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Multi-satellite time series of inherent optical properties in the California Current

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ABSTRACT

Satellite ocean color radiometry is a powerful method to study ocean biology but the relationships between satellite measurements and the in situ ocean properties are not well understood. Moreover, the measurements made with one satellite sensor may not be directly compatible with similar measurements from another sensor. We estimate inherent optical properties (IOPs) in the California Current by applying empirically optimized versions of the Quasi-Analytical Algorithm (QAA) of Lee et al. (2002) to satellite remote sensing reflectance (Rrs) from four ocean color sensors (OCTS, SeaWiFS, MODISA and MERIS). The set of estimated IOPs includes the total absorption coefficient at 490 nm (a490), phytoplankton absorption coefficient at 440 nm (aph440), absorption by dissolved and detrital organic matter at 440 nm (adg440) and particle backscattering coefficient at 490 nm (bbp490). The empirical inversion models are created by minimizing the deviations between satellite match-ups with in situ measurements and between the estimates of individual overlapping satellite sensors. The derived empirical algorithms were then applied to satellite Level-3 daily Rrs to create merged multi-sensor time series of the near-surface optical characteristics in the California Current region for a time period of over 16 years (November 1996-December 2012). Due to the limited number of in situ match-ups and their uneven distribution as well as the large errors in the satellite-derived *Rrs*, the uncertainty in the retrieved IOPs is still significant and difficult to quantify. The merged time series show the dominant annual cycle but also significant variability at interannual time scales. The ratio of adg440 to aph440 is around 1 in the transition zone, is > 1 in the coastal zone and generally < 1 offshore. adg440 decreases towards south and towards offshore. The long-term (~ 16 years) trend in *aph440*, representative of phytoplankton biomass, shows a significant (P < 0.01) increasing trend in a wide band (~ 500 km) along the coast and a significant decreasing trends in the oligotrophic North Pacific gyre. The trend of increasing aph440 in the upwelling areas off California is positively correlated with the increasing wind speed along the coast. © 2013 Elsevier Ltd. All rights reserved.

Abbreviations: CalCOFI, California Cooperative Oceanic Fisheries Investigations; CCE-LTER, California Current Ecosystem Long Term Ecological Research; CCMP, Cross-calibrated multi-Platform wind data (Atlas et al., 2009); GAC, global area coverage; ENVISAT, ESA earth observation satellite; ESA, European Space Agency; ESRID, empirical satellite-in situ data (Gregg et al., 2009); IOP, inherent optical property; MERIS, medium resolution imaging instrument on ESA Envisat satellite; NASA, National Aeronautics and Space Agency; NOMAD, NASA bio-Optical Marine Algorithm Data set (Werdell and Bailey, 2005); OCTS, Ocean Color and Temperature Sensor on Japan ADEOS satellite; QAA, Quasi-Analytic Algorithm (Lee et al., 2002); QaaCalFit, empirically fitted QAA developed in this work; RR, reduced resolution (of MERIS data); SeaWiFS, sea-viewing wide field-of-view sensor; VIIRS, visible infrared imager radiometer suite

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1. Introduction

Oceanic phytoplankton play an important role in global carbon and energy budgets and any changes in the concentration, composition and turnover rates are therefore of special interest, especially in the context of the global climate change debate. Satellite observations of ocean color have become the most important method of monitoring global distributions of phytoplankton and ocean productivity, and validating various global climate models (McClain, 2009; Yoder et al., 2011). The primary output product of ocean color measurements has been the concentration of chlorophyll-a (*Chla*) which is also the main input to ocean primary productivity models (Behrenfeld and Falkowski, 1997). Operational *Chla* algorithms (O'Reilly et al., 1998; O'Reilly et al., 2000) are based on the ratio of remote sensing reflectance

| Notations aw hbn | coefficient of absorption by pure sea water (m^{-1}) | | |
|--|---|--|--|
| acoefficient of absorption (m^{-1}) bbpa490coefficient of absorption at 490 nm (m^{-1}) R^2 adgCoefficient of absorption by dissolved and detrital organic matter (m^{-1}) RMA adg440adg at 440 nm (m^{-1}) Rrs aphcoefficient of absorption by phytoplankton (m^{-1}) $Rrs412$ | bbp at 490 nm (m ⁻¹) coefficient of determination reduced major axis (regression) root mean square remote sensing reflectance (sr ⁻¹) remote sensing reflectance at 412 nm (sr ⁻¹) | | |

