ice surfaces will not be processed due to difficulties in the provision of proper surface emissivities. Also, footprints with contributions from coastal regions will be omitted. The spatial resolution will approximately be 60 km.

The above 1D-Var scheme for SSM/I observations will be adapted to allow the retrieval of TCWV from MWR Level 1 observations. The product will be available above ice-free oceans only. However, the MWR TCWV product is considered as not suitable to build up a global climate series but can be beneficial for other ENVISAT observation based products.

The retrieval accuracy of the SSM/I TCWV is estimated with a RMSE (root mean square error) of 3.0 kg/m^2 and a bias of 1.0kg/m^2. These values are with respect to the CMSAF validation documented in Jonas and Schulz (2009).

2.2.2.2 MERIS

The algorithm for the retrieval of total column water vapour from MERIS measurements is based on the differential absorption technique, exploiting the MERIS measurements of bands 14 (885 nm) and 15 (900 nm) close-by and within the $\rho\sigma\tau$-water vapour absorption around 935 nm. In order to provide proper error propagation, an optimal estimation algorithm (Rodgers et al, 1976) will be developed in the GlobVapour framework, allowing for a pixel-by-pixel uncertainty estimation. The optimisation is based on a gradient descent, where the measurement error (co-variances) as well as the forward model errors and the background knowledge are integrated into a cost function, assigning the lowest cost to the solution with the highest probability, following the Bayes' theorem. First guess and background information will be provided by ERA Interim data which will be the same as used for the SSM/I.

For the optimal estimation approach, a very fast forward operator for the simulation of the water vapour absorption is needed, since standard RTMs lack the computational efficiency to be used in iterative fitting techniques in the VIS/NIR spectral region. Both a single scattering model and an artificial neural network will be tested with respect to their accuracy and speed, as both methods are fast and allow for an analytic calculation of the Jacobian matrices. The usage of an artificial neural network for the efficient forward modelling within an optimal estimation algorithm has for example been successfully demonstrated for MERIS cloud retrievals by Lindstrot et al. (2010). However, both forward approximations have to be carefully validated against full RTM calculations using the FUB radiative transfer code MOMO (Fell and Fischer, 2001).

In case the planned forward approximations shape up as insufficient, the fall back procedure is the standard MERIS L2 retrieval, which is based on a multi-dimensional nonlinear regression. The regression coefficients were retrieved using the results of a large number of RTM simulations, covering the naturally occurring variability of surface properties, aerosol amounts and properties, temperature and water vapour profiles and amounts. In case the standard MERIS L2 algorithm is used, the pixel based error analysis will be based on look up tables from stratified error analyses. In a validation study against ground-based GPS- and MWR-derived TCWV, the standard MERIS L2 TCWV was found to have a root mean square error of less than 1.7mm with a bias of less than 1mm.

2.2.2.3 Kriging and combination of both products

As an intermediate step the Level 2 products will be projected to latitudinal/longitudinal grid boxes which are $(0.5^\circ)^2$ for SSM/I over ocean and $(0.05^\circ)^2$ for MERIS over land and converted to Level 3. The applied procedure is based on an objective analysis method (Kriging, see Lindau and Schröder, 2010) which will be adapted to 1D-Var retrievals and associated uncertainties from SSM/I and MERIS. This procedure accounts for spatial correlations in TCWV fields and provides grid-box-based mean values, their errors, and the number of independent observations. The horizontal correlation functions will also have to be determined for the TCWV fields within this project. The provided number of observations in each box is related to the number of satellite overpasses.

Prior to the application of Kriging a potential bias between MERIS and SSM/I estimates need to be removed. It is planned to use collocated SSM/I and MERIS sunglint retrievals which are very accurate over the ocean to homogenise the estimates. An alternative approach could be based on ECMWF reanalysis. Other problems related to diurnal variability and the coverage of coastal areas, need to be studied. The SSM/I data set will be produced at DWD, the MERIS data set at FUB and the combined data set at FUB.

As the final processing step both TCWV products will be blended. The combination will be carried out on Level 3 basis. Coastal regions will preferably be filled with MERIS TCWV information. In these regions the quality of the final product might exhibit reduced quality relative to both individual products.

2.2.3 Validation approach and required data

A subset of the Diagnostic Data Set (DDS), which contains ground-based observations as well as satellite estimates of total columnar water vapour, will be used to validate the GlobVapour SSM/I-MERIS TCWV product. While the ground-based observations such as radiosonde measurements, and GPS data will primarily be used for land surfaces, the validation over ocean will be against other satellite products (AIRS, Radio Occultation, MODIS, etc.). MWR results will be compared to SSM/I products.

