

# An analytical Case 2 water algorithm for the North Sea

A. Folkestad<sup>a,\*</sup>, A. Korosov<sup>b</sup>, K. Sørensen<sup>c</sup>, L. H. Pettersson<sup>a</sup>, D. V. Pozdnyakov<sup>b</sup>

<sup>a</sup>Nansen Environmental and Remote Sensing Center, N-5006 Bergen, Norway – are.folkestad@nersc.no

<sup>b</sup>Nansen International Environmental and Remote Sensing Center, St. Petersburg, Russia

<sup>c</sup>Norwegian Institute of Water Research, Oslo, Norway

**Abstract – An advanced inverse Case 2 water algorithm for the retrieval of concentrations of colour producing agents (CPAs) from satellite ocean colour data is applied to the Skagerrak region in the North-eastern part of the North Sea. A set of the CPAs' specific inherent optical properties (SIOPs) was developed for this area. Sensitivity tests show that the algorithm's retrieval accuracy of the chlorophyll concentration (Chl) is highly sensitive to the absorption and backscattering properties of total suspended matter (TSM). Nevertheless, given the presented SIOP set, the algorithm is capable of accurately retrieving CPA concentrations and performs better than standard MERIS algorithms.**

**Keywords:** North Sea, MERIS, SIOP, Case 2 waters, inverse algorithm, CPA

## 1. INTRODUCTION

An advanced inverse Case 2 water algorithm for the retrieval of concentrations of colour producing agents (CPAs) from satellite ocean colour data is applied to the Skagerrak region in the North-eastern part of the North Sea. This area contains a highly complex and dynamic pattern of various water masses originated from Atlantic waters, the Jutland current, the Baltic outflow and river runoff from the surrounding land areas. The optical conditions are correspondingly complex. The inverse algorithm relies on a predefined set of the CPAs' specific inherent optical properties (SIOPs) assumed to be representative for the region. However, SIOPs are generally known to vary on both seasonal and spatial scales. The sensitivity of the algorithm's retrieval accuracy to SIOP variability is therefore investigated under various optical conditions. Furthermore, *in situ* validation of the algorithm is carried out, and the performance of the advanced inverse algorithm and the equivalent standard MERIS algorithms is compared.

## 2. THE BIO-OPTICAL MODEL

A bio-optical model is applied to relate the in-water SIOPs and CPAs, to the sub-surface remote sensing reflectance,  $R_{rsw}$ . The CPAs are Chlorophyll (Chl), total suspended matter (TSM), and yellow substance (YS). The concentration of the latter is given in terms of absorption [ $m^{-1}$ ] at 442nm,  $a_{YS}(442)$ . Concentrations of Chl and TSM

are given in terms of weight per volume unit ( $mgm^{-3}$  and  $gm^{-3}$ , respectively). At a given wavelength the total absorption,  $a=a(\lambda)$ , is assumed to be the sum of absorption by pure water ( $a_w$ ) and absorption by the three CPAs ( $a_{TSM}$ ,  $a_{chl}$ , and  $a_{YS}$ ) (Eq. 1) The contribution from each of the CPAs is assumed to be the product of the corresponding SIOP and the concentration of the component (<CPA>). Similarly the total backscattering,  $b_b$ , is the sum of contributions from the water itself, TSM and Chl (Eq. 2).

$$a = a_w + a_{TSM}^* \cdot \langle TSM \rangle + a_{Chl}^* \cdot \langle Chl \rangle + a_{YS}^* \cdot a_{YS}(442) \quad (1)$$

$$b_b = b_{bw} + b_{TSM}^* \cdot \langle TSM \rangle + b_{Chl}^* \cdot \langle Chl \rangle \quad (2)$$

Equation 3 relates the sub-surface remote sensing reflectance,  $R_{rsw}=R_{rsw}(\lambda)$ , to the total absorption and backscattering coefficients:

$$R_{rsw} = k_1 + k_2 \cdot (b_b/a) + k_3 \cdot (b_b/a)^2, \quad (3)$$

where  $k_1 = -0.00036$ ,  $k_2 = 0.11$ , and  $k_3 = -0.0447$  (Jerome *et al.*, 1996). The forward bio-optical model is, together with a suitable set of SIOPs, used in an inverse algorithm for the retrieval of the CPAs from a set of spectral values of  $R_{rsw}$  obtained from satellite images. This approach is described in detail by Kondratyev *et al.* (1990) and Pozdnyakov *et al.* (in press) and applies the Levenberg-Marquardt optimization procedure (Levenberg 1944, Marquardt 1963). The algorithm has proved to accurately retrieve CPA concentrations from satellite retrieved  $R_{rsw}$  for various inland and coastal water bodies (e.g. Pozdnyakov *et al.*, 2003).