(*Rrs*) at blue and green wavelengths, which primarily represents a change in the total absorption coefficient at the blue wavelength (\sim 440 nm). However, the total absorption at \sim 440 nm is not determined solely by the absorption of phytoplankton pigments, $aph(\lambda)$, but also by the absorption by colored dissolved organic matter (CDOM), detritus, suspended solids and pure ocean water. The relative contributions of these individual components are not constant but vary over space and time. CDOM and detritus are often added together and their sum is called colored detrital and dissolved materials (CDM, Siegel et al., 2002) with the respective absorption component $adg(\lambda)$. CDOM and detritus are produced primarily during the remineralization of the sinking particulate organic matter (Swan et al., 2009) and CDOM is destroyed at the surface by solar bleaching (Nelson et al., 1998). The ratio of $adg(\lambda)$ to $aph(\lambda)$ is an inverse index of the proportion of autotrophic light absorption and varies over a wide range in the world ocean. Moreover, variations in the ratio $adg(\lambda)$ to $aph(\lambda)$ are causing systematic bias in the operational Chla products (Siegel et al., 2005; Sauer et al., 2012). It is obvious that empirical band-ratio estimates of *Chla* are expected to have errors in response to the seasonal, regional or long-term changes in the $adg(\lambda)$ to $aph(\lambda)$ ratio. Estimates of phytoplankton productivity are also affected as (1) most primary productivity models are based on Chla, and (2) absorption by components other than $aph(\lambda)$ are not contributing to primary production by phytoplankton. Therefore, instead of using the biased Chla estimate produced by the standard band ratio algorithms, it is more appropriate to estimate phytoplankton absorption $aph(\lambda)$ which can be converted to *Chla* using a locally validated model for *Chla*-specific absorption coefficient. Lee et al. (1996) proposed an algorithm for calculating phytoplankton primary productivity based on inherent optical properties (IOPs). IOPs are properties of the medium that do not depend on the ambient light field. As such, they are distinguished from apparent optical properties (AOPs), such as the remote sensing reflectance (Rrs). The so-called absorption-based productivity algorithm (Aph-PP) replaces *Chla* with $aph(\lambda)$ as its primary input. There are two advantages of using $aph(\lambda)$ instead of the *Chla* in models of net primary productivity. First, the influence of absorption by CDM is explicitly included in the inversion process; and second, the uncertainty associated with Chla-specific absorption coefficient is avoided. In addition, *aph* is a good index of phytoplankton dynamics (e.g. Shang et al., 2011).

The California Current is a major and well-characterized Eastern boundary current with monitoring programs such as CalCOFI going back many decades as well as process oriented programs such CCE-LTER (Ohman and Venrick, 2003). While there have been reports of a rapid global decline in oceanic phytoplankton biomass (Boyce et al., 2010), studies in the California Current have reported the opposite trends: increasing turbidity (Aksnes and Ohman, 2009) and increasing surface chlorophyll-a (*Chla*) and primary productivity in the coastal zone (Kahru and Mitchell, 2008; Kahru et al., 2009, 2012).

