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**EUMETSAT TOTAL PRECIPITABLE WATER ALGORITHM FOR THE
POLAR SYSTEM – SECOND GENERATION (EPS-SG)
VISIBLE/INFRARED IMAGER (METImage)**

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Abstract

Total precipitable water (TPW) products from the EPS-SG Visible and Infra-red Imager (METImage) will be retrieved and disseminated by EUMETSAT. We present the METImage “Day 1” TPW operational algorithm, which is based on measurements of reflected sunlight in the water vapour absorption band centred at $\sim 0.91\mu\text{m}$ compared to measurements in the nearby visible/NIR atmospheric window bands ($\sim 0.55\text{--}1.24\mu\text{m}$). While having strong heritage from MERIS/MODIS algorithms, the approach chosen for METImage presents several innovative features, such as a full 1D-Var approach and a ‘real-time’ modelling of the variable atmospheric status and solar/satellite geometries using a fast RTM. Preliminary results of the algorithm prototype using synthetic METImage and MODIS data are presented.

INTRODUCTION

The current EUMETSAT Polar System (EPS) will end in the time frame after 2020, requiring a follow-on programme, the so-called EPS Second Generation (EPS-SG), to be in place by then to continue operational meteorological measurements from polar orbiting satellites in the mid-morning orbit. The METImage instrument, developed by the German space agency (DLR), will fly as a payload on the Metop Second Generation (Metop-SG) satellites to fulfil the objectives of a Visible Infrared Imaging (VII) observation mission [8]. METImage is a medium resolution, multi-spectral imager/radiometer capable of measuring thermal radiance emitted and sunlight reflected by the Earth in 20 channels ranging from $0.443\mu\text{m}$ up to $13.345\mu\text{m}$, from a low-altitude Sun synchronous orbit over a minimum swath width of 2700 km with a sampling of 500m at nadir. The primary objective of the METImage mission is to provide high quality imagery data for global and regional Numerical Weather Prediction (NWP) and Nowcasting (NWC) through the provision of, among others, high resolution water vapour imagery products, whose user requirements are summarized in Table 1.

Retrieved parameter	TPW in kg/m^2 (integrated humidity, no vertical resolution)
Accuracy	5%
Continuity	No (no previous product from Metop/AVHRR)
Horizontal resolution	Breakthrough: 3 km (6×6 pix), Objective: 1 km (2×2 pix)
Processing environment	Near Real Time & Reprocessing
Processing time	Within ~ 15 min from acquisition time
Coverage	Regional and Global
Basic scenarios	Clear scenes, Day & Twilight, All surface types, All seasons
Critical scenarios	Cloud/aerosol contamination, dark surfaces (e.g., ocean)

Table 1: User requirements for METImage Level 2 water vapour operational products [12].

EUMETSAT will implement two algorithms to retrieve total precipitable water (TPW) from the infrared (TPW-IR) and the visible (TPW-VIS) bands of METImage, respectively.

This paper focus on the TPW-VIS algorithm. Clear-sky water vapor (WV) measurements in the visible part of the spectrum are affected by the surface reflectance and the presence of aerosols in the atmosphere; METImage is suitable to perform such measurement because, in addition to the WV absorption channel centered at $\sim 0.91\mu\text{m}$, it is equipped with a number of channels sensitive to the surface reflection and the aerosol scattering (Table 2). Historically, this is the most used and accurate method in remote sensing of retrieving WV from space. The algorithm developed for METImage has heritage from the MERIS [6], MODIS [1], and MTG/SEVIRI GII algorithm [5]. However, the approach chosen for METImage presents several innovative features, such as a full 1D-Var approach and a 'real-time' modelling of the variable atmospheric status and solar/satellite geometries using a fast RTM.

