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The Ocean Colour Climate Change Initiative: I. A methodology for assessing atmospheric correction processors based on in-situ measurements

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ABSTRACT

The Ocean Colour Climate Change Initiative intends to provide a long-term time series of ocean colour data and investigate the detectable climate impact. A reliable and stable atmospheric correction procedure is the basis for ocean colour products of the necessary high quality. In order to guarantee an objective selection from a set of four atmospheric correction processors, the common validation strategy of comparisons between in-situ and satellite-derived water leaving reflectance spectra, is extended by a ranking system. In principle, the statistical parameters such as root mean square error, bias, etc. and measures of goodness of fit, are transformed into relative scores, which evaluate the relationship of quality dependent on the algorithms under study. The sensitivity of these scores to the selected database has been assessed by a bootstrapping exercise, which allows identification of the uncertainty in the scoring results. Although the presented methodology is intended to be used in an algorithm selection process, this paper focusses on the scope of the methodology rather than the properties of the individual processors.

1. Introduction

Ocean-colour is recognised as an Essential Climate Variable (ECV) by the Global Climate Observation System (GCOS-154, 2011). Many geophysical and bio-optical variables retrieved from ocean-colour data from satellites, such as chlorophyll concentration and inherent optical properties of the ocean, are relevant to climate research. All these products are derived from spectrally-resolved water-leaving radiances or reflectances, which are extracted from top-of-the-atmosphere radiance values measured by satellites using atmospheric-correction algorithms. Given that the atmospheric signal is typically 80% or more of the total signal at the top of the atmosphere, accurate Atmospheric Correction (AC) is key to a successful implementation of all in-water algorithms in routine use today.

Currently, several algorithms and approaches are used by space agencies for atmospheric correction of ocean-colour data. For example, National Aeronautics and Space Administration (NASA) uses the SeaDAS (SeaWiFS Data Analysis System, current version 6.3, SeaWIFS: Sea Wide Field-of-view Sensor) processor, based on the algorithm of (Gordon & Wang, 1994) with several subsequent modifications and improvements (IOCCG, 2010). Initially developed for processing data from NASA sensors such as the Coastal Zone Color Scanner (CZCS), SeaWiFS, and the Moderate resolution Imaging Spectroradiometer (MODIS), the SeaDAS processor has now also been extended to incorporate additional sensors. For the Medium Resolution Imaging Spectrometer (MERIS), the European Space Agency (ESA) uses the “MERIS Instrument Processing Facility” (IPF), whose latest version is 6.04; equivalent to the MEGS-8 (MERIS Ground Segment data processing prototype version 8.0). The

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implementation of the algorithm based on Antoine and Morel (1999) will be further noted as MEGS (see Bourg, 2012). Both the MEGS and the SeaDAS processors rely on the satellite signal in the near-infrared wavelengths to infer the optical properties of atmospheric aerosol, which are then extrapolated into the visible domain to implement the atmospheric correction in those wavelengths.

Alternate algorithms have also emerged that use both visible and near infrared wavebands for atmospheric correction, using techniques such as neural networks (Schiller & Doerffer, 1999), spectral optimisation methods (Chomko & Gordon, 1998, 2001; Chomko, Gordon, Maritorena, & Siegel, 2003; Steinmetz, Deschamps, & Ramon, 2011) and spectral matching methods (Gordon, Du, & Zhang, 1997).

The performance of the atmospheric correction algorithms is evaluated in a point-by-point comparison of normalised water leaving reflectances derived from satellite with in-situ measurements close in time and space, so called “match-ups”. The analysis presented here, is confined to MERIS satellite data and match-up data from the “MERis MAtchup In-situ Database” (MERMAID). In order to define an objective selection process which identifies the most suitable AC processor, a methodology for in-situ comparisons is developed, which converts statistical parameters and their confidence intervals as representations of product quality into a relative score per processor. The influence of the match-up data selection on the scoring results is investigated. The stability and error of the scoring system is tested with the help of the bootstrap method and the results are discussed.

2. Preparation of in-situ data and satellite data with candidate processors

2.1. In-situ site selection

MERMAID has been created to allow an easy access to match-up data which combines normalised water leaving reflectances measured in-situ and derived from MERIS satellite data. The water leaving reflectance ρ is defined as (Eq. 1, Antoine & Morel, 1998)

$$\rho(\lambda,\theta_v,\theta_s,\Delta\phi) = \pi L_w(\lambda,\theta_v,\theta_s,\Delta\phi)/E_s(\lambda)cos(\theta_s) \quad (1)$$

with wavelength λ, sun zenith angle θ_s, viewing angle θ_v, azimuth angle difference $\Delta\phi$, water leaving radiance L_w and irradiance $E_s(\lambda)$. By normalisation the radiometric instances are converted into a state which is independent of the observation geometry, i.e. the sun position is at the zenith and the viewing direction is in the nadir.

