

OCEAN COLOUR UNCERTAINTIES.

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Abstract - Uncertainty analysis is essential for the quality control and validation of satellite data. The results from two linked studies are presented: determining uncertainties for ocean colour products as part of the Sentinel-3 Level 2 Optical Prototype Processor development (O-L2PP); an investigation into the dependence of Envisat's Medium Resolution Imaging Spectrometer (MERIS) variability on sub-pixel variability.

Keywords: Marine, Radiometry, Space, Coast, Mapping, Oceans, Oceanography

INTRODUCTION

The Quality Assurance framework for Earth Observation (QA4EO), see <http://qa4eo.org/>, was established and endorsed by the Committee on Earth Observation Satellites (CEOS) as a direct response to a call from the Group on Earth Observations (GEO). It's suggested that data generators need to:

- Assign to all data / information products a Quality Indicator (QI), which allows stakeholders to unequivocally evaluate the products' suitability for a particular application.
- Provide a definition for each QI. This should be based on a quantitative assessment of its traceability to an agreed reference or measurement standard (ideally SI), but can be presented as numeric or a text descriptor, providing the quantitative linkage is defined.

The quantification of errors (difference between the value and best estimate of the "true" value of the measurand) therefore allows potential users to evaluate the products without having specialised knowledge. In addition, satellite products are increasingly assimilated into oceanographic numerical models and it's inappropriate for these users to assume the products have no error associated with them.

As well as quantifying the error coming from the sensor performance (Level 1 input) plus processing, it's important we recognised a pixel (spatial resolution from hundreds of metres to approximately 1km) will have spatial variability's within it. Therefore, when comparing satellite to in-situ biogeophysical products, uncertainties (dispersion of the

quantity values) will contain a mixture of this sub-pixel scale variability and satellite product quantifiable error.

SENTINEL-3 LEVEL 2 OPTICAL PROTOTYPE PROCESSOR DEVELOPMENT

The Sentinel-3 satellite, scheduled to launch in 2013, is the third in a series of five space missions within the European Global Monitoring for Environment and Security (GMES) programme. The programme is aimed at delivering environment and security monitoring services (covering areas such as climate change, sustainable development and environmental policies) that will be devoted to oceanography and land vegetation monitoring including fire detection and radiative power mapping. The mission aims to produce consistent long-term datasets with both an improved accuracy and reliability, and carries both an advanced radar altimeter and visible-infrared optical imaging instruments; this paper concentrates on the Ocean & Land Colour Instrument (OLCI), which is based on Envisat's MERIS instrument. Applicable Sentinel-3 user requirements were identified through surveys conducted within the relevant user groups: Operational and Institutional Oceanography Groups; Oceanographic Research Users; Land Users. In the long term a series of satellites, each designed for a lifetime of 7 years, is designed to provide an operational service over 15 to 20 years.

Work is ongoing within the ESA funded Sentinel-3 project titled "Sentinel-3 L2 product and algorithm definition" with ARGANS Ltd as the prime contractor and sub-contractors including ACRI-ST, Brockmann Consult, the Rutherford Appleton Laboratory (STFC/RAL) and Telespazio S.p.A. formerly Eltag Datamat) alongside several European research institutions and universities (Sentinel-3 L2 Products and Algorithm Team):

- Chris Merchant, University of Edinburgh, UK
- David Antoine, Laboratoire d'Océanographie de Villefranche (LOV), UK
- Fred Prata, Nilu, Norway
- Gerald Moore, Bio-Optika, UK
- Jadunandan Dash, University of Southampton, UK
- John Remedios, University of Leicester, UK
- Jurgen Fischer, Freie Universität Berlin (FUB), Germany
- Martin Wooster, King's College London, UK
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- Roger Saunders, UK MetOffice, UK
- Roland Doerffer, Helmholtz-Zentrum Geesthacht Centre for Materials and Coastal Research (formerly GKSS Research Centre), Germany

The overall product tree structure is based on the MERIS and (A)ATSR heritage plus the continuity of the SPOT-VGT mission (availability of the full spectral range provided by the two instruments); integrating the individual sensor (OLCI & SLSTR) and synergy (SYN) processors within a single environment. This single environment is called the Sentinel-3 Level 2 Optical Prototype Processor (O-L2PP).

