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Calibration and validation of a generic multisensor algorithm for mapping of total suspended matter in turbid waters

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ABSTRACT

Mapping of total suspended matter concentration (TSM) can be achieved from space-based optical sensors and has growing applications related to sediment transport. A TSM algorithm is developed here for turbid waters, suitable for any ocean colour sensor including MERIS, MODIS and SeaWiFS. Theory shows that use of a single band provides a robust and TSM-sensitive algorithm provided the band is chosen appropriately. Hyperspectral calibration is made using seaborne TSM and reflectance spectra collected in the southern North Sea. Two versions of the algorithm are considered: one which gives directly TSM from reflectance, the other uses the reflectance model of Park and Ruddick (2005) to take account of bidirectional effects.
Applying a non-linear regression analysis to the calibration data set gave relative errors in TSM estimation less than 30% in the spectral range 670–750 nm. Validation of this algorithm for MODIS and MERIS retrieved reflectances with concurrent *in situ* measurements gave the lowest relative errors in TSM estimates, less than 40%, for MODIS bands 667 nm and 678 nm and for MERIS bands 665 nm and 681 nm. Consistency of the approach in a multisensor context (SeaWiFS, MERIS, and MODIS) is demonstrated both for single point time series and for individual images.

1. Introduction

Mapping of total suspended matter concentration (TSM) from satellites and airborne imagery has become a valuable tool for marine scientists to assess and monitor suspended sediment distribution, which is a key element of water quality in coastal areas. Remote sensing (RS) data have been used in various ways: combined with *in situ* measurements to draw up sediment transport maps e.g. van Raaphorst et al. (1998), as input boundary conditions and validation data to sediment transport models by Fettweis and Van den Eynde (2003), assimilated in transport models by Vos and Gerritsen (1997) and Blaas et al. (2007), or used in the light forcing of an ecosystem model e.g. Lacroix et al. (2007). With the continuous optimisation of satellite capabilities e.g. improvement of wavelengths used for MODIS after the SeaWiFS experiment as described in Esaias et al. (1998), the more bands and higher spatial resolution of the MERIS instrument, and the development of algorithms for retrieval of water constituents, the accuracy and reliability of RS products is increasing. A historical overview of TSM algorithm evolution from 1974 to 2005 is given in Acker et al. (2005).

TSM algorithms were first designed for open ocean waters as a function of chlorophyll *a* (CHL) concentration, as established in Morel (1980), Sturm (1980) and Viollier and Sturm (1984), because suspended solids in the deep sea consist mainly of plankton and associated organic detrital matter. The form commonly adopted for CHL algorithms and inherited by TSM algorithms is a reflectance band ratio, characterizing the high CHL absorption around 440 nm and low absorption in 550 nm. However, as underlined by Tassan (1993), CHL and TSM do not co-vary in coastal waters because of the presence of particles arising from re-suspension, shore erosion or river discharge, making the blue:green band ratio algorithms unsuitable for TSM retrieval.

Curran et al. (1987) and Novo et al. (1989) investigated the form of the relationship between TSM and reflectance in coastal waters and showed that single band algorithms may be adopted where TSM increases with increasing reflectance. A variation of these relations with viewing geometry was observed by Novo et al. (1989). Empirical calibration of different data sets followed during the last decade, establishing log-linear models as function of reflectance or radiance in the visible range. Calibration has been made using variously: laboratory TSM and reflectance data by Chen et al. (1991), with *in situ* reflectances over the Rhône river plume by Forget and Ouillon (1998) and with MODIS 645 nm-reflectance over Tampa Bay by Hu et al. (2004). Non-linear equations have been tested by Myint and Walker (2002) for TSM and AVHRR data, concluding that the best model is a linear one with AVHRR channel 2 (725 nm–1100 nm) with non-linear models being better adapted for shorter wavelengths.

Although these models might be efficiently applied to satellite images concurrent with calibration data sets, their accuracy may be reduced outside the conditions of the calibration data set because of the empirical basis. Semi-analytical approaches have overcome such a

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limitation with models based on physical knowledge of the relationship between reflectance and TSM. The reflectance model of Gordon et al. (1988) used for open sea waters and validated for inland turbid waters by Dekker et al. (1997), has been intensively used to retrieve TSM in estuarine e.g. Stumpf and Pennock (1989) and Dekker et al. (1998), in coastal and deep waters by Van Der Woerd et al. (2000), Van Der Woerd and Pasterkamp (2004) and Eleveld et al. (2008). In very turbid waters Doxaran et al. (2002, 2003) used a NIR band ratio model to remove the effects of particle size distribution and of the bidirectional variation of the remote sensed reflectance.

Analytical approaches have been developed since the last decade aiming to solve the reflectance model with water constituents as the unknowns, by parameterization of specific IOPs (inherent optical properties) e.g. Forget et al. (1999), Lahet et al. (2000) and Haltrin and Arnone (2003). Vasilkov (1997) used non-linear least square regression, with parameterization of particle backscattering coefficient and coloured dissolved organic matter (CDOM) absorption. Multi-spectrum multi-component analytical retrieval algorithms are emerging, where the reflectance spectrum is inverted to derive simultaneously TSM, phytoplankton pigment and CDOM, e.g: Hoogenboom et al. (1998) and Sterckx and Debruyn (2004) using matrix inversion of the reflectance model and Schiller and Doerffer (1999) used a neural network technique. The multi-component models (e.g. TSM, CHL and CDOM) generally use hyperspectral information or at least many bands in the visible range, to discriminate each component.