In general, the validation of the products draws on four pillars:

- The validation over land using instantaneous reference data from ground based observations.
- The validation over ocean using instantaneous reference data over ocean, if available.
- The validation of long term products over land using time series from reference stations as GUAN or ARM sites.
- The comparison of instantaneous and of long term over ocean with other satellite retrieval schemes.

The comparison of satellite retrieval results over ocean to independent reference data is rather complicated due to the low number of ground based measurements in these regions. Often occurring problems for validation over land and ocean are the non-negligible errors in the instrument characterizations of the reference systems. Further, the chosen reference observations are never perfectly collocated in space and time. To overcome these problems, Rodgers (2000), Rodgers and Connor (2003) and Pougatchev (2008) developed methods to assess many of the mentioned error sources. Within this validation we will address possible inconsistencies of the TCWV product in those regions where SSM/I and MERIS retrievals where combined, i.e. coastal regions.

One validation limitation will be that over Africa and South America not many long term data sources are available. Considering the task that GlobVapour aims at producing long-term data sets also the long term stability of the ground based data needs to be investigated. We will rely on information given by the editors of the ground based data or on related publications.

2.2.4 Assumptions and limitations

Due to the relative low spatial resolution of SSM/I, with an oval retrieval footprint of about 60 km x 40 km at 22 GHz, the resolution of the final TCWV product was chosen to be $(0.5°)^2$ over ocean which exceeds the defined horizontal resolution over land by a factor of 10. This still meets the Requirements Baseline (AR-5) and the over land and over ocean spatial resolutions perfectly match.

The quality of the combined TCWV product will contain some deficiencies over coastal regions. The TCWV values in these regions will be taken from the MERIS retrieval which is known to have lower accuracy if water surfaces contaminate the MERIS field of view. The quality of the MERIS TCWV retrieval is unknown over mountainous and/or ice-covered areas, mainly caused by uncertainties in cloud detection.

A further restriction arises from the fact that the MERIS retrieval algorithm relies on measurements in the visible channels. For this reason, the TCWV will only be retrieved from MERIS day time overpasses over land. A diurnal variation of the atmospheric water vapour is therefore not captured but the differences can be assessed at least over oceans using day and night SSM/I products.

Another limitation is that the MERIS level 2 water vapour products will only be generated under clear sky conditions. The filling of cloud gaps is an unresolved issue. Studies on the so called clear sky bias exist and indicate that cloudy areas should not be filled with values from neighbouring clear sky pixels. Another issue, not dealt within this document, is the homogenisation of the radiance time series. The SSM/I time series will rely on existing homogenisations, and MERIS stability is not considered as critical due to the relatively short length of the time series. However, attention will be paid on this.

2.2.5 Compliance with requirements baseline

In Table 2-5 differences between the Requirements Baseline and the Technical Specifications for the combined SSM/I+MERIS TCWV product are summarized. The following remarks explain such differences.

Temporal coverage is constrained by the availability of MERIS Level 1 data. Above oceans an SSM/I only product can be provided. Its temporal coverage is oriented at the temporal coverage of the other GlobVapour TCWV products.

The accuracy estimate is expected to be better than threshold accuracy but slightly larger than breakthrough accuracy.

Table 2-5: Compliance matrix between Requirements Baseline (RB) and Technical Specifications (TS). Columns are present only, if differences between RB and TS occur (order of values from RB: goal, breakthrough, threshold).

ID	**Spatial coverage**		**Accuracy**			**Temporal coverage**	
			Bias (kg m^{-2})	**RMSE (kg m^{-2})**			
Reference	TS	RB	TS	TS	RB	TS	RB
GVAP-SMT	Ocean, land, ice-free	Ocean, land, global	1 (SSM/I) 1 (MERIS)	3 (SSM/I) 2 (MERIS)	1, 2, 5	ocean: Jan 1996 - Dec 2002 (SSM/I) land/ocean: Jan 2003 - Dec 2008 (MERIS,SSM/I)	>20 years

2.3 ATSR/AATSR

2.3.1 Overview

The (A)ATSR(-2) TCWV product will be based on an analysis of the observations of ATSR-2 on ERS-2 (1996-on) and AATSR on ENVISAT (2002-on). The algorithm will be applied during day and night and therefore allows an analysis of day/night effects on daily averages of water vapour products from MERIS. It will be applicable above both water and land surfaces. Since the spatial resolution is similar to that of MERIS reduced resolution measurements, the (A)ATSR(-2) L3 product grid will be equally spaced (0.05°).

