DUE GLOBVAPOUR

Algorithm Theoretical Basis Document
L2 SSM/I and MWR

Issue 1 Revision 0

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1 Introduction

1.1 Purpose

This document provides the Algorithm Theoretical Basis of the Level 2 SSM/I total column water vapour product for the ESA DUE GlobVapour project. Some text passages were adopted from the below listed documents, e.g. NWP SAF User Guide, the ATBD of water vapour products of CM SAF, etc.

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

1.2 Definitions, acronyms and abbreviations

AMSU	Advanced Microwave Sounding Unit
ATBD	Algorithm Theoretical Basis Document
DMSP	Defense Meteorological Satellite Programme
DWD	Deutscher Wetterdienst
L1	Level 1
L2	Level 2
L3	Level 3
MWR	Microwave Radiometer
NWP SAF	Satellite Application Facility Numerical Weather Prediction
RTM	Radiative Transfer Model
RTTOV	Name of a Radiative Transfer Model
SSM/I	Special Sensor Microwave/Imager
SSMIS	Special Sensor Microwave Imager and Sounder
TCWV	Total Column Water Vapour
WACMOS	Water Cycle Multimission Observation Strategy

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, iss. 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] DUE GLOBVAPOUR Algorithm Theoretical Basis Document (ATBD) for L2 MERIS, issue 1, revision 0, dated 29 October 2010.

[RD-2] DUE GLOBVAPOUR Algorithm Theoretical Basis Document (ATBD) for L3 SSM/I+MERIS, issue 1, revision 0, dated 29 October 2010.

[RD-3] Andersson, A., C. Klepp, K. Fennig, S. Bakan, H. Grassl, and J. Schulz, 2009: The HOAPS climatology: Essential water cycle components over global oceans derived from satellite data. Accepted by J. Appl. Met. Clim.

[RD-4] CM SAF, 2009: ATBD for Total Column Water Vapour Retrieval from SSM/I, SAF/CM/DWD/ATBD/HTW_SSMI, 6 January 2009.

[RD-5] Deblonde G., 2001: NWP SAF User's Guide: Standalone 1D-var scheme for the SSM/I, SSMIS and AMSU., NWPSAF-MO-UD-001 Version 1.0, 22 August 2001.

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[RD-13] Press W.H., Flannery B.P., Teukolsky S.A. & Vetterling W.T., 1989: Numerical Recipes in Pascal; The Art of Scientific Computing Cambridge University Press, Cambridge

[RD-14] Saunders, R., Matricardi, M., and Geer, A., 2008: RTTOV 9.1 Users Guide, NWP SAF report, Met. Office, 57 pp.

[RD-15] Rodgers, C. D., 1976: Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation, Rev. Geophys., 14(4), 609–624.

[RD-16] Tarantola, A., and B. Valette, 1982: Generalized nonlinear inverse problems solved using the least squares criterion, Rev. Geophys., 20(2), 219–232

1.5 Structure of the document

Section 2 gives a short overview of algorithms used, illustrated with the processing flow. The algorithm description occurs in section 3, where all theoretical and practical important steps of the algorithm will be explained in detail. Assumptions and limitations can be found in section 4. The conclusion is written in section 5.

2 Algorithm overview

The core of the algorithm used to derive total column water vapour from SSM/I as well as MWR observations is based on a 1D-Var scheme developed at ECMWF by Phalippou (1996). The scheme was initially build for the SSMIS microwave imager/sounder and AMSU. It was further extended to be a stand-alone scheme applicable to SSM/I, SSMIS and AMSU (Deblonde, 2001). The actual utilisation of the scheme is given in Deblonde (2001).

Within the GlobVapour project, the total integrated column water vapour (TCWV) is derived from brightness temperatures of SSM/I over ice-free ocean using the mentioned scheme. The best estimate of the atmospheric state, composed of atmospheric temperature and moisture as well as surface variables temperature and wind speed, is determined by an iterative adjustment of the state vector to match the simulated satellite radiances with the measurements. The term best estimated refers to the optimal estimation theory and describes the state that is most likely considering the errors in the background information and in the measurements. This methodology also enables the provision of a retrieval error.

In practical application the 1D-Var scheme uses ERA-Interim atmospheric and surface fields as background information and inter-calibrated and homogenized SSM/I brightness temperatures (level 2) from various DMSP satellites.