In the present study a single band algorithm for TSM retrieval based on a reflectance model is developed (Section 2) and calibrated (Section 3) using seaborne reflectance and TSM measurements collected in the southern North Sea area. A second version of the algorithm is calibrated using the reflectance model of Park and Ruddick (2005) to take into account the bidirectional effects (Sections 2.1 and 2.2). Unlike the papers available in literature up to now, this TSM algorithm innovates by its hyperspectral calibration, its strong theoretical basis and its simple application to multiple ocean colour sensors. The hyperspectral calibration is used to identify the best spectral interval for TSM retrieval from remote sensed reflectance, while the semi-empirical approach takes into account assumptions on spatial and temporal variability of specific IOPs, whose impact on TSM estimation are discussed in “Web Appendix 1 — Theoretical error of estimates”, hereafter referred to as WA1. The results of the generic hyperspectral calibration and the specific calibration for MERIS, MODIS and SeaWiFS sensors are presented (Section 4). The results of the calibration using the reflectance model of Park and Ruddick (2005) are presented in “Web Appendix 2 — BRDF algorithm variant”, denoted by WA2 and the method to remove outliers from the calibration dataset is given in “Web Appendix 3 — Treating outliers in regression analysis” (WA3). Validation of the algorithm is carried out using MERIS and MODIS imagery (Section 5) and model errors are assessed using *in situ* matchups. TSM time series from the MERIS standard product using the neural network technique Schiller and Doerffer (1999) and from MODIS and SeaWiFS using the current algorithm are shown (Section 6). The performance of the single band algorithm is demonstrated with TSM concentration maps retrieved from the three ocean colour sensors (Section 7). Finally conclusions synthesize the method and the results and consider future possibilities of TSM retrieval in a synergistic multisensor perspective (Section 8).

2. Theory

The aim of this section is to derive the mathematical form of the model allowing TSM concentration, S, to be estimated from the water-leaving reflectance defined by:

$$\rho_w(\lambda) = \pi R_{rs}(\lambda) \tag{1}$$

where R_{rs} is the remote sensing reflectance at wavelength λ (dropped hereafter for simplicity): $R_{rs} = \frac{L_w^{0+}}{E_d^{0+}}$, L_w^{0+} and E_d^{0+} are respectively the water-leaving radiance, corrected for air–sea interface reflection, and the downward irradiance just above the sea surface. S is first related to the ratio of total backscattering b_b to total absorption a, $\omega_b' = \frac{b_b}{a}$. Two alternative approaches are then offered here. In the first approach the inherent optical property ω_b' is estimated from water-leaving reflectance by inversion of the reflectance model of Park and Ruddick (2005). In the second approach, the simple first order analytical reflectance model of Gordon et al. (1988) is used. It is assumed in these models that bottom effects do not contribute to water-leaving reflectance (optically deep water column).

2.1. Inherent optical property model

For the purposes of deriving a total suspended matter retrieval algorithm, ω_b' is most conveniently divided into the contributions to backscatter and absorption from particles (both non-algal and algal) and all other non-particle optically-active substances (essentially the pure water molecules and coloured dissolved organic matter):

$$\omega_b' = \frac{b_{bp} + b_{bnp}}{a_p + a_{np}} \tag{2}$$

where the subscripts p and np denote the particle and non-particle contributions. A number of assumptions and approximations regarding these inherent optical properties (IOPs) are then made in order to relate S directly to ω_b'. The validity of these assumptions is obviously crucial to the accuracy of the consequent retrieval algorithm and is assessed in detail in the error analysis of WA1. Starting with the most important, these assumptions are as follows:

1. Particulate backscatter is assumed proportional to TSM concentration via the constant TSM-specific particulate backscatter coefficient, b_{bp}^*:

$$b_{bp} = b_{bp}^* S \tag{3}$$

   This is the most important of the 4 assumptions made regarding IOPs since natural variability of b_{bp}^* will give a direct, linear error to S retrieval. Both specific-scattering studied in Babin et al. (2003a) and the scattering:backscattering ratio examined by Boss et al. (2004) are known to vary in relation with space or time variations of particle size and composition, and b_{bp}^* is expected to be significantly different between algae and non-algae particles (as well as being variable within these two groups). If the natural variability of b_{bp}^* could be characterised in some way *a priori*, then it may be possible to improve on this assumption. The quantification of the errors associated with differences in b_{bp}^* between algae and non-algae particles is given in WA1, Section I.1.
2. Space and time variabilities of non-particulate absorption, a_{np} is assumed to be negligible. For validity of this assumption in areas of high CDOM absorption, e.g. coastal waters with river plumes, it is necessary to choose the wavelength for retrieval such that the pure water absorption is dominant. The impact of variability of a_{np} on retrieval errors is quantified in WA1, Section I.2.
3. Particulate absorption is assumed proportional to TSM concentration via the constant TSM-specific particulate absorption coefficient, a_p^*:

$$a_p = a_p^* S. \tag{4}$$

   It is well known that there is considerable variability in a_p^* as stressed by Babin et al. (2003b), both in magnitude and spectral variation, according to the size and composition of particles. This is particularly significant when comparing algae particles with non-algae particles. However, the impact of this variability on retrieval accuracy can be