The ATSR instrument series has hardly been used for the retrieval of columnar water vapour in the past, since the primary focus of the mission is on the retrieval of sea and land surface temperature. A careful analysis of the validation results will therefore be necessary in order to assess the quality and the usefulness of (A)ATSR(-2) measurements for the GlobVapour production of long time series data sets. However, the (A)ATSR(-2) series started already in 1995 and allows retrievals during day and night.

Table 2-6: Technical Specifications for the GlobVapour ATSR TCWV product.

ID	Name	Acronym	Input satellite data	Dissemination			Spatial		Temporal	
				type (NRT/ off-line)	Means	Format	coverage	resolution	coverage	resolution
GVAP-AP	Total Column Integrated Water Vapour (kg m^{-2})	WV_ATSR	AATSR	Offline	ftp or web	netCDF CF standard	Global	$(0.05°)^2$	1996-present	Daily, monthly

Accuracy		Verification method	Applications and users
Bias (kg m^{-2})	RMSE (kg m^{-2})		
TBD	TBD	ground based measurements, Inter-satellite comparison	NMHSs, climate research

Table 2-6 shows the technical specifications of the final GlobVapour (A)ATSR TCWV product. Reduced quality can be expected above ice-covered areas due to strong dependencies on unknown and strongly variable surface emissivities. It is planned to estimate the (A)ATSR TCWV accuracy during the validation of the prototype products, that is, at the end of 2010.

2.3.2 Description of methodology

(A)ATSR(-2) measurements in the thermal infrared at 10.8 µm and 12 µm contain information on the atmospheric water vapour content. The algorithm for the estimation of TCWV will be based on the so called split window technique, relying on the different impact of water vapour on measured emitted radiances in these two channels. The impact of varying surface emissivity and absorbing aerosols will be studied in a sensitivity analysis. Following the results of this investigation either the same surface emissivity at 11 and 12 µm will be assumed or a correction term, correlated with a NDVI value, will be introduced. During nighttime observations, additional information for the retrieval of TCWV from (A)ATSR(-2) measurements will be provided by the 3.7 µm channel, which shows a strong sensitivity to water vapour. A decision about the methodology to be applied will be made on the basis of a preliminary sensitivity study. In either case, the algorithm will be applicable above land and ocean during day and night but will exhibit the highest accuracy above ocean during nighttime. Above land surfaces, the uncertainty introduced by the surface emissivity will reduce the quality of the derived TCWV. In similar approaches based on AVHRR and MSG SEVIRI data, a TCWV accuracy of 6mm (rmse) with a bias of 3mm was achieved (Kleespies and McMillin, 1990; Schroedter-Homscheidt et al, 2008)

In case the (A)ATSR TCWV product exhibits comparable or better quality than TCWV from MERIS, SSM/I and GOME a 1D-Var algorithm for (A)ATSR will be developed.

2.3.3 Validation approach and required data

A subset of the Diagnostic Data Set (DDS), containing ground-based observations as well as satellite estimates of TCWV, will be used to validate the GlobVapour (A)ATSR(-2) TCWV product. Above land surfaces, the (A)ATSR(-2) TCWV product will be validated against GPS and radiosonde data. Additionally, a cross-comparison with the highly accurate and temporally simultaneous MERIS TCWV retrieval will be performed.

The validation above ocean will mainly be based on inter-comparison with other satellite products (AIRS, Radio Occultation, MODIS, etc.) with additional validation based on independent reference data, where available.

2.3.4 Assumptions and limitations

The planned algorithm is based on the analysis of the differing water vapour impact on the (A)ATSR(-2) channels at 10.8 and 12 µm. For this we must assume that the surface emissivities do not differ substantially between the two bands, which is reasonable for most cases, in particular above water surfaces. Nevertheless, NASA’s emissivity archive (Baldridge et al, 2009) will be analyzed to prove this assumption and to optionally use the NDVI as a proxy for slight deviations. Nevertheless, reduced quality can be expected above ice-covered areas due to strong dependencies on unknown and strongly variable surface emissivities.

The local equator crossing time of ERS-2, carrying ATSR-2, is 30 minutes after that of ENVISAT, carrying AATSR. This has to be regarded in the analysis of the long term data set.