A set of SIOPs has been developed for this study. The specific absorption coefficients,  $a_{chl}^*$ ,  $a_{TSM}^*$ ,  $a_{YS}^*$  (Fig. 1) as well as  $b_{TSM}^*$  were retrieved from *in situ* data sampled in the Norwegian Coastal Current (NCC) outside the Norwegian west coast (Folkestad *et al.*, in prep). The specific chlorophyll backscattering coefficient,  $b_{chl}^*$ , as presented by Bukata *et al.* (1991) was adopted for this study. Spectral values of  $a_w$  and  $b_{bw}$  are selected from Pope and Fry (1997) and Smith and Baker (1981), respectively.

## 3. SENSITIVITY TEST

### 3.1. Sensitivity test setup

A sensitivity test was performed in order to quantify the influence of SIOP variability on the inverse algorithm retrieval accuracy. By varying the spectral values for each individual SIOP, the resulting variations in the modelled remote sensing reflectance ( $R_{rsw}$ ) and further in the inversely retrieved CPAs were investigated. The sensitivity test was performed for four different optical conditions; open ocean (Case 1) waters, sediment dominated (Case 2S) waters, yellow substance dominated (Case 2Y) waters, and finally for a high biomass bloom (HBB). For each of these conditions, a reference  $R_{rsw}$  spectrum was simulated (Fig.2)

\*Corresponding author.

\*\*The work was performed through the MORAN project funded by the Norwegian Research Council. Data for the validation was provided from the EU-project FerryBox (EVK2-CT-2002-00144).

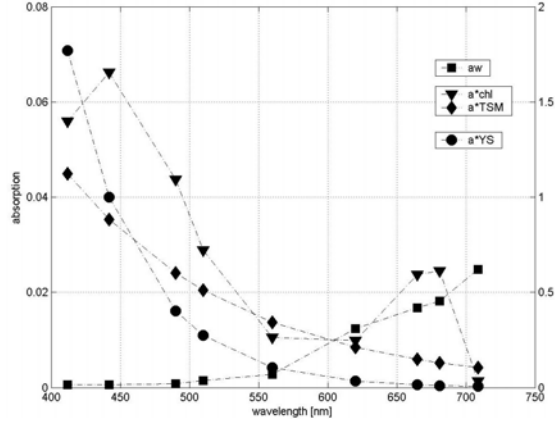


Figure 1. Specific absorption coefficients ( $a^*_{chl}$ ,  $a^*_{TSM}$ , and  $a^*_{YS}$ ) applied in this study, for MERIS wavelengths.  $a^*_{chl}$  and  $a^*_{TSM}$  are given on the left-hand side y-axis. Units are  $m^2 \cdot mg^{-1}$  and  $m^2 \cdot g^{-1}$ , respectively.  $a^*_{YS}$  is normalized to  $a_{YS}(442)$ , and is given on the right-hand side y-axis in dimensionless units.  $a_w$  is given on the right-hand side y-axis with absorption units ( $m^{-1}$ ).

by the forward model using the corresponding CPA concentrations (Table 1) and the reference SIOP set as specified above. Next, in order to test the  $R_{rsw}$  response to SIOP variability (i.e. the  $R_{rsw}$  deviation from the reference spectrum) the same combinations of CPAs were applied, but now each SIOP's spectral values were shifted by either +50% or -50% from their respective values in the reference SIOP set. Thus, for each SIOP two  $R_{rsw}$  spectra were generated. Consequently, given the five SIOPs, for each optical condition a total of 10 spectra were generated. These spectra together with the reference SIOP set were applied as input to the inverse retrieval algorithm. The difference between the inversely retrieved CPA concentrations ( $CPA_r$ ) and the initial CPA concentrations used to generate the spectra ( $CPA_i$ ) is entirely caused by the shift in SIOP values and is therefore a measure of the inverse algorithm's sensitivity to the SIOP variability.