Channel Name	Channel ID	λ (μm)	FWHM (μm)	Comments
VII-4	1	0.443	0.03	Atmospheric window band (aerosol scattering)
VII-8	2	0.555	0.02	Atmospheric window band (aerosol scattering)
VII-12	3	0.668	0.02	Atmospheric window band (aerosol scattering)
VII-15	4	0.752	0.01	Continuum narrow-band near O ₂ A-band (aerosol scattering)
VII-16	5	0.763	0.01	O ₂ A-band (aerosol scattering)
VII-17	6	0.865	0.02	Atmospheric window band (surface reflection)
VII-20	7	0.914	0.02	WV absorption band
VII-22	8	1.240	0.02	Atmospheric window band (surface reflection)

Table 2: METImage spectral channels used by the TPW-VIS algorithm.

THE TPW-VIS ALGORITHM

The basic principle of the TPW-VIS algorithm is the comparison of the radiance measured in the WV absorption band centred at $\sim 0.91\mu\text{m}$ to close by bands with no or few absorption features (Table 2). Under the assumption of zero path radiance (no atmospheric scattering) and zero gaseous absorption in the out-of-band channels, the reflectance difference is directly attributable to the WV absorption/transmittance in the in-band channel ([6], [1]). Because these assumptions are not strictly met in practice, the observed reflectances must be related to TPW via RTM simulations that include scattering and absorption in all bands. The WV transmittance is modelled including atmospheric scattering and the influence of the temperature ($T(p)$) and pressure (p) profile on the absorption line; critical factors affecting the WV retrieval from the VIS/near-IR (i.e., aerosols and surface reflectance) are taken into account. The 1D-Var approach is used to retrieve the WV profile ($Q(p)$), the surface Bidirectional Reflectance Distribution Function (BRDF), and (in the future) the aerosol optical depth (AOD) as a function of the measured reflectances (ρ), with prior information obtained from the forecast for $Q(p)$ and auxiliary database daily or weekly updated for the BRDF and AOD. The forward model is RTTOV in version 11.2 or higher [4], which is able to simulate the top of atmosphere radiances in VIS/near-IR channels for the given profile of temperature/humidity as well as aerosols loading. The TPW is determined by integrating the solution $Q(p)$ between the surface pressure and the top of the atmosphere. The TPW-VIS retrieval scheme is implemented using a full 1D-Var approach whose processing steps are shown in Figure 1. The maximum probability solution (i.e., the final state vector x) is found by (equivalently) minimizing the cost function J given by:

$$J(x) = [F(x) - y]^T \cdot [F(x) - y] + (x - x_a)^T \cdot S_a^{-1} \cdot (x - x_a)$$

The 1D-Var parameter setting is still under optimization and we report here the set-up of the current in-house prototype algorithm, highlighting future improvements/updates:

- The measurement vector (y) consists of up to four reflectances to effectively provide information on TPW ($0.91\mu\text{m}$), surface BRDF ($0.86\text{-}1.24\mu\text{m}$ for interpolation to $0.91\mu\text{m}$) and potentially aerosol loading ($0.44\text{-}0.7\mu\text{m}$). However, how they are technically represented and whether additional measurements in other channels may improve the retrieval is still to be defined, and several possibilities will be explored/tested:

$y = [0.4\text{-}0.7\mu\text{m}, 0.86\mu\text{m}, 0.914\mu\text{m}, 1.24\mu\text{m}]$ or combination (e.g., ratios)

The effect of different definition does not fundamentally change the information content of the measurements but can potentially change the linearity of the problem and/or simplify the definition of the associated error covariance. A reflectance ratio or difference, for example, can eliminate partially or otherwise a source of error common to both channels (e.g., an undefined aerosol scattering contribution). Moreover, both two-channel and three-channel ratios may be used depending on the surface type to optimize the algorithm for land/sea surfaces [1].