The project is organised into several distinct steps (definition, specification, implementation and maintenance) with responsibly assigned to the various partners. Phase 1 was concluded with a Preliminary Design Review (PDR) in September 2009 and the next step (the Critical Design Review, CDR, closed end 2010) has involved finalising the Algorithm Theoretical Basis Documents (ATBDs) and hence methodologies for determining uncertainties. The list of ATBDs is extensive (21 in total where each describes one or more algorithms):

- Pixel classification
- Gas corrections, instrumental corrections and confidence check
- Water vapour product
- White caps & glint correction
- Standard Atmospheric Correction (SAC) over clear and turbid (bright) waters
- Alternative AC (AAC) – use of a Neural Net to perform the atmospheric correction including a glint correction
- Ocean colour for clear and turbid waters plus transparency products
- PAR (Photosynthetically Active Radiation)
- OLCI ICOL - adjacency correction (adopted ATBD to be implemented over a longer timescale)

The land products are less extensive and include:

- Rayleigh correction over land
- FAPAR (Fraction of Absorbed PAR)
- OLCI Terrestrial Chlorophyll Index (OTCI)

For each baseline output product, the aim is to determine a method that will allow error estimates/uncertainties to be calculated on a pixel-by-pixel basis. However, as the science is at different levels of maturity the proposed algorithms and uncertainty estimates span an operational readiness range. Therefore, some of the fields will contain default values in the shorter term.

Including this pixel-by-pixel uncertainty has the potential to double the size of the products. However, it's foreseen that the implementation of NetCDF v4 with data compression could be used to offset this growth in product size and network speeds will continue to improve with external impetus imposed by the general public increasingly using the

internet to download high volume content such as videos and films.

Example: Glint

The OLCI glint correction ATBD (Lavender and Kay, 2010) was developed from the heritage of the MERIS (Montagner *et al.*, 2003) and SeaWiFS (Wang and Bailey, 2001) approaches. The amount of sun glint will be reduced compared to MERIS as the OLCI field-of-view (FOV) is tilted to reduce the sun-glint pollution (maximum Operating Zenith Angle, OZA, of 55°).

For MERIS, all water pixels are tested for glint by comparing the reflectance to the predicted glint reflectance (ACRI, 2006), see Equation 1:

$$\rho_g = \frac{\pi \rho(\omega) \rho(\xi, \eta)}{4 \cos \theta_s \cos \theta_v \cos^4 \beta} \quad (1)$$

Where $\rho(\omega)$ is the Fresnel reflectance (approximated as a constant, 0.02, for incidence angles between 0 and 50 degrees), $\rho(\xi, \eta)$ is the probability distribution function (PDF) for the sea surface slope, and β is the zenith angle of the wave facet calculated from the specular reflection angle (ω).

As input variable (Level 1) PDFs aren't currently available, current research has focused on the sensitivity analysis approach. The predicted glint radiance is non-linear in all input variables except the atmospheric transmittance, which itself is a function of the illumination and viewing geometries. Therefore, the calculated radiance is highly sensitive to changes in the input variables in at least parts of their ranges. This can be demonstrated by evaluating how the glint function changes as a result of a 5% change in each input variable, using values from across the across the full range of all variables, see Figure 1 for some of the parameters, (Saltelli *et al.*, 2006).

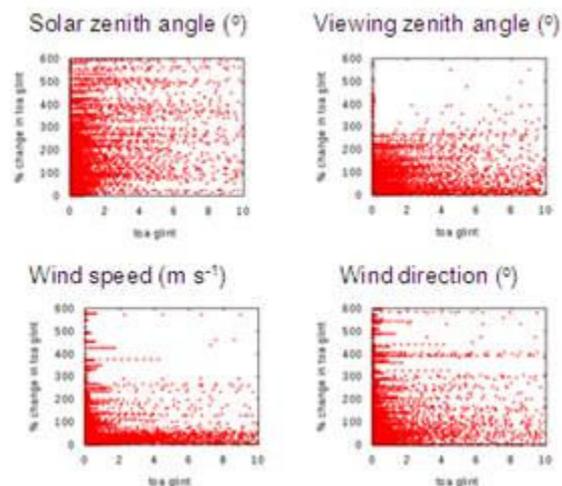


Figure 1. Relative change in glint for 5% change in input variable against glint reflectance.

Figure 2 and Table 1 show an example of sensitivity estimation for 6 pixels in a MERIS image. In this case, the wind speed has been varied by 5% and the corresponding change in glint reflectance is shown. The high percentage uncertainties in the low glint region will not impact on the final uncertainty as these reflectances are too low to be considered as medium glint. However, the uncertainty at pixel C will lead to uncertainty in the corrected reflectance and the uncertainty at D could change the classification of the pixel as high/medium glint.