### 3.2. Sensitivity test results

The sensitivity of the retrieval algorithm to SIOP variability is expressed as the percentage error,  $\Delta CPA / CPA_i$ , between the inversely retrieved and the initial CPA concentrations (Table 1), where  $\Delta CPA = (CPA_r - CPA_i)$ . This error is presented in Table 2 for the three CPAs (Chl, TSM and  $a_{YS}$ ), for the four optical conditions (Case 1, Case 2S, Case 2Y, and HBB), and as a result of a 50% positive or negative shift (indicated by '+' and '-', respectively) in the various SIOPs. Table 2 shows that a 50% shift in  $a^*_{chl}$  results in a Chl retrieval error of the same magnitude as the shift itself, i.e. 43-51%. This result seems not to depend significantly on the optical condition.

Table 1. CPA sets used in the sensitivity test.

Optical condition	Chl [ $mg/m^3$ ]	TSM [ $g/m^3$ ]	$a_{YS}(442)$ [1/m]
Case 1	1.0	1.0	0.10
Case 2S	1.0	5.0	0.10
Case 2Y	1.0	1.0	0.50
HBB	10	5.0	0.10

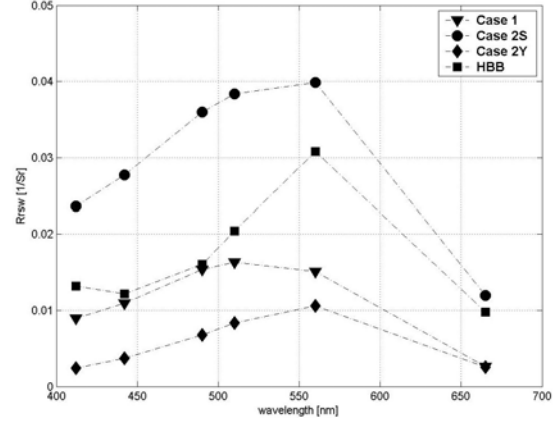


Figure 2. Reference  $R_{rsw}$  spectra for the various optical conditions applied in the sensitivity test. The spectra are obtained by the bio-optical model using the SIOP set as specified in the text and CPAs given in table 2.

The errors in TSM and  $a_{YS}$  retrievals are much less influenced. A change in  $b^*_{chl}$  will not dramatically influence any of the CPA retrievals due to its low value relative to  $b^*_{TSM}$ . The impact of a shift in  $a^*_{TSM}$  is much bigger for the retrieval error of Chl (all optical conditions) and of  $a_{YS}$  (Case 2S and HBB) than of TSM itself. In fact, a Chl retrieval error of 99-116% is observed for Case 2S waters when  $a^*_{TSM}$  is shifted. The same features are seen for a shift in  $b^*_{TSM}$ , with the exception that also TSM is retrieved with an error of 52-54%. The Chl and TSM retrieval errors resulting from a 50% shift in  $a^*_{YS}$  is effectively zero, while  $a_{YS}(443)$  is retrieved with an error of exactly 50%. This result is rather intuitive, as YS is not backscattering. Therefore a specified percentage shift in  $a^*_{YS}$  will have an impact on the forward modelled  $R_{rsw}$  spectral values that is identical to the impact caused by the same percentage shift in  $a_{YS}(443)$ , as long as the spectral slope is fixed, which is the case in the present study.

## 4. ALGORITHM *in situ* VALIDATION

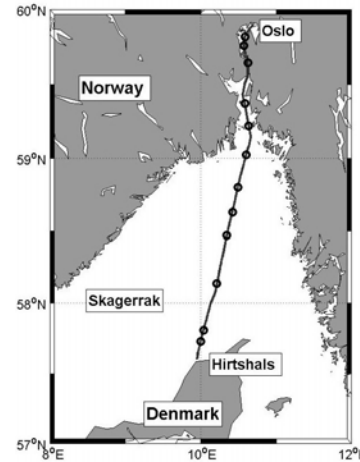


Figure 3. Map of the "Color Festival" ferry transect between Oslo and Hirtshals. Circles indicate positions where water samples are collected for the determination of Chl on March 28, 2003.