The preparation of the combined SSM/I+MERIS product using the swath-based L2 retrieval data from MERIS and SSM/I is documented in the GlobVapour ATBD for L3 SSM/I+MERIS products.

The retrieval scheme was further implemented to make use of the microwave observations measured with the MWR on-board the ENVISAT satellite. The MWR retrieval code underwent only small adaptations which are described at the end of section 3.

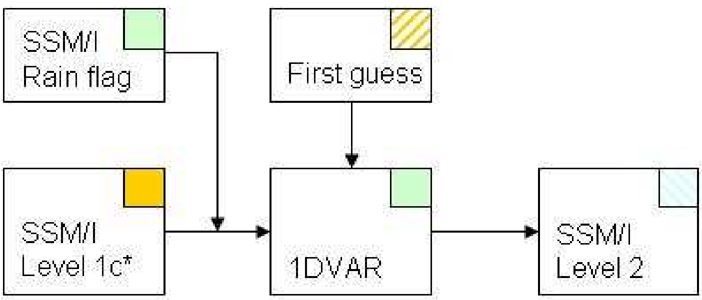

Figure 1: Flow chart of the SSM/I processor. Input data is marked orange (orange shaded: higher level input data), products are marked blue (blue shaded: instantaneous level 2 products) and software development is marked green. The MWR processor follows the same construction.

3 Algorithm description

3.1 Theoretical description

SSM/I (Special Sensor Microwave Imager)

The SSM/I is a conical scanner with a scan angle (satellite view angle with respect to nadir) of ~45° which corresponds to an earth incidence angle of ~53°. The altitude is ~833 km. All channels have dual polarisation except the 22 GHz channel (see Table 1). The first SSM/I instrument was onboard the F08 of the DMSP (Defence Military Satellite Project), launched in 1987. The last one was sent onboard the F15. The L2 end product is supposed to consist of combined data from the satellites F13, F14 and F15.

Table 1: Spectral characteristics of the SSM/I instruments aboard the DMSP satellites.

Central Frequency (GHz)	First Sideband (GHz)	Half-bandwidth (MHz)	Polarization	Ground resolution* (km)	NeΔT (K)
19.35	0.13	120	V,H	70 x 45	0.8
22.235	0.13	120	V	60 x 40	0.8
37.0	0.55	450	V,H	38 x 30	0.6
85.5	0.8	700	V,H	16 x 14	1.1

*The ground resolution is based on the 3dB antenna footprint and the integration time of ~8 ms.

MWR (Microwave Radiometer)

The MWR principal duty is the measurement of 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. The MWR instrument on board Envisat is a derivative of the radiometers used on the ERS-1 and ERS-2 satellites. It is a dual-channel nadir-pointing Dicke-type radiometer, operating at frequencies of 23.8 and 36.5 GHz (ESA Earthnet, 2010).

Radiative Transfer

The following section about radiative transfer was adopted from CM SAFs ATBD of water vapour products.

The radiative transfer is approximated by the following equation (1):

$$I_\nu = \epsilon_\nu B_\nu(T_s)\tau_\nu^* + \int_{p_s}^{0} B_\nu(T)\frac{\partial \tau_\nu}{\partial p}dp + (1-\epsilon_\nu)\tau_\nu^* \int_{0}^{p_s} B_\nu(T)\frac{\partial \tau_\nu}{\partial p}dp \qquad (1)$$

where ν is frequency, T is temperature, T_s is surface temperature, ε_ν is surface emissivity, B_ν is the Planck function, p is pressure, p_s is surface pressure, τ_ν is transmission and τ_ν* is total atmospheric transmission. The three right-hand terms may be interpreted as follows:

- the first term gives the proportion of surface emission at temperature T_s and emissivity ε_ν, transmitted through the atmosphere with transmissivity τ_ν*.
- the second term describes the upwelling emitted radiation of the atmosphere integrated from the surface to the top (in pressure coordinates). The emission $B_\nu(T)$ is weighted by the vertical derivative of transmission as function of atmospheric pressure.
- the last term describes the downwelling atmospheric radiation that is reflected at the surface with the reflectivity 1-ε_ν and transmitted through the atmosphere with the total transmissivity τ_ν*. Note that for this, it has been assumed that $\varepsilon_\nu + \rho_\nu = 1$, i.e. the penetration depth of radiation for the SSM/I channel wavelengths has been set to zero which is a reasonable approximation.