The best known and most used ocean color sensor, SeaWiFS, stopped providing data in the end of 2010 and extending

consistent ocean color time series beyond 2010 has been a problem. Here we create satellite algorithms that are empirically tuned to in situ datasets of inherent optical properties and minimize the sensor to sensor differences at the same time. As output of our optimized models we have selected the following inherent optical properties: total absorption coefficient at 490 nm (a490), phytoplankton absorption coefficient at 440 nm (aph440), absorption by dissolved and detrital organic matter at 440 nm (adg440) and particle backscattering coefficient at 490 nm (bbp490). These are also the inputs to the Lee et al. (2011) absorption-based productivity model where the a490 and bbp490 values are required for the calculation of euphotic zone depth and aph440 replaces Chla as the major input to the production model per se. We merge satellite data from four ocean color sensors (OCTS, SeaWiFS, MODISA and MERIS) into a unified time series of several IOPs and evaluate their variability during the last 16 years (1996-2012).

2. Data and methods

2.1. In situ measurements of the inherent optical properties of seawater

In situ measurements were made on a number of cruises that were part of the CalCOFI (from CAL9610 to CAL0304) and CCE-LTER (P0704, P0810) programs.

The spectral backscattering coefficient, $bb(z, \lambda)$, was determined from in situ measurements with Hydroscat-6 sensors (HobiLabs, Inc.), each with six wavebands in the visible range from 440 to 676 nm. Data were processed with the methods described by Maffione and Dana (1997), Boss and Pegau (2001) and Allison et al. (2010). The coefficient *bb* is considered to be the sum of contributions from pure water backscattering, *bbw*, and particle backscattering, *bbp*. The near-surface data (at depths less than ~5 m) were discarded because of significant fluctuations at these shallow depths and the subsurface values were extrapolated to the surface.

The spectral particulate absorption coefficient, $ap(\lambda)$, was measured with a filter-pad technique (Mitchell et al., 2002). Discrete water samples were collected from CTD/rosette casts and filtered onto GF/F filters. The spectrophotometric measurements on the filters were made in the transmittance mode on freshly collected samples. The data were acquired in the spectral range from 300 to 800 nm with a 1 nm interval and the correction for the pathlength amplification factor was made following Mitchell (1990). After the $ap(\lambda)$ measurement, the GF/F filter was treated with 100% methanol to remove phytoplankton pigments, and the spectrophotometric measurements were then taken on the "bleached" filters to determine the spectral absorption coefficient of non-algal (detrital) particles, $ad(\lambda)$ (Kishino et al., 1985). Assuming that the total particulate absorption, $ap(\lambda)$, is the sum of the detrital absorption, $ad(\lambda)$, and phytoplankton absorption, $aph(\lambda)$, the latter was calculated as $aph(\lambda) = ap(\lambda) - ad(\lambda)$.

The determinations of the absorption by chromophoric dissolved organic matter (CDOM) or gelbstoff, $ag(\lambda)$, were made following Mitchell et al. (2002). Samples of seawater were filtered through 0.2 µm Nuclepore filters, the filtrate was collected in acidwashed combusted glass bottles and the spectral absorption coefficient $ag(\lambda)$ was measured between 250 and 750 nm with a spectrophotometer on freshly prepared samples using a blank of a standard purified deionized water (Milli-Q) in 10 cm quartz cuvettes. The spectra were corrected for an offset measured at 650 (± 5) nm, which can be attributed mainly to scattering effects. The exponential fit was made to these spectra and a blank spectrum was subtracted to achieve the final $ag(\lambda)$ values. The sum of $ag(\lambda)$ and $ad(\lambda)$ is referred to as $adg(\lambda)$ and represents the sum of absorption by detrital and dissolved organic matter. We use only the near-surface estimates of $bbp(\lambda)$, $aph(\lambda)$, $adg(\lambda)$, as well as the total absorption coefficient, $a(\lambda) = aw(\lambda) + aph(\lambda) + adg(\lambda)$, for the blue and green spectral wavebands (440 and 490 nm). All of the near-surface points were within both the mixed layer and the first optical depth. The pure water absorption values, $aw(\lambda)$, were taken from Pope and Fry (1997) and those of $bbw(\lambda)$ from Morel (1974).