Table 2. Sensitivity test results given as the percentage error between inversely retrieved ( $CPA_r$ ) and initial ( $CPA_i$ ) concentrations ( $\Delta CPA = CPA_r - CPA_i$ ). Results are obtained by applying a positive or negative (indicated by '+' or '-', respectively) SIOP shift of 50% for four optical conditions –Case 1, 2S, 2Y waters (C1, C2S and C2Y) and High Biomass Bloom -HBB).

SIOP	$\Delta Chl/Chl_i$ [%]				$\Delta TSM/TSM_i$ [%]				$\Delta a_{ys}/(a_{ys})_i$ [%]			
	C1	C2S	C2Y	HBB	C1	C2S	C2Y	HBB	C1	C2S	C2Y	HBB
$a_{chl}^*$ +	48.7	51.0	49.7	43.0	-5.3	-1.1	-5.4	-12.5	-1.9	-0.3	-2.0	-5.9
$a_{chl}^*$ -	-50.4	-51.4	-51.2	-49.6	5.3	1.1	5.5	11.8	1.8	0.3	1.9	3.4
$b_{b*chl}^*$ +	0.4	-1.3	-0.7	3.2	5.3	1.1	5.5	12.4	1.8	0.3	2.0	4.0
$b_{b*chl}^*$ -	-0.6	1.2	0.5	-3.5	-5.3	-1.1	-5.5	-12.1	-1.9	-0.3	-2.1	-6.0
$a_{TSM}^*$ +	21.5	115.5	20.3	10.3	-3.7	-4.1	-2.8	-3.6	3.0	24.1	0.3	26.6
$a_{TSM}^*$ -	-22.2	-98.5	-21.1	-10.5	3.7	3.3	2.8	3.4	-3.2	-34.4	-0.4	-28.3
$b_{b*TSM}^*$ +	-22.4	-98.9	-22.2	-10.7	54.2	51.7	53.0	52.9	-3.6	-35.3	-0.5	-31.7
$b_{b*TSM}^*$ -	20.7	105.7	18.5	7.8	-52.9	-54.7	-52.3	-53.6	2.5	19.6	-0.1	25.7
$a_{YS}^*$ +	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	50.0	50.0	50.0	50.0
$a_{YS}^*$ -	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-50.0	-50.0	-50.0	-50.0

#### 4.1. Ship borne data

Estimates of *in situ* Chl were obtained from water samples collected by the ferrybox system onboard the passenger ferry 'Color Festival' cruising twice a day between Oslo, Norway, and Hirtshals, Denmark. The sampling points along the ferry transect is indicated in Fig. 3. The Chl were sampled at depths of 3-4m and determined with the HPLC method according to the MERIS validation protocols and described by Sørensen *et al.* (2003). Additionally the turbidity (Formazine Nephelometric Units –FNU) was measured continuously by the ferrybox system along the ferry transect. For practical use, turbidity is equivalent to TSM in this area. The data were used for validation of the inverse retrieval algorithm using synoptically sampled cloud free MERIS data as input to the algorithm.

#### 4.2. Satellite EO data

MERIS Reduced Resolution Level 2 data from a total of 13 dates in 2003 and 2004 that coincided with synoptic ferrybox measurements were collected and used for validation of the inverse retrieval algorithm. Standard MERIS retrieval algorithms are presented in the MERIS Product Handbook and in (Antoine and Morel 1999, Moore *et al.* 1999, Morel and Antoine 2000). The MERIS surface reflectance ( $\rho_w$ ) in 9 bands (412-705nm) were converted to  $R_{rsw}$  and applied as input to the inverse algorithm. The algorithm's Chl and TSM outputs were compared both to the ship borne data, and to the equivalent standard MERIS products. Additionally the yellow substance and bleached particle absorption (YSBPA) at 442nm is a standard MERIS product and was compared to the equivalent output from the inverse algorithm, which was calculated as  $YSBPA(442) = a_{YS}(442) + TSM \cdot a_{TSM}(442)$ .