The ATSR instrument series has hardly been used for the retrieval of columnar water vapour in the past, since the primary focus of the mission is on the retrieval of sea and land surface temperature. A careful analysis of the validation results will therefore be necessary in order to assess the usefulness of (A)ATSR(-2) measurements for the GlobVapour TCWV production.

Another limitation is that the level 2 water vapour products will only be generated under clear sky conditions. The filling of cloud gaps is an unresolved issue. Studies on the so called clear sky bias exist and indicate that cloudy areas should not be filled with values from neighbouring clear sky pixels.

2.3.5 Compliance with requirements baseline+

In Table 2-7 differences between the Requirements Baseline and the Technical Specifications for the (A)ATSR(-2) TCWV product are summarized. The following remarks explain such differences.

Temporal coverage is constrained by the availability of operational ATSR Level 1 data.

The accuracy estimate is expected to be better than threshold accuracy. (A)TSR(-2) was designed for surface temperature retrievals and not for water vapour retrievals. The infrared channels are affected by water vapour. However, they are mainly influenced by continuum absorption and by tails of absorption lines what might lead to reduced sensitivities.

Table 2-7: Compliance matrix between Requirements Baseline (RB) and Technical Specifications (TS). Columns are present only, if differences between RB and TS occur (order of values from RB: goal, breakthrough, threshold).

ID	**Accuracy**			**Temporal coverage**	
Reference	**Bias (kg m^{-2})**	**RMSE /(kg m^{-2})**			
	TS	TS	RB	TS	RB
GVAP-AP	TBD	TBD	1, 2, 5	Jun 1996 - Dec 2008	>20 years

3. Water vapour profile products

3.1 IASI-SEVIRI

3.1.1 Overview

The GlobVapour water vapour profile product will be based on merging two separate water vapour products, one derived from IASI and the other derived from SEVIRI, respectively. Corresponding retrieval schemes are based on the optimal estimation theory incorporating forecasts as background constrains. Both instruments observe water vapour differently and have different error characteristics. The IASI scheme is expected to be of very high quality performed on relatively high vertical resolution. It is proposed to initially perform a retrieval assessment for 5 IASI retrieval systems using a common validation data set. The SEVIRI scheme especially provides water vapour information on high spatial and temporal resolution. This scheme will be based on the NWC-SAF optimal estimation Radio Occultation, retrieval. The sensor merged product will contain water vapour content in at least 3 atmospheric layers for the SEVIRI disc. The product includes land and ocean areas.

The exact accuracy of the final product will naturally depend on the accuracies of both used retrieval schemes. According information about the actual product accuracy, which will arise from the assessed retrieval errors and the sensor merging method used, will be a part of the final product.

The activities in GlobVapour do not create a climate time series for this product, since only a short common time period is available for this work. However, this part of the project is very beneficial for investigating the quality of the existing retrieval methods and to explore ways to combine the estimates into a higher value product.

Table 3-1 shows the technical specifications of the GlobVapour water vapour profile product. The accuracy values are taken from WACMOS (2009).

Table 3-1: Technical Specifications for the GlobVapour SEVIRI/IASI water vapour profile product.

ID	Name	Acronym	Input satellite data	Dissemination			Spatial		Vertical resolution	Temporal	
				type (NRT/ off-line)	Means	Format	coverage	resolution		coverage	resolution
GVAP-ISP	Layered Vertically Integrated Water Vapour ($kg\ m^{-2}$)	WV_IASI_SEVIRI	SEVIRI, IASI	Offline	ftp or web	netCDF CF standards	Full Meteosat disc	$(0.25°)^2$	3 layers	planned from: Oct. 2007 - Dec 2008	Three hourly, monthly

Accuracy		Verification method	Applications and users
Bias ($kg\ m^{-2}$)	**RMSE ($kg\ m^{-2}$)**		
Layer 1: 0.2 Layer 2: 0.6 Layer 3: 0.8	Layer 1: 0.8 Layer 2: 2.0 Layer 3: 3.0	ground based measurements, Inter-satellite comparison	NMHSs, climate research