- The covariance matrix S_y contains the uncertainty on the measurement data (i.e., instrument noise and channel co-registration error). No bias and RTM errors (i.e., inaccuracies in the RTM simulations due to errors in fixed model parameters such as forecast temperature profiles, etc.) are considered in the current prototype, although the scheme allows for their inclusion. S_y is assumed to be diagonal (i.e., errors in different channels are uncorrelated).
- The state vector x contains the parameters to be retrieved, i.e., $Q(p)$ and more or fewer elements of the channel surface BRDF and in the future AOD (not yet included in the current prototype). As for the measurement vector, the final form of the state vector is still to be defined. The most intuitive definitions are:

$$x = [Q(p), \text{BRDF}(\lambda), \text{AOD}(\lambda)] \text{ over land}$$

$$x = [Q(p), \text{BRDF}(\lambda) \text{ or wind speed}, \text{AOD}(\lambda)] \text{ over ocean}$$

- The *a priori* state vector x_a and the covariance matrix S_a contain the prior values of the parameters to be retrieved and the covariance of their errors, respectively. This information can be effectively disregarded downweighted (if required) by assuming very large values for S_a . Whether to use it or not within the TPW-VIS retrieval will be established during the algorithm testing. In the current prototype the prior value for $Q(p)$ is derived from the ECMWF forecast [7], the prior BRDF is obtained from the MODIS MCD43A1 products over land and from RTTOV simulations [3] over ocean using the ECMWF forecast wind speed, and the prior AOD from the ECMWF/MACC database [2]. The covariance matrix S_a is constructed using static NWP error standard deviation for $Q(p)$ (to be potentially replaced by the flow-dependent ECMWF/Ensemble Long-Window data assimilation in the operational algorithm), MCD43A1 uncertainty for land BRDF (~10%), and an empirical uncertainty for ocean BRDF (~100%) estimated over glint areas using the forecast wind speed error. Errors on $Q(p)$ /BRDF are assumed to be uncorrelated, BRDF errors at 0.86 and 1.24 μm 70% correlated. AOD errors are not yet included in the prototype;
- $F(x)$ is the forward model which calculates the expected measurements corresponding to the current state vector x . $F(x)$ is computed at each iteration by RTTOV, which is capable of simulating reflectances in the METimage channels of interest for the specific viewing geometry and auxiliary information (such as surface type, surface pressure and temperature, atmospheric temperature profile, etc.) and for varying WV profile, surface BRDF and AOD. RTTOV provides also the gradient (Jacobian matrix K) quantifying the change of simulated reflectances due to a change in $Q(p)$, BRDF and AOD. It shall be noted that RTTOV simulations are performed in 'real-time'. The advantage of this approach is that the best available auxiliary information (e.g., atmospheric temperature, vertical WV profile and potentially aerosol loading) is introduced and directly accounted for, thus avoiding the implicit errors that climatological assumptions affecting other RTM methods (e.g., look-up tables) would give, while maintaining a processing speed suitable for an operational algorithm.

The state vector x is adjusted iteratively to find optimal (statistically) values with respect to the measurements and the prior using the Levenberg-Marquardt (LM) minimization method [10]. The minimisation is assumed achieved when the cost J is lower than a pre-determined threshold or the rate of change of J becomes acceptably small. The minimization procedure is also terminate if a maximum number of allowed iterations is reached. If the convergence criteria are met, the solution covariance matrix S_x describing the uncertainty to be associated with the retrieved state parameters is calculated:

$$S_x = (S_a^{-1} + K^T \cdot S_y^{-1} \cdot K)^{-1}$$

The TPW is determined by integrating the retrieved WV profile $Q(p)$ over all pressure levels between the surface pressure (p_{surf}) and the top of the atmosphere (p_{toa}):

$$TPW = \frac{1}{g} \sum_{i=p_{\text{surf}}}^{p_{\text{toa}}} \overline{Q(p_i)} \cdot \Delta p_i$$

where g is the Earth gravitational acceleration, $\overline{Q(p_i)}$ is the average humidity and Δp_i the pressure difference in the layer defined by each pair of levels. The uncertainty to be associated to the TPW is obtained from the elements of S_x corresponding to $Q(p)$:

$$err_TPW = \frac{1}{g} \cdot \sqrt{(\delta p) \cdot S_x(Q(p)) \cdot (\delta p)^T}$$

where δp contains the pressure difference between each pair of consecutive levels in the WV profile.

