DUE GLOBVAPOUR

Algorithm Theoretical Basis Document
L2 MERIS

Issue 1.0 Revision 0

21 March 2011

Project nr: ESRIN/AO/1-6090/09/I-OL

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

Technical Officer: Bojan Bojkov
ESA
bojan.bojkov@esa.int

Document Change Record

Document, Version	Date	Changes	Originator
DOC, v1.0	2010.11.01	Original version	Rasmus Lindstrot

Table of Contents

1 Introduction

1.1 Purpose

This document provides the Algorithm Theoretical Basis of the Level 2 MERIS total column water vapour product for the ESA DUE GlobVapour project.

Two L2 and one L3 ATBD are available for the combined SSM/I + MERIS product.

1.2 Definitions, acronyms and abbreviations

DOAS	Differential Optical Absorption Spectroscopy
MERIS	Medium Resolution Imaging Spectrometer
MOMO	Matrix Operator Model
SSM/I	Special Sensor Microwave Imager
TCWV	Total Columnar Water Vapour

1.3 Applicable Documents

[AD-1] DUE GLOBVAPOUR Requirements Baseline Document (RBD), issue 1, revision 0, dated 16 April 2010.

[AD-2] DUE GLOBVAPOUR Technical Specification Document (TSD), issue 1, revision 0, dated 16 April 2010.

[AD-3] DUE GLOBVAPOUR Software Development Plan (SDP), issue 1, revision 0, dated 16 April 2010.

[AD-4] DUE GLOBVAPOUR Summary Report on Existing Algorithm Comparison and Validation Reports (SVR), issue 1, revision 0, dated 29 July 2010.

[AD-5] ESRIN Statement of Work, EOEP-DUEP-EOPS-SW-09-0003, issue 1 rev. 1, 13.05. 2009

[AD-6] DUE GLOBVAPOUR Proposal, issue 1 revision 3, dated 9 July 2009

1.4 Reference Documents

[RD-1] Bennartz, R. and Fischer, J., 2001. Retrieval of columnar water vapour over land from backscattered solar radiation using the Medium Resolution Imaging Spectrometer, Remote Sensing of Environment, 78 (3), 274-283, DOI: 10.1016/S0034-4257(01)00218-8.

[RD-1] Fischer, J. and Bennartz, R., 1997. Retrieval of total water vapor content from MERIS measurements. Algorithm Theoretical Basis Document PO-NT-MEL-GS-005, ESA-ESTEC.

[RD-2] Leinweber, R. and Fischer, J., 2010, Water vapor retrieval from MERIS satellite measurements over cloud free land surfaces, submitted to Journal of Applied Meteorology and Climatology.

[RD-3] Rothman, L.S. and coauthors, 2009, The HITRAN 2008 molecular spectroscopic database, Journal of Quantitative Spectroscopy & Radiative Transfer 110, 533-572.

[RD-5] DUE GLOBVAPOUR Metadata Defintion, issue 1, revision 2, dated 07 September 2010

[RD-6] Guanter, L., Alonso, L. and Moreno, J., 2004, Atmospheric correction of CHRIS/PROBA data acquired in the SPARC campaign, Proc. of the 2nd CHRIS/Proba Workshop, ESA/ESRIN, Frascati, Italy, 28-30 April (ESA SP-578, July 2004)

[RD-7] Fischer, J. and Grassl, H., 1984, Radiative transfer in an atmosphere—ocean system: an azimuthally dependent matrix-operator approach, Applied Optics 23 (7), 1032-1039 (1984), doi:10.1364/AO.23.001032

[RD-8] Fell, F., and Fischer, J., 2001, Numerical simulation of the light field in the atmosphere-ocean system using the matrix-operator method, Journal of Quantitative Spectroscopy & Radiative Transfer 69, 351-388.

[RD-9] McClatchey, R., R. Fenn, J. Selby, F. Volz, and J. Garing, 1972: Optical Properties of the Atmosphere. Air Force Cambridge Research Laboratories, 3rd edition.