3.1.2 Description of methodology

We will utilise SEVIRI Level 1.5 data, the CM-SAF cloud mask and the NWC-SAF optimal estimation software package (NWC-SAF ATBD, 2010) to retrieve humidity profiles. Level 1c data will be used for the IASI retrieval. Since the IASI and SEVIRI retrievals are based on optimal estimation theory, retrieval uncertainty information will be provided. The instantaneous spatial resolution of the derived SEVIRI and IASI Level 2 products is 3 and 12 km at nadir. The temporal sampling is 15 min for SEVIRI and ~12 hours for IASI. The vertical resolution of the derived IASI Level 2 product depends on the internal number of levels of the utilised RTM. In case RTTOV will be used the Level 2 will consist of 90 levels. However, the number of independent observations from IASI is smaller, with a reasonable average vertical resolution of 2 km for humidity (~10 layers). The vertical resolution and centre altitude of each layer will be a function of the current atmospheric situation and is a priori not known. In general, the IASI retrieval properties are expected to be similar to ILPG (2009). The produced SEVIRI Level 2 product will be given for 43 levels according to the use of the RTTOV model. However, the number of independent information is only 3 (from 6.2 µm, 7.3 µm, and window channel differential absorption). The quality of the water vapour profile information from SEVIRI needs to be analysed. Recent validation efforts at CM-SAF have shown low quality of mid to low tropospheric water vapour products from SEVIRI particularly in the Tropics depending on humidity (Bennartz et al., 2008). Water vapour above 500 hPa shows good quality in comparisons to radiosondes fulfilling the user requirements. In spring 2009 the NWC-SAF presented a new and improved water vapour algorithm package that is capable to derive the vertically integrated water vapour with a higher accuracy by incorporating a-priori information. This approach is expected to improve the water vapour retrieval in lower tropospheric layers.

Table 3-2: Proposed layer definitions for GlobVapour water vapour profile product.

Layer	1	2	3
Pressure [hPa]	500-200	850-500	Surface-850

The envisaged end product consists of tropospheric integrated water vapour content for at least 3 tropospheric layers with a three-hourly temporal sampling. The proposed vertical grid resolution is shown in Table 3-2.

The sensor merged product combines the high vertical sampling and expected high quality of IASI products with the high temporal sampling of SEVIRI products to provide a sensor merged product for the full MSG disc, roughly covering the complete Africa, Europe, and the Atlantic Ocean.

The instantaneous water vapour products from SEVIRI and IASI are retrieved under clear-sky conditions only. A spatiotemporal interpolation into non clear-sky regions is a challenging task, mainly due to anisotropic correlations and strong gradients in water vapour content, e.g., in the vicinity of fronts. In principle, gaps can be filled by the objective analysis. However, Sohn and Bennartz (2008), Mieruch et al. (2010), and Xavier et al. (2010) demonstrated a systematic difference between TCWV within clouds and in clear sky regions. In addition, this difference is a function of location. Therefore, gap filling of clear sky only products is not feasible.

Both the SEVIRI and the IASI product are transformed onto a longitude/latitude grid with 0.25° spatial resolution. The first step of the sensor merging procedure will be the determination of the spatial and temporal correlation functions. The correlation will be analysed on an exemplary data set, e.g., one month of data. Based on the results the correlation functions will be defined. A likely approach will be an exponential decrease of the spatial correlation functions, similar as in Lindau and Schröder (2010) and a spherical function for the temporal correlation. Furthermore, an analysis of the pixel based retrieval error, if present, and the variance is necessary for both uncertainty estimation and normalisation.

Before the sensor merging can be applied a couple of pre-processing steps need to be carried out. For both new products quality monitoring of retrieval results is required in order to analyse quality flags and to identify possible extreme outliers in the difference between the observations and problematic geographical areas (similar to the approach in Lindenbergh et al., 2008). The latter can be achieved by comparing mean absolute and absolute relative differences between the collocated data. Systematic differences between data streams entering the Kriging approach need to be eliminated. This can be done by taking one as reference.

For both data products an objective analysis method (Kriging) will be applied to achieve an interpolation with the possibility to also provide uncertainty information for the sensor merged products. We will employ the approach of Lindenbergh et al. (2008), which leads to a technical extension of the currently used CM-SAF operational Kriging approach described in Lindau and Schröder (2010).

3.1.3 Validation approach and required data

The validation of the products draws on four pillars:

- The validation of retrieval schemes using instantaneous reference data from field experiments.
- The validation of long term products using time series from reference stations as GUAN or ARM sites.
- The comparison of products with each other to assess the relative quality of the products.
- The use of products in applications.

The comparison of satellite retrieval results to independent reference data is rather complex. Often occurring problems for validation are for example that reference systems also have specific instrumental characterisation with non-negligible errors, and chosen reference observations are never perfectly collocated in space and time. To overcome these problems, Rodgers (2000), Rodgers and Connor (2003) and Pougatchev (2008) developed methods to assess many of the mentioned error sources.