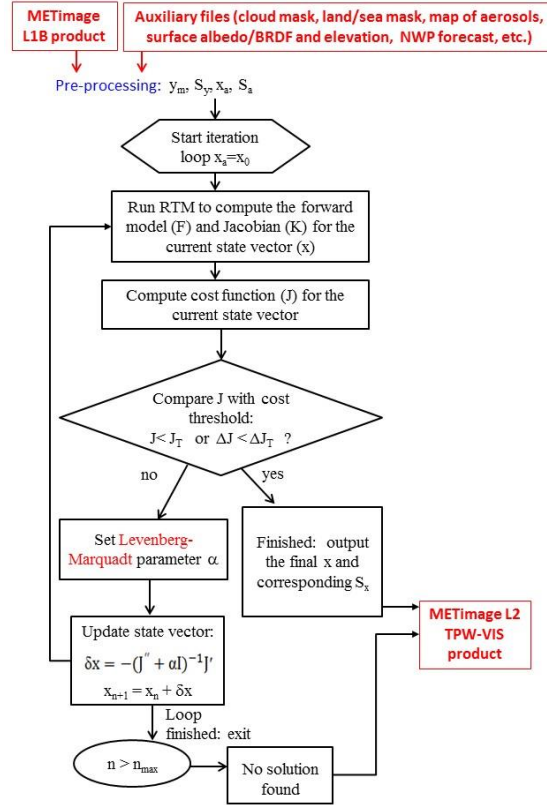


Figure 1: Flow diagram of TPW-VIS algorithm for METImage.

TEST RETRIEVAL USING METIMAGE SIMULATED DATA

The TPW-VIS algorithm has been first applied to in-house simulated METImage radiances. This exercise offers the advantage to have of the full knowledge of the true surface and atmospheric parameters and, hence, test the algorithm performance is an ideal case.

METImage radiances were simulated using the geolocation and geometry of an AVHRR granule acquired on the 12 Sept 2007 at 8:43 AM and the closest ECMWF forecast atmospheric profiles (12 Sept 2007 9:00 AM) and surface BRDF (MCD43A1, 5 Sept 2007). The granule covers 4200×3144 pixel locations over central Europe (Figure 2), including land, dark ocean and Sun glint areas. Radiance in the METImage channels were simulated using RTTOV v11.2 assuming cloud-free situations, no contamination by atmospheric aerosols, and taking into account the current specifications of the instrument noise model (i.e., shot noise model [9], channel co-registration errors ~6% and inhomogeneity noise ~0.5%). The retrieval was then performed introducing controlled errors on the prior information with respect to the true values used in the simulations:

- Two test retrievals were performed using an input prior forecast obtained 3h and 9h later than the true forecast, respectively. This time-shift in the forecast affects both the $Q(p)$ and ocean BRDF retrieval, because this last is estimated by RTTOV using the forecast wind speed;
- The prior land BRDF was shifted 1 pixel with respect to the true BRDF used in the simulations to effectively mimic a ~10% error.