[RD-10] Li, Z.; Muller, J.-P.; Cross, P.; Albert, P.; Hewison, T.; Watson, R.; Fischer, J. and Bennartz, R., 2003, Validation of MERIS Near IR water vapour retrievals using MWR and GPS measurements, MERIS user workshop, ESA ESRIN, Frascati, Italy, 10-13 Nov 2003.

1.5 Structure of the document

Section 2 gives an overview of the MERIS instrument and the retrieval algorithm scheme developed within the Globvapour project. The used methods, models and preparatory works are introduced. In section 3 both the theoretical basis of the algorithm as well as the practical application are detailed. Necessary assumptions and limitations are described in section 4. Section 5 gives a conclusion.

2 Algorithm overview

The algorithm for the retrieval of TCWV from measurements of MERIS is based on the exploitation of the pronounced water vapour absorption band around 950 nm using the differential absorption of water vapour. A similar approach was described by, e.g., [RD-1] and implemented in the MERIS ground segment ([RD-2]; [RD-3]). The retrieval is limited to daytime observations above cloud-free land, sea ice and sun glint regions.

MERIS is a wide field-of-view imaging pushbroom spectrometer, providing measurements in 15 spectral channels between 400 nm and 900 nm. The spatial resolution in the reduced resolution mode is 1*1 km^2 and the swath width is roughly 1150 km. MERIS is one out of ten core instruments on ENVISAT and therefore provides continuous observations since March 2002. ENVISAT is flying in a sun-synchronous orbit, descending node, with a constant equator crossing time of 10 LT.

The full MERIS spectrum is used in the retrieval scheme, whereupon the majority of the spectral bands are exploited for cloud screening. Ultimately, three spectral channels are used for the retrieval of water vapour: Channels 13 and 14, located at 865 nm and 885 nm, respectively, provide measurements in the atmospheric window region whereas channel 15, located at 900 nm, at the shortwave edge of the φϕτ-absorption band, is strongly influenced by atmospheric water vapour. Here the ratio of MERIS bands 15 and 14 allows for the approximation of the atmospheric transmittance in the water vapour absorption band which is closely related to the total column amount. In order to avoid errors due to the spectral variation of the surface reflectivity between 885nm and 900nm, MERIS band 13 is additionally used for the linear extrapolation of the surface reflectivity from MERIS bands 13 and 14 to 15.

The algorithm does not rely on auxiliary data except for information about the aerosol optical thickness that is available from MERIS L2 data. In a first step, the MERIS L1B data is screened for clouds, using an Artificial Neural Network developed at FUB. In the next step, the surface reflectance at 865 nm and 885 nm is derived from MERIS L1B data, assuming a Lambertian surface and single scattering conditions. The surface reflectance at 900 nm is then inferred from a linear extrapolation of the window channels reflectances. The gaseous absorption coefficients, based on HITRAN 2008 data ([RD-4]) and pre-calculated using an advanced k-distribution routine from [RD-1], are chosen according to the most appropriate temperature profile, depending on latitude and season. Finally, the total columnar water vapour is inferred by matching the channel ratio *R* of MERIS bands 15 and 14 with the modelled channel ratio, using the simplified single scattering model. The optimization routine is based on the secant method.

Due to the strong water vapour sensitivity of the MERIS measurements, the algorithm does not rely on prior knowledge and background information like water vapour from ERA Interim reanalyses. Reliable aerosol information is beneficial but not crucial. Figure 1 shows a flow chart of the MERIS L2 algorithm for the retrieval of TCWV.