A subset of the Diagnostic Data Set (DDS), which contains ground-based observations as well as satellite estimates of water vapour products, will be used to validate the GlobVapour water vapour profile product. This subset firstly includes radiosonde measurements, maintained by national weather services and available via the Global Telecommunication System (GTS), and secondly, radio occultation satellite data. Furthermore, other satellite water vapour profile retrievals, such as from AIRS, will be included.

3.1.4 Assumptions and limitations

The level of maturity of the sensor merged product will be assessed as a part of this project. However, there exist some reasons, why the maturity will probably be limited:

In the past, not much experience has been gained in the geostatistical combination of different sensor data that could guide the development of the new sensor merged products. Besides the difference in spatiotemporal samplings, differences in water vapour estimates from different spectral regions are present and not fully understood.

Preliminary validation results (WACMOS, 2010) exhibited promising quality of the recently released NWC-SAF software for the retrieval of water vapour from SEVIRI. As it can be expected from SEVIRI channel characteristics, lowest quality was found in the mid-troposphere. Further validation, in particular, over semi-arid to arid surfaces as present in the AMMA region (Niamey, Niger) need to be performed to finally decide, if the full disc SEVIRI+IASI product is feasible only for the upper troposphere (p<500 hPa).

Another limitation is that the level 2 water vapour products will only be generated under clear sky conditions. The filling of cloud gaps is an unresolved issue. Studies on the so called clear sky bias exist and indicate that cloudy areas should not be filled with values from neighbouring clear sky pixels. Another issue, not dealt within this document, is the homogenisation of the radiance time series. IASI and SEVIRI stability is not considered as critical due to the relatively short length of the time series. However, attention will be paid on this. Finally, more sophisticated ways of combining satellite observations at retrieval level could also be carried out but are beyond the scope of this study.

3.1.5 Compliance with requirements baseline

In Table 3-3 differences between the Requirements Baseline and the Technical Specifications for the sensor merged IASI+SEVIRI water vapour profiles are summarized. The following remarks explain such differences.

During the validation of the CM-SAF water vapour profile products it became obvious that relative accuracies for water vapour at upper tropospheric levels are not appropriate measures to define specifications. The reason is, that at such altitudes average water vapour contents are very small, and therefore small biases transform into large relative uncertainties. E.g., average specific humidities at pressure levels around 200 hPa are ~ 0.02 kg/m^2. A small relative accuracy value will be beyond the accuracy that can be expected from infrared satellite observations. This leads to a need for the provision of the required accuracy in absolute values.

In the 2008 CM-SAF annual validation reports (Validation Report, 2008a) it has also been shown that the quality of reference observations such as radiosonde measurements, considerably varies among the different stations. Different calibration procedures and various ages of radiosondes can influence the quality of the measurements. The latter issue can have a large effect on the bias of relative humidity observations as shown by Miloshevich et al. (2004). They further analyzed the dry bias of relative humidity observations and found a temperature depend bias ranging from -4 to -10% with significant scatter. In presence of ice saturation the bias largely increases. It is very unlikely that stations apply the proposed correction algorithm of Miloshevich et al. (2004) in their routine observations. This already indicates that validation and also definitions of accuracy specifications at upper tropospheric levels are very ambitious and difficult. It further explains the deviation of TS from RB in changing relative accuracies into absolute accuracies.

Temporal coverage is constrained by the availability of operational IASI Level 1 data.

Table 3-3: Compliance matrix between Requirements Baseline (RB) and Technical Specifications (TS). Columns are present only, if differences between RB and TS occur (order of values from RB: goal, breakthrough, threshold).

ID	**Accuracy**			**Vertical resolution**		**Temporal coverage**	
	Bias (kg m^{-2})	**RMSE**					
Reference	TS	TS (kg m^{-2})	RB (%)	TS	RB	TS	RB
GVAP-ISP	Layer 1: 0.2 Layer 2: 0.6 Layer 3: 0.8	Layer 1: 0.8 Layer 2: 2.0 Layer 3: 3.0	5, 8, 20	3	2, 5, 10	Oct. 2007 - Dec. 2008	>20 years

4. Conclusions

This document summarises the Technical Specifications for the GlobVapour water vapour products based on GOME-SCIAMACHY-GOME2, SSM/I(MWR)-MERIS, (A)ATSR, and SEVIRI-IASI. For each product a compliance matrix provides a direct comparison of the Technical Specifications and the Requirements Baseline. Also, an overview of the methodologies, the validation approaches and assumptions as well as limitations are given.