2.2. Study area

In order to examine various time series in different regions of the California Current we used the grid of 3 by 4 areas (Fig. 1A) from offshore (approximately 300–1000 km from coast) through a transition zone (100–300 km from coast) to the coastal zone (0–100 km from coast), and from north to south as Central California (areas 1–3), Southern California (areas 4–6), Northern Baja California (areas 7–9) and Southern Baja California (areas 9–12). This grid has been used in the past (e.g. Kahru and Mitchell, 2001) and derives from the work of Lynn and Simpson (1987) who showed that the variability structure of dynamic height in the California Current can be divided into offshore, transition and coastal bands that are roughly parallel to the coast.

2.3. Match-ups between satellite and in situ data

The validation of satellite products using quasi-simultaneous and spatially collocated measurements (match-ups) of satellite and in situ data followed the general procedures of previous studies (e.g. Kahru and Mitchell, 1999; Werdell and Bailey, 2005; Bailey and Werdell, 2006; Antoine et al., 2008; Kahru et al., 2012). The latest available versions of Level-2 (i.e. processed to surface quantities but unmapped) data from four ocean color satellite sensors were used: 2010.0 for OCTS (1996-1997), 2010.0 for SeaWiFS (1997-2010), 2012.0 for MODIS-Aqua (MODISA, 2002-2012), and 3rd reprocessing for MERIS (2002-2012). We used the full resolution (\sim 1 km) Level-2 data for SeaWiFS and MODISA, the GAC Level-2 (\sim 4 km) for OCTS and the RR data (\sim 1 km) for MERIS. For OCTS each GAC pixel is every 4th full resolution pixel both along and across the track of the satellite with a ground separation of about 4 km. The MERIS RR data have approximately the same 1 km spatial resolution as the full-resolution SeaWiFS and MODISA data. OCTS. SeaWiFS and MODISA Level-2 data were obtained from NASA's Ocean Color website (http://oceanco lor.gsfc.nasa.gov/) and MERIS Level-2 data were obtained from ESA's MERIS Catalogue and Inventory (http://merci-srv.eo.esa.int/ merci/welcome.do). For each Level-2 pixel we used the corresponding Level-2 flags. A pixel was determined valid if none of the following flags were set: ATMFAIL, LAND, HISATZEN, CLDICE, CHLFAIL, SEAICE, NAVFAIL, HIPOL and PRODFAIL. Standard ESA MERIS processing procedures use different flags. If any of the following MERIS flags was set then the pixel was considered invalid: LOW SUN, HIGH_GLINT, ICE_HAZE, SUSPECT, COASTLINE, PCD_19, PCD_18, PCD_17, PCD_16, PCD_15, PCD_14, PCD_1_13, CLOUD and LAND. All variables in Level-2 files were extracted from 3×3 pixel windows centered at the pixel nearest to the in situ sample. As satellite pixels close to cloud edges or land have increased errors, we included only those match-ups with at least 3 valid pixels (out of 9). The maximum time difference with in situ sample was set at 24 h; however, most match-ups were within 2 h and had at least 7 valid pixels. The mean $Rrs(\lambda)$ value of valid pixels within the 3×3 pixel window was used as input to the QAA model. The spatial distribution of match-ups with in situ measurements of IOPs is shown in Fig. 1B.

2.4. Satellite to satellite match-ups

For a comparison of products between different satellite sensors we created satellite to satellite match-ups plotting the same pixel in Level-3 globally mapped 9-km images for the same day over the California Current region. Daily Level-3 data are binned using the best quality Level-2 data and exclude questionable pixel values that are present in Level-2 datasets. Temporally overlapping daily data are available from three sensors (SeaWiFS,



Fig. 1. (A) Grid of 12 selected areas from northern California to the southern tip of Baja California parallel and across the mean coastline: coastal (0–100 km, areas 3, 6, 9, 12), transition (100–300 km, areas 2, 5, 8, 11) and offshore (300–1000 km, areas 1, 4, 7, 10). The north–south bands are called Central California, Southern California, Northern Baja California and Southern Baja California, respectively. (B) Locations of the in situ match-ups (circles) and satellite to satellite match-ups (*).