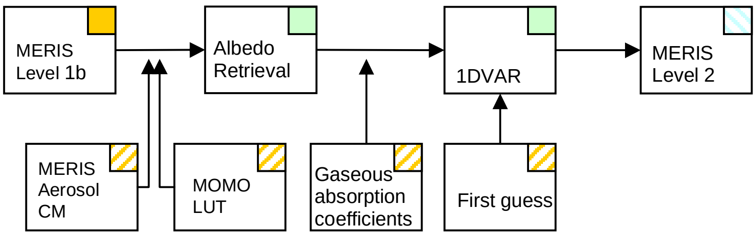

Figure 1: Flow chart for the MERIS L2 processor. Input data is marked in orange (orange shaded: higher level input data), products are marked in blue (blue shaded: instantaneous level 2 products) and software development is marked in green. (CM: cloud mask, LUT: Look-up table)

The resulting MERIS L2 data are stored in NetCDF files that are fully compliant with the NetCDF Climate Forecast convention. A detailed description of the output file format can be found in [RD-5].

3 Algorithm description

3.1 Theoretical description

Measurements within the φϕτ-band around 950 nm provide a good sensitivity to the total columnar water vapour in the atmosphere since the absorption band is pronounced but not saturated for the range of water vapour amounts occurring on a global scale and measured under MERIS observation geometries. The transmittance, carrying the information about the absorber mass, cannot be measured directly but is approximated by the ratio of two spectral channels inside and close-by the absorption band, respectively, using the common DOAS approach.

The two MERIS channels utilized in the retrieval algorithm are spectrally separated by 15nm. Despite this close band setting, it is important to account for the spectral dependence on any of the parameters contributing to the signal in order to avoid errors in the approximated transmittance. A spectral dependency of the surface reflectivity is particularly momentous, since the resulting difference in the reflection of the solar radiation strongly impacts the channel ratio. If not accounted for, this effect causes systematic errors in the retrieved water vapour amount because the virtual change in transmittance is falsely attributed to the strength of the water vapour absorption. Since the surface reflectance cannot be derived in absorption channels without exact knowledge of the absorber mass, the surface albedo at 900 nm is linearly extrapolated from the window channels at 865nm and 885nm.

The forward model used within the retrieval framework is based on a simplified description of the radiative transfer under single-scattering conditions. Under the assumption of an isotropic surface reflectance, the normalized top-of-atmosphere radiance signal L^N_{TOA} can be calculated by a simple analytical expression accounting for the interaction of the radiation reflected by the surface with the atmosphere (e.g. [RD-6]):

$$L^N_{TOA} = T_{Gas}(L^N_{Path} + \frac{\alpha\, T^{\uparrow} T^{\downarrow}}{1 - H\alpha})$$

where T_{Gas} is the gaseous transmittance, L^N_{Path} is the normalized path radiance, α is the surface reflectance, $T^{\uparrow}$ and $T^{\downarrow}$ are the up- and downward diffuse and direct transmittances due to scattering, and H is the hemispherical albedo, mainly accounting for multiple scattering events between the surface and the atmosphere.

Under single scattering conditions it is feasible to further reduce this expression by assuming $H = 0$. Inverting the expression then leads to

$$\alpha = \left(\frac{L^N_{TOA}}{T_{Gas}} - L^N_{Path}\right) / \left(T^{\uparrow}T^{\downarrow}\right)$$

It is thus possible to derive the surface reflectance for the window channels 13 at 865 nm and 14 at 885 nm, since

- T_{Gas} is close to 1 with a negligible dependency on the unknown water vapour amount and can be estimated for the known viewing geometry.
- L^N_{Path}, $T^{\uparrow}$ and $T^{\downarrow}$ can be pre-calculated using exact radiative transfer codes like MOMO ([RD-7], [RD-8]) for a given aerosol loading.

As mentioned above the surface reflectance at 900 nm is then inferred via a linear extrapolation.

The gaseous absorption in the water vapour absorption band is calculated using an advanced k-distribution technique from [RD-1]. The absorption line data was extracted from the HITRAN 2008 data base ([RD-4]). In order to account for the temperature and pressure dependent line-broadening effects in the atmosphere, the absorption coefficients were calculated for a number of standard temperature effects taken from [RD-9].