Specific stations of the AERONET-OC (“AErosol-RObotic-NETwork-Ocean-Color” component, Zibordi et al. (2009), Zibordi et al. (2010)) (AAOT [Aqua Alta Oceanographic Tower], Helsinki Lighthouse, Gustav Dalén Tower) are selected as well as the two major buoys located in deep open-ocean waters; the Marine Optical Buoy (MOBY, Clark et al., 1997), and the buoy for the acquisition of long-term optical times series BOUSSOLE (Bouée pour l'acquisition de Séries Optiques à Long Terme, Antoine et al., 2008). In addition, the data ensembles from different cruises (Plumes and Blooms, NOMAD Werdell & Bailey, 2005, SIMBADA Deschamp, Fougnie, Frouin, Lecomte, & Verwaerde, 2004) are considered. These stations are supposed to comprise chlorophyll dominated optical water types (case 1 water) which cover most of the open oceans. In a stricter definition of case 1 the dataset is restricted to spectra with reflectances at 560 nm smaller than 0.01.

For the AERONET sites, MERMAID provides the data with site specific band-shift correction as not all in-situ radiometers share the same spectral bands as MERIS (Zibordi et al., 2009). To NOMAD and SIMBADA data, an empirical band-shift is applied at 555 nm to 560 nm and 670 nm to 665 nm respectively, where necessary. The empirical band-shift utilises in-situ data from NOMAD, where in-situ measurements at 555 and 560 nm or 665 and 670 nm have been taken simultaneously. Their dependence can be described by a linear relationship, if bias-corrected logarithmic reflectances ρ are considered. The linear fit assumes errors for both variables. To correct the spectral mismatch at 555 nm to 560 nm the following empirical relationship (Eq. 2) is applied:

$$\log_{10}\rho(560) = bias + a + b \cdot \log_{10}\rho(555) \quad (2)$$

with $bias = 0.0172$, $a = 0.1735$ and $b = 1.0768$. The band-shift from 670 to 665 nm uses a $bias = 0.0751$, $a = -0.0198$ and $b = 1.035$. Even though this empirical approach is not ideal, it serves the purpose of the analysis to increase the number of exhaustive spectra (Table 1).

2.2. AC processor selection

The candidates for the atmospheric correction procedure is the standard processor for MERIS, here noted as MEGS, the SeaDAS 6.3, the POLYMER processor in the algorithm's version 2.4.1 (Steinmetz et al., 2011), and an implementation of the ForwardNN, which is a modification of the MERIS' standard processor for retrieval of case 2 water constituents. MERIS IPF-6, commonly referred to as MEGS8, has a NeuralNet-algorithm applied for atmospheric correction specific for the retrieval of case 2 water constituents (Doerffer, 2011).

The MEGS processor has been developed specifically for the MERIS sensor and has undergone continuous improvement and optimisation.

SeaDAS started with CZCS, was optimised and applied to SeaWIFS and MODIS and was recently extended to other sensors such as MERIS. Especially being applicable to many sensors makes it a prominent candidate for producing a multi-sensor long-term climate data record.

The processors MEGS and SeaDAS incorporate algorithms, which rest on the assumption that there is no signal coming from the water in the NIR. They are therefore by definition only valid in case 1 water, which holds this assumption. The atmospheric contribution is then extrapolated to the visible part of the spectrum. To further the application beyond case 1 waters, a bright pixel correction has been introduced in MEGS8.

Other algorithms that utilise both visible and near-infrared bands have been developed. The first algorithm of this type used operationally, had been included in the IPF-6. This neural net approach is optimised for case 2 waters and has been designed to work in sun glint conditions (Doerffer, Schiller, Fischer, Preusker, & Bouvet, 2008). This algorithm has been recently modified to a combined forward-NN and an iterative optimisation method to allow usage with a flexible subset of a total 35 wavelength bands. A prototype version of this ForwardNN approach has been included in the analysis, which is known to suffer from an implementation error. The angular specifications are faulty which lead to a large loss of data to invalid products on the right hand side of each satellite orbit. Nevertheless this severe error does not strongly deteriorate the quality of the water leaving reflectance when compared to in-situ match-ups. As this paper focusses on the selection methodology, it has been decided to keep the uncorrected results of the ForwardNN. After a future revision of the processor results are expected to change for the better.

Another independent algorithm development of this type is the POLYMER processor. It also uses many wavelength bands in the visible and the near infrared region. Similarly to the NN-processor, it is capable of handling radiance data, which is strongly affected by sun glint and by successfully retrieving water leaving reflectances. A three-day composite map of chlorophyll derived from MERIS with the standard MEGS processor and the POLYMER processor, depicts the increase in spatial and temporal coverage vividly (Fig. 1).

2.3. Selection and preparation of match-up data

The selection of data points from the MERMAID database relies on several levels of combined quality information:

1. The satellite overpass has to be within a three hour interval before or after the in-situ measurement. All sky conditions are allowed, while the maximum wind speed is 9 m/s.