The solution of the radiative transfer equation in the microwave part of the spectrum requires a description of the transmission of the atmosphere and the quantification of the surface emission. As the atmospheric transmissivity is concerned, water vapour and oxygen are – apart from hydrosols – the relevant absorbers as is shown in Figure for the spectral range of SSM/I observations. The extinction coefficients at varying atmospheric conditions have been fully described by Liebe (1985).

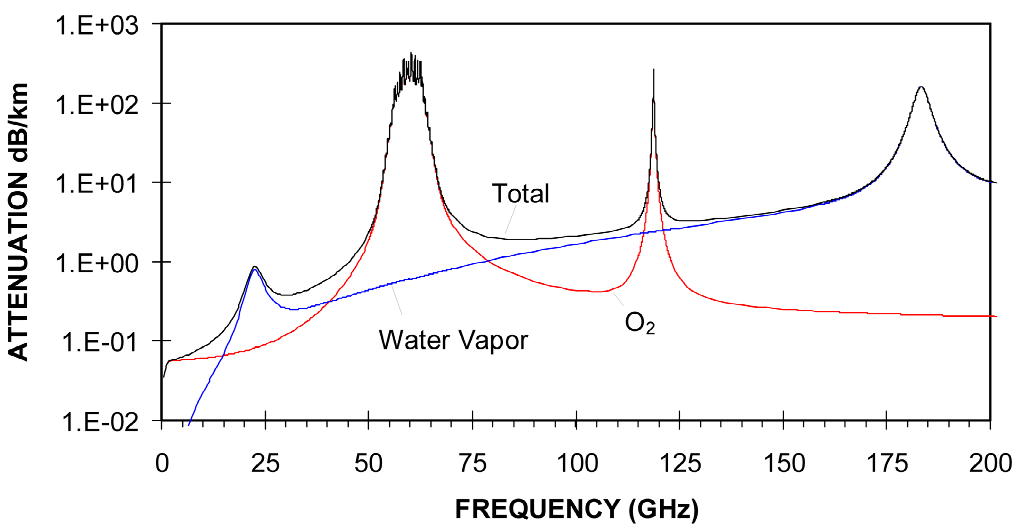

Figure 2: Microwave attenuation of water vapour and oxygen (after Liebe, 1985).

Hydrometeors do also affect the atmospheric transmissivity by scattering. As this process is not covered by the radiative transfer model (RTM) applied for the retrieval of total column water vapour, atmospheric conditions including heavy rain have to be filtered out prior to the application of the algorithm.

The SSM/I 1D-Var retrieval scheme

This section largely follows the outline in NWP SAF User Guide and Deblonde (2001).

The SSM/I 1D-Var solves for atmospheric temperature, atmospheric water vapour, oceanic surface wind speed and either liquid water path or total water content. The scheme requires as input atmospheric profiles (background profiles) that are spatially and temporally collocated with the satellite observations and returns solution profiles that optimally fit both the observations and the background profiles. The optimal fit is determined by the relative weight of the background error covariances and the observation errors. The forward model (here the radiative transfer model) is RTTOV6.7 modified so that SSMIS, SSM/I and AMSU brightness temperatures and their Jacobians can be computed. The fast emissivity ocean model Fastem Version 2.0 (Deblonde and English, 2001, English and Hewison, 1998) is used. This model has been included in RTTOV versions 7 and onwards.

Variational Assimilation Technique

A variational retrieval is applied in which the a priori or background information of the atmosphere and surface (x^b), and the measurements y^o (observed brightness temperatures) are combined in a statistically optimal way (with a Bayesian analysis) to estimate the most probable atmospheric state x. The approach is common to a number of areas where non-linear inverse problems are encountered and has been described in detail by many authors (e.g. Rodgers, 1976, Tarantola and Valette, 1982, Lorenc, 1986). Gaussian error distributions are assumed and consequently, obtaining the most probable state is equivalent to minimising a cost function $J(x)$ also referred to as a penalty function. Following the notation of Ide et al. (1997), $J(x)$ may be written as:

$$J(x) = \frac{1}{2}(x - x^b)^T B^{-1}(x - x^b) + \frac{1}{2}[y^o - H(x)]^T (E + F)^{-1}[y^o - H(x)] + J_s \qquad (0.1)$$

where B, E and F are respectively, the background, the instrumental, and the representativeness (includes errors of the forward model) error covariance matrices. J_s is a cubic function that limits the supersaturation and acts as a weak constraint (Phalippou 1996):

$$J_s = a(x - x_s)^3 \qquad (0.2)$$

x_s is the value of the control variable at saturation. $H(x)$ is the forward operator that maps the control vector x into measurement space. Here $H(x)$ is the radiative transfer model RTTOV6.7. The superscripts T and –1 denote matrix transpose and inverse respectively.