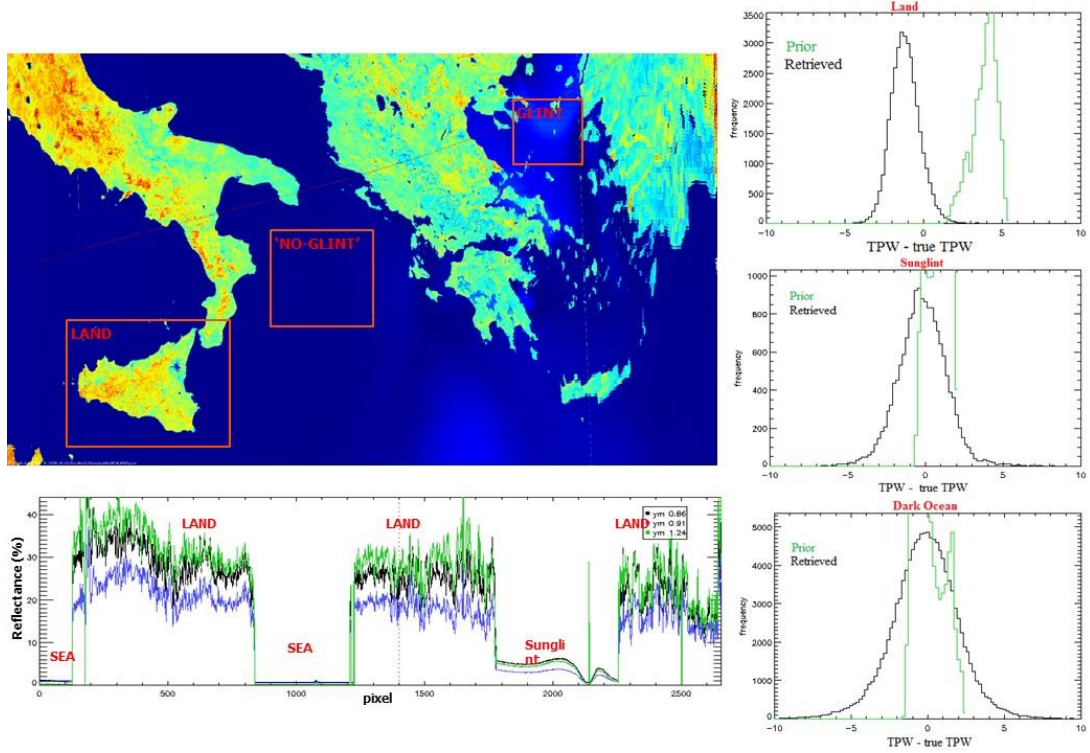


Figure 2: Simulated METImage clear-sky radiance image at 0.86μm (top-left) and corresponding plot along a line (bottom-left). Right panels: histogram of the difference between the TPW and the true TPW used in the simulations for land, Sun glint and dark ocean areas.

The algorithm performance was quantified using the following diagnostic parameters:

- Rate of convergence (conv_rate);
- Average number of iterations before convergence (N_{iter});
- Average solution cost (J);
- Measurement residuals Δy (i.e., difference between measurement radiances and simulated radiance at last iteration);
- Errors on the retrieved parameters with respect to the prior errors;
- Degree of freedom for signal (d_s) and noise (d_n) and information content (IC) of the retrieval defined according the theory of the inverse method [11]:

$$d_s = \text{trace}[S_x \cdot (K^T S_y^{-1} K)], d_n = \text{trace}(S_x \cdot S_a^{-1}), IC = -\frac{1}{2} \cdot \ln(S_x \cdot S_a^{-1})$$

It shall be noted that in the current 1D-Var set-up, the state vector x contains 56 elements (WV values for 54 pressure levels and surface BRDF values in 2 window channels), while the measurement vector y contains 2 measurements in 2 window channels and 1 measurement in the WV channel. Thus, d_s is expected to be no better than ~ 1 for TPW and ~ 2 for the surface BRDF, while the rest of the degrees of freedom goes to noise (i.e., $d_n \sim 43$ for TPW and ~ 0 for BRDF).