This illustrates how uncertainty in the calculated glint radiance can lead to two types of error:

- Uncertainty in the size of the corrected radiance for the medium glint region (e.g. pixel C in Figure 2). This will lead to an uncertainty that propagates along the downstream processing chain.
- A pixel can be wrongly categorised as low, medium or high glint (e.g. pixel D in Figure 2). This is more difficult to quantify at later stages of processing, but can at least be reported to the user.

It remains to be determined how many repeated runs are needed to give an accurate estimate of uncertainty. For the 6 pixels used here, 100 runs gave a relative uncertainty consistent to within 3-4%, and a mean glint within about 3% of the reported value, 1000 runs gave consistency in the uncertainty to 2-3% and a mean within 1% of the reported value. 10000 runs gave more reliable results, but may be too demanding of computation time for practical use. Note that consistency was much worse for the low glint values, but this should not matter for values below the medium glint threshold.

Example: Atmospheric Correction

In order to determine the errors resulting from the OLCI SAC, combination of a clear water atmospheric correction and bright water adjustment, a sensitivity analysis has been performed by ACRI-ST (Lamquin, 2010). The two near infra-red (NIR) wavelengths used for the determination of aerosol properties in the AC algorithm of MEGS (MERIS prototype processor) have been modified with additive Gaussian noise. Then, statistics of departures from the original retrieval (selection of aerosol models, marine reflectances...) have been computed for MERIS observations.

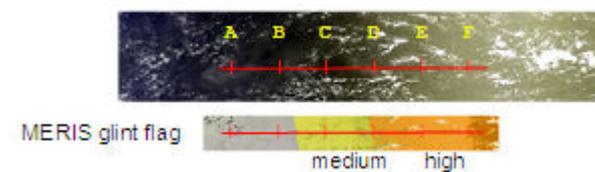


Figure 2. Section of a MERIS image of the Pacific Ocean, showing the position of 6 pixels A-F. Main view is a Level 1 RGB image with the pixel also shown in reference to the application of the glint flag.

Table 1. Glint reflectance and uncertainty produced by a 5% change in wind speed for the 6 pixels shown in Figure 2. Atmospheric transmittance has been taken as 1.

Position	Glint flag	TOA glint reflectance	Absolute uncertainty	Relative uncertainty (%)
A	none	1.60×10^{-7}	6.75×10^{-7}	420
B	none	0.0006	0.00062	101
C	medium	0.0185	0.00282	15
D	high	0.0327	0.00175	5.4
E	high	0.0547	0.00005	0.1
F	high	0.0777	0.00179	2.3

As computation of output uncertainties from noise simulation is very time consuming in near-real time, the aim is to create

Look-Up-Tables (LUTs); these will be built once and then

called during data retrieval for faster error estimation. A preferred method is based on an equation linking the water-leaving reflectance to the atmospheric path (Rayleigh + aerosol) reflectances and transmission as it directly relates the error in the NIR to output reflectances at other wavelengths. The tabulation of the relationships between these quantities and the aerosol optical depth has been tested and show that water-leaving reflectance can accurately be determined by a comparison between computed and simulated uncertainties for a single bracketing pair of aerosol models (4,8), see Figure 3. Further analysis and optimizations are currently being investigated to evaluate this method for all aerosol couples (thus all oceanic pixels).

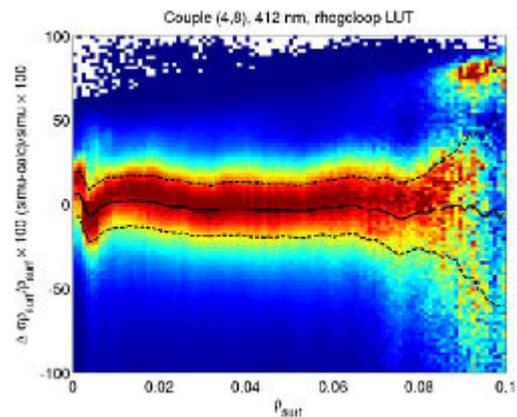


Figure 3. Relative difference between the simulated and calculated uncertainties standard deviation (water-leaving reflectance) as a function of water-leaving reflectance for all observations; bracketing pair of aerosol models (4, 8). Source: Lamquin (2010)

MERIS SUB-PIXEL VARIABILITY

The investigation involved the analysis of averaged MERIS geophysical data between 7x7, 5x5, 3x3 and 1 Reduced Resolution pixel sizes. An IDL routine was written (based on initial routines developed at ACRI-ST) which interrogated MERIS Level 2 products for all clear (no cloud) Case-1 flagged water pixels (only 'water' and 'BPAC' flags raised);

with the intention of extending the analysis to Case-2 waters in the future.