#### 4.3. Validation results

For all 13 dates in the dataset, retrievals of the three CPAs by the inverse algorithm, the standard MERIS algorithms, and *in situ* measurements (where available) were plotted for the ferry transect between Oslo and Hirtshals. Examples from March 28, 2003, are shown in Fig. 4. Satellite retrievals from pixels north of 59.1°N were abandoned, due to adjacent land pixels. In the example plot of Chl (Fig. 4a), the inverse algorithm generally retrieves Chl values very close to ship borne values. The standard MERIS algorithms are generally over-estimating the Chl

values as compared to the ship borne results. A strong Chl gradient is indicated by the satellite retrievals between 57.6 and 57.7°N. The ship borne data indicates a similar gradient but its position is shifted to the north (between 57.7 and 57.8°N). However, this location is close to the Danish coast where sediment re-suspensions occur frequently. Consequently, it is known that Chl sampled at depths of 3-4m may not be representative for the remotely sensed signal in this region. North of the gradient, a very good agreement is furthermore observed for TSM between both the two different satellite algorithms and the turbidity parameter measured by the ferrybox system. In Fig. 4c YSBPA obtained by the inverse algorithm and the standard MERIS algorithm are shown. The discrepancy between the two YSBPA products are increasing from the southern to the northern range of the transect. Generally, the inverse algorithm retrieves higher values.

The agreement between the satellite and the ship borne data was also investigated for the other dates not shown. For some of the dates the discrepancy was substantially larger than for the examples shown in Fig. 4. This discrepancy is expected to arise from various sources. If the MERIS atmospheric correction fails to produce high quality estimates of the surface reflectance, realistic CPA retrievals cannot be expected. Furthermore, for the inverse algorithm a single set of SIOPs was applied. However, at present it is not known to what extent this set is representative for the whole study area and for all optical conditions that are present for the 13 dates. Especially, variations in  $b_{b*TSM}^*$  and  $a_{TSM}^*$  are seen to highly influence the retrieval accuracy of Chl. The focus of ongoing and future research is therefore to further investigate the validity of these SIOPs for the various optical conditions present in the study area.

## 5. CONCLUSIONS

The sensitivity test performed in this study highlighted that the retrieval accuracy of Chl is especially sensitive to variability in  $a_{TSM}^*$  and  $b_{b*TSM}^*$  in addition to  $a_{chl}^*$ . Given the SIOP set applied in this study, the agreement between the inverse algorithm retrievals and ship borne data is nevertheless seen to be very good for several of the 13 dates in the presented dataset, and in general better than the standard MERIS algorithms.