The diagnostic parameters for the two test retrievals described above are summarized in Table 3. Based on these numbers, we can conclude that over bright surface (i.e., land surfaces and Sun glint areas) and under the assumption of clear-sky and no aerosol contamination, the current set-up of the algorithm performs as expected and, in particular:

- Results are independent from the quality of the prior forecast (i.e., no significant difference is seen in the retrieval when the prior forecast is degraded with a delay of 3h to 9h with respect to the truth);
- The converge rate is always very high ($>90\%$);
- The solution cost is always low (<2);
- The measurement residuals are always very low ($<1\%$ of signal);
- Values of d_s and d_n for both TPW and BRDF are very close to the expected maximum values, and IC values shows that the retrieval is improving the knowledge of the truth with respect to the prior;
- The error on the retrieved parameter (both TPW and BRDF) are significantly improved (by a factor always >5) with respect to the prior errors;

- The average number of iterations to obtain convergence is reasonably small (~3 on the average) and this ensures a fast processing time, which is a crucial point for an operational algorithm.
- On the other hand, the algorithm performance over dark ocean is not promising, as expected because of the low measured signal (Figure 2), an issue known to affect other analogous algorithms such as those developed for MODIS and MERIS ([1], [6]). Our test retrieval over dark ocean shows that:
- The performance of the retrieval strongly depends on the quality of the prior forecast. Indeed, the converge rate drops from 30% to 0% when the prior forecast is degraded with a delay of 3h to 9h with respect to the truth (i.e., the retrieval is not even possible if the input forecast is significantly different than the true atmospheric status at the moment of observation);
 - In case of convergence, the average solution cost (<2) and residuals (<1%) are still low but more iterations (>5) are required, and this implies a longer processing time;
 - In case of convergence, the d_s , d_n , and IC for both the TPW and the BRDF are much lower than the land/Sunglint case and not significant within the errors (i.e., the retrieval is not improving the knowledge of the truth with respect to the prior).

	Land	Glint	Dark ocean
<i>Test 1 (prior forecast 3h shifted and prior BRDF 10% shifted with respect to truth)</i>			
conv_rate	99%	90%	30%
Average N_{iter}	3	3	5
Average J	1.37	0.53	1.23
Average Δy (in the range 0.86-1.25 μm)	<1%	<1%	<10%
Average prior error TPW / retrieved error TPW	9.3	6	1.5
d_s (TPW)	1.00 $\pm$ 0.02	0.98 $\pm$ 0.01	0.85 $\pm$ 0.20
d_n (TPW)	53.01 $\pm$ 0.05	53.04 $\pm$ 0.13	53.82 $\pm$ 0.45
IC(TPW) with respect to prior	2.88 $\pm$ 0.39	2.10 $\pm$ 0.54	2.58 $\pm$ 0.95
Average prior error BRDF/retrieved error BRDF	12*	30*	30*
Average d_s (BRDF)	1.96 $\pm$ 0.10	1.99 $\pm$ 0.01	1.84 $\pm$ 0.28
Average d_n (BRDF)	0.02 $\pm$ 0.11	0.01 $\pm$ 0.01	0.01 $\pm$ 0.01
Average IC(BRDF)	7.80 $\pm$ 0.53	5.52 $\pm$ 0.56	4.70 $\pm$ 0.14
<i>Test 2 (prior forecast 9h shifted and prior BRDF 10% shifted with respect to truth)</i>			
conv_rate	95%	90%	0%
Average N_{iter}	3	3	20 (max allowed)
Average J	1.57	1.06	NA
Average Δy	<1%	<1%	NA
Average prior error TPW / retrieved error TPW	9.2	5.7	NA
d_s (TPW)	0.99 $\pm$ 0.02	0.92 $\pm$ 0.17	NA
d_n (TPW)	53.01 $\pm$ 0.03	53.06 $\pm$ 0.14	NA
IC(TPW) with respect to prior	2.71 $\pm$ 0.34	1.83 $\pm$ 0.55	NA
Average prior error BRDF/retrieved error BRDF	12*	80 *	NA
Average d_s (BRDF)	1.95 $\pm$ 0.13	2.00 $\pm$ 0.01	NA
Average d_n (BRDF)	0.05 $\pm$ 0.14	0.00 $\pm$ 0.01	NA
Average IC(BRDF)	4.48 $\pm$ 0.73	4.32 $\pm$ 0.56	NA

Table 3: Diagnostics of TPW-VIS retrieval applied to METimage simulated radiances (*=value strongly dependent on our assumption for BRDF prior error).