MODISA and MERIS). OCTS, SeaWiFS and MODISA Level-3 datasets were downloaded from NASA's Ocean Color website (http:// oceancolor.gsfc.nasa.gov/) and MERIS Level-3 data were obtained from ESA's GlobColour Project at ftp://hermes.acri.fr/meris_13. MERIS data were remapped to the same grid as the NASA data.

The number of potential satellite-to-satellite match-ups is orders of magnitude higher than the small number of available match-ups with in situ IOP data. In order to have approximately comparable weight from the in situ match-ups we reduced the number of satellite to satellite match-ups used in the algorithm tuning while keeping a representative set of points covering the full range of data. We first created sensor to sensor (MODISA to SeaWiFS in 2004. MERIS to SeaWiFS in 2004. MERIS to MODISA in 2012) match-ups for the *Rrs412* band for a selected year. We then sorted these match-ups by Rrs412 value of the first satellite sensor (SeaWiFS in the first two comparisons and MODISA in the third comparison), deleted the lowest ten and highest ten match-ups and then picked every Nth match-up. N was varied to produce approximately 30–40 match-ups. We then added all the other Rrs bands of the same pixel and same day to create the full spectral Rrs match-up data used as input to the QAA models. As a result, we created a representative dataset of 34 MODISA vs. SeaWiFS matchups, 37 MERIS vs. SeaWiFS match-ups and 31 MERIS vs. MODISA match-ups. The procedure allowed us to reduce the number of satellite-to-satellite match-ups but to keep a representative range of Rrs values while also removing the lowest and highest values where we would expect additional between-sensor errors (Kahru et al., 2012). The spatial distribution of these satellite-to-satellite match-ups is shown in Fig. 1B.

2.5. Fitting the QAA model to match-ups with in situ data

The Quasi-Analytical Algorithm (QAA) developed by Lee et al. (2002) is a method to derive the absorption and backscattering coefficients by inverting the spectral remote-sensing reflectance, $Rrs(\lambda)$. QAA starts with the calculation of the total absorption coefficient $a(\lambda)$ at a reference wavelength and then propagates the calculation to other wavelengths. Component absorption coefficients $adg(\lambda)$ and $aph(\lambda)$ are further algebraically decomposed from the total absorption spectrum. The coefficients used in QAA were derived using synthetic (modeled) data. Satellite estimates of Rrs spectra contain significant errors due to problems with sensor calibration, atmospheric correction, unresolved surface effects like glint and foam, sensor saturation and recovery from bright targets like clouds, the effect of sub-pixel clouds, etc. Satellite estimation of Rrs is inherently a difficult problem due to the small signal to noise ratio as over 90% of the signal at the top of the atmosphere is created by the atmosphere and not by the underlying ocean (Siegel et al., 2000). As QAA and other semi-analytic algorithms are very sensitive to such errors, the application of such algorithms to noisv and biased satellite data is problematic. The updated version of QAA (version 5) as described in http://www.ioccg.org/groups/Soft ware_OCA/QAA_v5.pdf was used here. QAA version 5 includes 10 coefficients that are estimated from modeled data or from theoretical considerations. We treat these 10 coefficients as tunable parameters that can be optimized by minimizing the absolute deviations from the measured values, with an implicit assumption that field-measured values were error-free. We use the values of the coefficients in the standard QAA as the starting point of the minimization process which optimizes the values of these 10 coefficients for each of the 4 sensors, i.e. 40 coefficients in total. For the optimization we used the Trust-Region method, a variant of the Levenberg-Marquardt method as implemented in the NMath 5.2 numerical libraries (http://www.centerspace.net/). As both observed and predicted values of IOPs cover a range of several orders of magnitude, we used log₁₀ transformed IOP data.