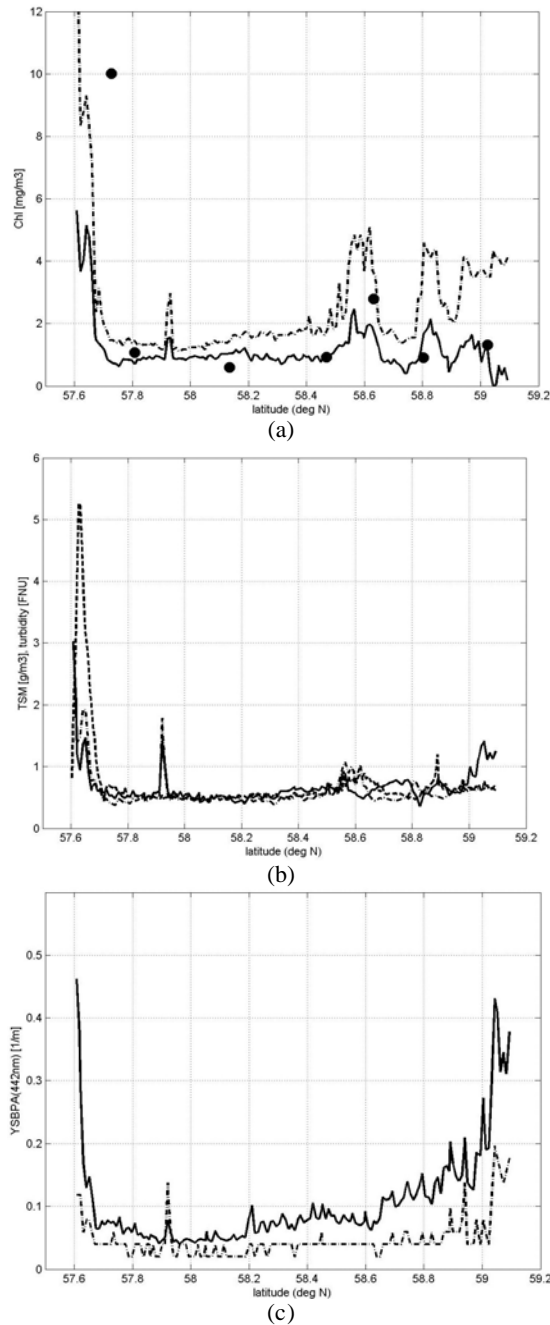


Figure 4. CPAs as retrieved along the ferry transect (Fig. 3) by the inverse algorithm, the MERIS standard algorithms, and ferrybox *in situ* measurements. Results are shown for (a) Chl obtained by the inverse (solid line) and standard MERIS (dashed line) algorithms, and ferrybox system (filled circles), (b) TSM obtained by the inverse (solid line) and standard MERIS (dot-dash line), and turbidity obtained by the ferrybox system (dashed line), and (c) YSBPA obtained by inverse (solid line) and standard MERIS (dot-dash line) algorithms. No ferrybox measurements of YSBPA are undertaken.

## 6. REFERENCES

- Antoine, D., and A. Morel, "A multiple scattering algorithm for atmospheric correction of remotely sensed ocean colour (MERIS instrument): principle and implementation for atmospheres carrying various aerosols including absorbing ones", *Int. Journ. Rem. Sens.*, vol 20, p.p. 1875-1916, 1999.
- Bukata, R. P., J. H. Jerome, K. Ya. Kondratyev, and D. V. Pozdnyakov, "Estimation of organic and inorganic matter in inland waters: Optical cross sections of Lakes Ontario and Ladoga", *J. Great Lakes Res.*, vol 17, p.p. 461-469, 1991.
- Folkestad A., A. Korosov, K. Sørensen, L. Pettersson, "Parameterization and application of a bio-optical model for the North Sea", in preparation.
- Jerome, J. H., R. P. Bukata, and J. R. Miller, "Remote sensing reflectance and its relationship to optical properties of natural water", *Int. Journ. Rem. Sens.*, vol 17, p.p. 3135-3135, 1996.
- Kondratyev, K. Ya., D. V. Pozdnyakov, and V. Yu. Isakov, "Radiation and hydrooptical experiments on lakes", Leningrad: Nauka Press, 115 pp. (in Russian), 1990.
- Levenberg, K., "A method for the solution of certain non-linear problems in least squares", *Quantitative and Applied Mathematic*, vol 2, p.p. 164-168, 1944.
- Marquardt, D. W., "An algorithm for least-squares estimation of non-linear parameters", *Journal of the International Society of Applied Mathematic*, vol 11, p.p. 36-48, 1963
- MERIS product Handbook, issue 1.2, September 2004, <http://envisat.esa.int/dataproducts/meris/>
- Moore, G., J. Aiken, and S. J. Lavender, "The atmospheric correction of water colour and the quantitative retrieval of suspended particulate matter in Case II waters: application to MERIS", *Int. Journ. Rem. Sens.*, vol 20, pp 1713-1733, 1999.
- Morel, A. and D. Antoine, "Pigment index retrieval in Case I waters", MERIS ATBD 2.9, Laboratoire de Physique et Chimie Marines, France, 2000.
- Pope, R. M., and E. S. Fry, "Absorption spectrum (380-700nm) of pure water. II. Integrating cavity measurements", *Appl. Optics*, vol 36, pp 8710-8723, 1997.
- Pozdnyakov, D. V., L. H. Pettersson, O. M. Johannessen, A. V. Lyaskovsky, N. N. Filatov, and L. P. Bobylev, "SeaWiFS maps water quality parameters of the White Sea", *Int. Journ. Rem. Sens.*, vol 24, pp 4065-4071, 2003.
- Pozdnyakov, D. V., A. Korosov, H. Grassl, and L. H. Pettersson, "An advanced algorithm for operational retrieval of water quality from satellite data in the visible", *Int. Journ. Rem. Sens.*, in press.
- Smith, R. C., and K. S. Baker, "Optical properties of the clearest natural waters (200-800nm)", *Appl. Optics*, vol 20, pp 177-184, 1981.
- Sørensen, K., E. Aas, J. Høkedal, G. Severinsen, R. Doerffer, and E. Dahl, "Validation of MERIS water products in the Skagerrak", *Proceedings from Envisat MAVT-2003 –working meeting on MERIS and AATSR Calibration and Geophysical validation*, 2003.