TEST RETRIEVAL USING MODIS DATA

After assessing the algorithm performance with METimage simulated data, the TPW-VIS algorithm has been applied to radiance data obtained with MODIS. This exercise offers the advantage to test the algorithm in a real case, where observed radiances are likely to be contaminated by undetected clouds and atmospheric aerosol (which are not taken into account in the current algorithm set-up). Moreover, this test is valuable because the MODIS WV channel (centered at 0.905 μm) and the reference channels for BRDF (centered at 0.858 μm and 1.24 μm) are very similar to METimage's channels.

In order to allow a straightforward comparison with the retrieval performed on the simulated METimage data, we selected the MODIS/Terra radiance product acquired on the 12 Sept 2007 at 10:15 AM, i.e.,

more or less at the same time of our simulated METImage observations, and covering more or less the same area over central Europe (Figure 3). The granule covers 2030×1554 locations with a spatial resolution of 1 km (i.e., half of the METImage resolution) and was processed using the best available (i.e., closet in time) prior forecast (12 Sept 2007 9:00 AM) and surface BRDF (MCD43A1, 5 Sept 2007). The MODIS instrument noise model was taken into account in the set-up of the S_y matrix of the 1D-Var (i.e., shot noise model [13], channel co-registration errors ~12% and inhomogeneity noise ~1.5%).

The main conclusions of this test retrieval are as follows:

- As shown in Table 4, the diagnostics parameters confirm the algorithm behaviour over land, Sun glint and dark ocean established on the basis of METImage simulated data (Table 3);
- The diagnostic specifically calculated over (visually identified) cloud-contaminated areas (Table 4, last column) show that the algorithm is able to identify possible undetected cloud. Indeed, it is converging poorly over clouds (~30% of the cases only) and, when converging, both the retrieval cost (Figure 3) and measurement residuals (Table 4) are significantly higher than in clear-sky situations, allowing a flagging for anomalous algorithm behaviour;
- The comparison between the TPW retrieved by our TPW-VIS algorithm and the TPW obtained from the operational MODIS WV product (MOD05 L2 NIR TPW, 12 Sept 2007 at 10:15 AM) shows a good agreement, with no significant bias within the errors (Figure 3).

	Land	Glint	Dark ocean	Cloudy areas
conv_rate	99%	91%	44%	30%
Average N_{iter}	1	6	5	4
Average J	2.5	4.7	5.8	>10 up to 10^2
Average Δy	<1%	<1%	<6%	20-60%
Average prior/retrieved error (TPW)	4.8	4.1	4.3	5
d_s(TPW)	0.98±0.04	0.86±0.26	0.99±0.01	0.98±0.02
d_n(TPW)	53.19±0.05	53.12±0.26	53.02±0.01	53.00±0.02
IC(TPW) with respect to prior	1.84±0.53	1.38±0.55	1.80±0.38	2.60±0.38
Average prior/retrieved error (BRDF)	4.9*	8*	5*	2.9*
Average d_s(BRDF)	1.71±0.39	1.84±0.32	1.64±0.29	1.62±0.30
Average d_n(BRDF)	0.28±0.38	0.16±0.32	0.38±0.29	0.38±0.30
Average IC(BRDF)	2.61±0.80	3.42±1.24	2.09±0.45	2.09±0.65

Table 4: Diagnostics of TPW-VIS retrieval applied to MODIS radiances (*=value strongly dependent on our assumption for BRDF prior error).

CONCLUSIONS AND FUTURE DEVELOPMENTS

We have developed and tested the prototype of the METImage L2 operational algorithm for the retrieval of TPW using the 0.91 μ m water vapour absorption band and nearby visible window channels. The retrieval is based on a full 1D-Var approach and has been successfully applied to both METImage simulated radiances and MODIS radiances over land and Sun glint areas, while with the current set-up the performance is poor over dark ocean.