Initial results of the study, presented at the MERIS Validation Team (MVT) Meeting in March 2010, have highlighted the relationship between variability (wavelength dependent) and the:

- size of the Region Of Interest (ROI), also known as the macro-pixel size;
- ratio of the pixel size to the ROI;
- scale of the ratio between pixel/ROI ratio.

Using a subset of 40 Reduced Resolution products covering a large number of open ocean regions, analysis found that the relationship between variability and the pixel/ROI ratio follows a power law (Figure 4), while there is only a linear dependence of variability with regard to scale of the ratio (Figure 5).

Efforts are currently focused on identifying and quantifying any variability resulting from the MERIS AC. Therefore, analysis is currently being performed on a number of corresponding Level 1 and Level 2 MERIS products over open oceans to assess the AC input at all wavelengths. Following this assessment, analysis will then be performed in more complex coastal waters.

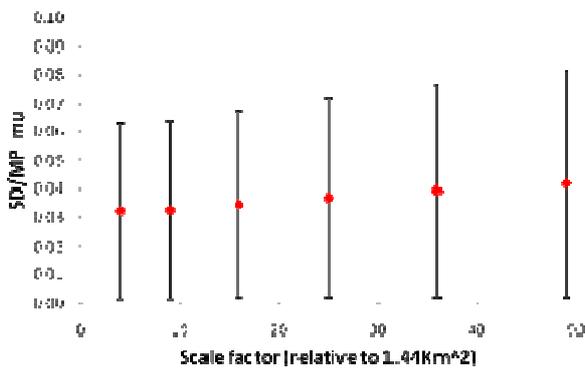


Figure 4. A linear relationship between the macro-pixel standard deviation divided by the mean, and scale of sub-macro pixel area. The ratio of sub-pixel to macro-pixel area is 1:4, and for 412 nm.

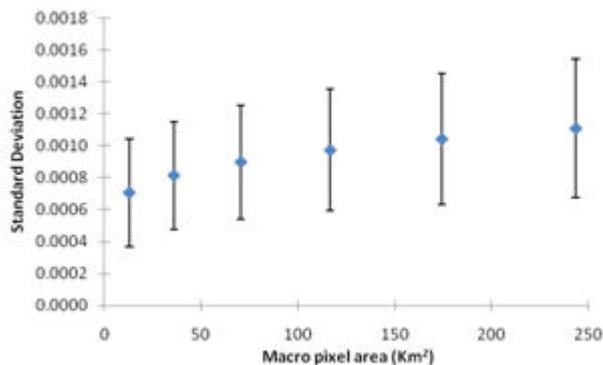


Figure 5. A power-law relationship between the macro-pixel standard deviation divided by the mean, and increasing macro-pixel size (constant sub-pixel size), for 412 nm.

CONCLUSIONS

- Determination of Quality Indicators is not easy, but is seen as a real benefit to the eventual users of the data.
- There is an assumption that Level 1 will derive uncertainties so that these can feed into Level 2, but uncertainties will also be needed for auxiliary data and the algorithm/modelling process (at each step/known assumption).
- Based on the MERIS study, there should also be a consideration of variability at sub-pixel scales.

REFERENCES

- ACRI, 2006. "MERIS Level 2 Detailed Processing Model", http://earth.esa.int/pub/ESA_DOC/ENVISAT/MERIS/MERIS_DPML2_i7r2A_re-issued.pdf.
- N. Lamquin, "Error Propagation in the Atmosphere Correction"
- S3-L2-SD-01-C01-ACR-TN_OLCIACErrorPropagation, September 2010.
- S. Lavender, and S. Kay, "OLCI Glint Correction ATBD SD-03-C09", S3-L2-SD-03-C09-ARG-ATBD_GlintCorrection_v2.0, April 2010.
- Montagner, F., Billat, V., and Belanger, S., "MERIS ATBD 2.13 Sun Glint Flag Algorithm", 2003. http://envisat.esa.int/instruments/meris/atbd/atbd_2_13.pdf.
- A. Saltelli, M. Rattoa, S. Tarantola, F. Campolongo, And European Commission, Joint Research Centre of Ispra, "Sensitivity analysis practices: Strategies for model-based inference. Reliability Engineering & System Safety", 91(10-11), p.p. 1109-1125, 2006.
- M. Wang, And S. Bailey, "Correction of sun glint contamination on the SeaWiFS ocean and atmosphere products", Applied Optics, 40(27): p.p. 4790-4798, 2001.