The control vector x consists of temperature (at 43 fixed pressure levels defined by the radiative transfer model), the natural logarithm of specific humidity (defined for the lowest 19 levels of the radiative transfer model) and the oceanic surface wind speed. Optionally, the liquid water path (LWP) defined below can also be added to the control vector.

$$LWP = \frac{1}{g}\int_0^{P_s} q_L(P)dP \qquad (0.3)$$

where g is the gravitational constant, P_s is the surface pressure and q_L is the cloud liquid water content ($kgkg^{-1}$).

If LWP is not chosen as a control variable, then one solves for the natural logarithm of total water content. The total water content is defined as follows:

$$q_{total}(P) = q(P) + q_L(P) \qquad (0.4)$$

where q is the specific humidity ($kgkg^{-1}$).

In general, the minimum of the cost function can be found by the iterative solution of (Newtonian iteration):

$$J''(x_n)(x_{n+1} - x_n) = -J'(x_n) \qquad (0.5)$$

and

$$J'(x_n) \rightarrow 0 . \qquad (0.6)$$

x_n and x_{n+1} are the n^{th} and $(n+1)^{th}$ approximation of x, J' and J'' are the first and second derivatives of the cost function with respect to x. These are given by:

$$J'(x_n) = B^{-1}(x_n - x^b) - H'(x_n)^T (E+F)^{-1}(y^o - H(x_n)) \quad (0.7)$$

where $H'(x_n)$ is the Jacobian matrix and contains the partial derivatives of $H(x)$ with respect to x. In the linear limit,

$$J''(x_n) = B^{-1} + H'(x_n)^T (E+F)^{-1} H'(x_n) = A^{-1} \quad (0.8)$$

where A is the error covariance matrix of the solution if $H(x)$ is linear. $J''(x_n)$ is also referred to as the Hessian of the cost function. A is also called the analysis error covariance matrix and in this document A will be referred to as the theoretical error.

Accounting for clouds

To properly account for the absorption of cloud particle in the retrieval system, the liquid water path (*LWP*) is included in the state vector. Thus the control vector consists of the profile of natural logarithm of specific humidity (lnq), the oceanic surface wind speed (SWS) and the liquid water path. Thus x=(lnq, SWS, LWP).

During the minimisation process of Eq. (0.1), LWP is allowed to vary while the cloud structure S(P) is maintained fixed. The cloud structure S(P) is defined as follows.

$$S(P) = q_L(P)/LWP \quad (0.9)$$

with $q_L(P)$ as the profile of cloud liquid water. If there is a cloud in the background profile, then S(P) is given by:

$$S(P) = q_{LB}(P)/LWP_B \quad (0.10)$$

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

If there is no cloud in the background profile, then a non-zero cloud structure is generated where the relative humidity of the background profile exceeds a pre-set threshold value (e.g. 80%). If there is still no cloud, then a non-zero cloud structure is assigned to the lowest levels of the profile. In all cases, the first guess LWP is set to 0.1 kgm^{-2}.

The inclusion of the LWP in the state vector allows the retrieval to converge and retrieved meaningful water vapour values in the presence of cloud.

An alternative option is to retrieved the total water content instead of cloud liquid water and water vapour separately which follows closely the same concept as that developed in Blankenship et al. (2000). After each iteration step the total water content, as included in the control vector is spilt into the liquid and vapour part to be able to calculate the Jacobians with RTTOV. This option has not been tested within the GlobVapour project. The reader is referred to Deblonde (2001) for further details on both options.

<u>Minimization technique</u>

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

3.2 Practical application

The 1D-Var scheme was implemented at DWD, including the procedure of adjustment of the corresponding interfaces. The main task here was the development of an interface software that provides first guess data to the 1D-Var. This contains the collocation of the SSM/I and MWR observations and background data. Therefore, a tool was implemented into the 1D-Var to choose between ERA-Interim forecast data and climatologies as background data. The 1D-Var was modified to read input files in netCDF format and to write data in updated GlobVapour metadata information in netCDF format following the CF-1.4 standard.