The algorithm development plan aims at tackling this last issue by optimizing the measurement vector (e.g., refining the channel selection, use of 2- and 3-channels reflectance ratios [1]) and state vector definition (e.g., use of wind speed over ocean, inclusion of aerosols, etc.). Moreover, the algorithm will be tested using the total column water vapor from the EPS-SG Microwave Sounder (MWS) as prior over ocean, to overcome forecast dependency.

Further algorithm developments include: i) the continuous update of measurement covariance matrix (S_y) following METImage development for performance modeling; ii) the error characterization and anomaly mitigation (e.g. residual cloud); iii) the algorithm validation; iv) the possible extension of the 1D-Var scheme to combine the use of METImage visible and near-IR water vapour absorption bands.

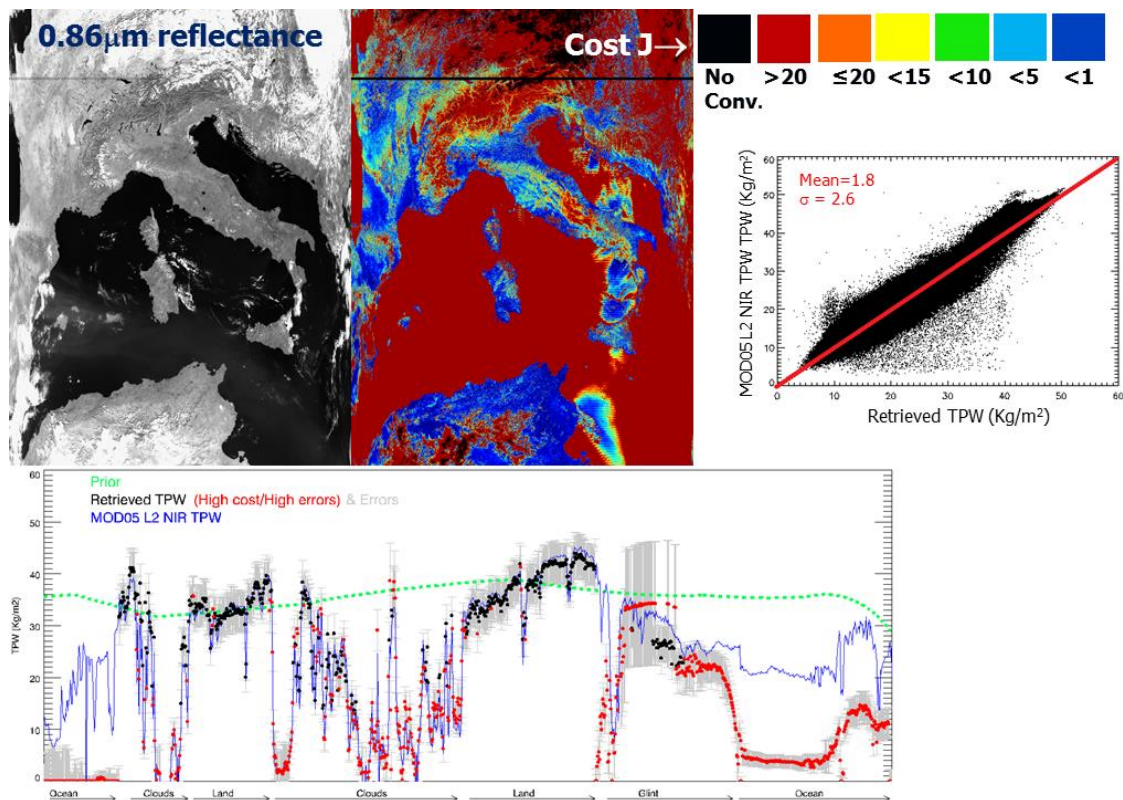


Figure 3: MODIS radiance image at 0.854μm (top-left) and corresponding map of solution cost (top-central). The bottom panel shows the retrieved TPW along a line compared to the forecast prior and the MOD05 L2 NIR TPW product. The top-right panel shows the same comparison for the full image.

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