The resulting total columnar water vapour is found by minimizing the difference between measured and simulated water vapour transmittance. The forward model used in the iterative optimization routine is again based on the simple single-scattering model. The ratio *R* of MERIS channels 15 and 14 is simulated using

$$R = \frac{T^{15}_{Gas}}{T^{14}_{Gas}} \frac{\alpha^{15}}{\alpha^{14}} \left(L^{15N}_{Path}/\alpha^{15} + (T^{\uparrow}T^{\downarrow})^{15}\right) / \left(L^{14N}_{Path}/\alpha^{14} + (T^{\uparrow}T^{\downarrow})^{14}\right)$$

with the indices 15 and 14 indicating the appropriate values for MERIS band 14 and 15, respectively. Using pre-calculated values of L^N_{Path}, $T^{\uparrow}$ and $T^{\downarrow}$, the forward simulation can be performed with high speed.

Since the algorithm is based on the optimal fit of merely one parameter, namely the channel ratio $R = L^N_{15}/L^N_{14}$, and no additional background knowledge is needed to be included, the optimization was chosen to be performed by the simple, well known secant method, a finite difference approximation of Newton's method.

The theoretical error of the MERIS water vapour retrieval was predicted by [RD-1] in an extensive error analysis. Accounting for both instrumental effects like sensor noise and spectral misregistration and geophysical influences like variable aerosol scattering and surface reflectance, they found a theoretical accuracy of better than 2 kg/m^2. This finding was supported by validation exercises of the operational MERIS L2 product ([RD-10]; [RD-3]).

3.2 Practical application

The algorithm can be roughly divided into three steps:

1. Cloud screening above land, coast and ice/snow regions.
2. The estimation of the surface reflectivity at 885 nm and 900 nm, assuming a Lambertian surface and single-scattering conditions,
3. The subsequent retrieval of the vertically integrated water vapour content based on a Newton secant method for the iterative matching of measurements and forward simulation. The single scattering model is used for the efficient forward simulation.

The cloud screening is performed using Artificial Neural Networks (ANN) developed at FUB. Differing ANNs for cloud screening above land and ocean surfaces were developed using a large number of MOMO simulations of the full MERIS spectrum, returning the probability of cloudiness. In order to exclude all cloudy pixels, all pixels with a cloud probability above 10% are disregarded. Above snow or ice surfaces, the cloud screening is performed using a snow index *SI* calculated from MERIS bands 13 and 14:

$$SI = {(L_{13} - L_{14})}/{(L_{13} + L_{14})}$$

A limit of SI = 0.025 is used to discriminate clouds from snow or ice on land or ocean. The threshold was defined clear-sky-conservative in order to exclude all cloudy samples. Therefore, a significant number of presumably clear sky scenes above snow / ice are flagged as cloudy and bypassed in the retrieval algorithm.

For the remaining clear sky pixels above land, sun glint and sea ice the surface reflectance at 885 mn and 900 nm is determined, as detailed in section 3.1. TCWV is then derived by matching simulated and measured channel ratio *R* using the secant method.

4 Assumptions and limitations

The retrieval algorithm is applicable over land, sea ice and sun glint only since the reflectivity of the ocean surface is too small outside the direct reflection of the sun and the resulting signal is dominated by the uncertain optical properties of the aerosols. Outside of the direct sun glint, the algorithm produces significantly biased results over ocean pixels.

The MERIS L2 aerosol optical thickness product is only available over dark surfaces like dense dark vegetation. An aerosol optical thickness of 0.15 is used elsewhere. There is no information about the aerosol type and vertical distribution. A non-absorbing continental aerosol residing between 0km and 2km was used in the radiative transfer simulations.

5 Conclusions

The GlobVapour MERIS L2 algorithm used for the TCWV retrieval is described in detail in this document. It is based on the exploitation of the differential absorption of water vapour in the near infrared, as measured by MERIS bands 14 and 15. The algorithm builds on previous developments at

FUB and provides the total columnar water vapour over cloud free land, sea ice and sun glint regions. The output is used for the generation of gridded L3 products, namely daily composites and monthly means, in combination with SSM/I observations above ocean.