L1 data source

SSM/I Level 1C data, including a homogenization with respect to F11 (Anderson, 2010), is utilized in the applied 1D-Var. The statistical approach utilizes SSM/I on F11 as reference and is described in and Andersson et al. (2009). The Level 1 data set provides SSM/I swath-based information for brightness temperatures on four frequencies and for horizontal and vertical polarizations including additional information (see Table 2-1).

First guess input

The 1D-Var has to be filled with a first guess information. Therefore, the use of ERA-Interim forecast data has been established within the GlobVapour project. For each processed day one representative ERA-Interim data file is chosen. This background data is collocated with SSM/I footprints. The data contains the atmospheric profiles for temperature, specific humidity and liquid water content provided on pressure levels as well as the surface values for wind speed, temperature and pressure.

As a second option, climatological profiles can be chosen as background. However, the correspondingly large background errors might not be well represented in the currently used background error covariance matrix.

SSM/I rain flag

The 1D-Var is only applied in non-precipitating scenes which is filtered using an internal scattering index module which rejects cases with strong scattering suggesting large particle of rain or ice. This step is necessary since scattering is not accounted for in the radiative transfer model.

Spatial coverage

Furthermore, the algorithm is only applied to footprints completely filled with ocean surfaces. Land and ice surfaces are not processed due to difficulties in the provision of proper surface emissivities. Also, footprints with contributions from coastal regions will be omitted. The spatial resolution is approximately 60 km.

Quality Control

A quality flag exists in the SSMI/I 1D-Var output. The data are marked by following parameters: default (99), data not in valid range (0), good value (1) and data not above sea surface or brightness temperature is not correct (2).

The pixel-based quality check is applied within the 1D-Var. The valild range for TCWV is set to 0.1 to 90 kg/m^2. Retrieved values exceeding the threshold are blacklisted by setting the quality flag to 0.

L2 data output

The Level 2 data set provides swath-based global information for each day. It contains the retrieved data of the total column water vapour, the background equivalent, and the corresponding retrieval error. All values are given in kg/m^2. Some additional data, as for example q quality flag, is also a standard L2 output.

Adaptation for ENVISAT MWR

The same 1D-Var framework has been adjusted to enable the retrieval of TCWV from the microwave radiometer (MWR) on-board the ENVISAT satellite. The major adjustment made a listed in the following:

- Defining MWR as satellite instrument in RTTOV.
- Composing the absorption coefficient file to be used as input for RTTOV (Collection of the Instrument characteristics for the MWR, e.g. central wavelength, bandwidth, polarization, etc.).
- Defining MWR as one input option in the 1D-Var which consisted of some minor but numerous code changes.

However, some difficulties occur within the practical application. Due to the nadir-only looking nature of the instrument and its spectral characteristics, no scattering signal can be observed. For this reason and since the instrument has only two channels, no scattering index can be calculated, thus no rain and/or ice cases can be filtered out.

Further, no ice mask is provided in the L1 data. Retrieval results in regions with potential sea-ice coverage will be subject to increased errors. As temporary solution the ice mask from SSMI measurements is collocated to the MWR footprints. However, this is only been done with a time resolution of one month.

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 is a factor of 10 lower than the horizontal resolution of the MERIS product $(0.05°)^2$ over land. This still meets the Requirements Baseline (AD-1), and the spatial resolutions over land and over ocean perfectly match.

An aspect that has not been analysed in detail within this project and elsewhere is the impact of background uncertainties on retrieval quality. This issue should be tackled in future assessments of satellite (climate) products.

5 Conclusions

A 1D-Var retrieval scheme, which is based on Deblonde (2001), has been implemented at DWD within the ESA DUE GlobVapour project. The scheme is used to retrieve total columnar water vapour (TCWV) using microwave satellite radiances. It can be applied to ice-free oceans. The derived TCWV is an optimal estimate considering the provided background information and the satellite measurements with their associated errors. The derived TCWV values are on L2 satellite swath resolution. The TCWV quality is estimated to be of high standard.

Some further improvements might be able with respect to the background error covariance matrix, the scattering index used as rain flag, and some tuning of the bias correction and observation errors.

The L2 TCWV products are used to compose a combined L3 product in conjunction with MERIS VIS/NIR TCWV retrieval over land and coastal regions.