After running the minimization procedure there was still residual bias which was removed with the following empirical adjustment: YAdjusted = (Y - intercept)/slope, where Y is the vector of predicted values after applying the coefficients derived in the optimization procedure, YAdjusted is the adjusted vector of output values, *intercept* and *slope* are respectively the intercept and slope of the reduced major axis (RMA) regression between Y and the vector of in situ measurements X. RMA regression is more appropriate than the standard ordinary least squares regression as the independent variable (either the measured in situ IOP values or the estimates using another satellite sensor) is measured with error (Sokal and Rohlf, 1995). The resulting sets of optimized QAA coefficients and the coefficients of adjustment (*intercept* and *slope*) are used in the QAA model and the procedure is called the QaaCalFit model.

2.6. Wind data

We used Cross-Calibrated Multi-Platform (CCMP) ocean surface winds (Atlas et al., 2009) derived through cross-calibration and assimilation of data from SSM/I, TMI, AMSR-E, SeaWinds on QuikSCAT, and SeaWinds on ADEOS-II (http://podaac-ftp.jpl.nasa.gov/allData/ccmp/L3.5a/). These data sets are combined with conventional observations and with a starting estimate of the wind field using a variational analysis method. For this study, we used wind speed (U, m/s) Level 3.5 monthly data with 25 km spatial resolution.

2.7. Statistical estimates of model performance

We used three statistical measures to assess the performance of the different algorithms in comparisons between satellite products and in situ observations (satellite to in situ match-ups) or between satellite products of multiple sensors (satellite to satellite matchups). In satellite to in situ match-ups O_i is the *i*th observation of an in situ variable and P_i is the corresponding predicted satellite variable. In satellite to satellite match-ups the choice of the observed versus predicted variable is arbitrary. All the estimates of performance were done with log_{10} transformed values. The coefficient of determination (R^2) shows how well one variable can be predicted from another. An estimate of scatter between observation and prediction, *delta*, was calculated as (following Lee et al., 2011):

$$RMSD = \sqrt{\text{AVERAGE}\left[\log_{10}\left(\frac{O_i}{P_i}\right)\right]^2},$$

 $delta = (10^{RMSD} - 1) \times 100\%$

An estimate of the bias between observation and prediction (*Bias*) was calculated as the median of the absolute percent error *Abs* $((P_i - O_i)/O_i)$. The median is multiplied by 100 to be expressed in percent.

3. Results

3.1. Comparison of remote sensing reflectance from different sensors

We are fortunate to have temporally overlapping sensor pairs: MODISA with SeaWiFS: from 4 Jul 2002 to 11 Dec 2010, MERIS with SeaWiFS: from 1 Jul 2002 to 11 Dec 2010 and MERIS with MODISA: from 4 Jul 2002 to 8 Apr 2012. We can therefore compare directly the same pixel value on the same day from a pair of sensors. Different sensors have different optical characteristics even for the same nominal waveband, e.g. 412 nm; they have different sensitivities, signal to noise ratios, calibration and degradation histories. Additionally, different satellite orbits lead to different observation times, observation geometries, variable influences by sun glint, solar zenith angle, and clouds. In this paper, we do not intend to accomplish a comprehensive analysis of the differences and errors between the various *Rrs* bands of the different sensors. We show by examples that both random and systematic differences in *Rrs* exist and are significant. We use these differences and errors as a justification for designing empirical algorithms for IOPs that are optimized for the real satellite data and not for the ideal data that we may hope to have.

Using 2004 as an example we found nearly 440,000 same day *Rrs412* match-ups between MODISA and SeaWiFS in the California Current region using 9-km Level-3 data and about 214,000 match-ups between MERIS and SeaWiFS *Rrs412* (Fig. 2). The approximately 2 times fewer match-ups with MERIS are at least partly due to the narrower swath of the MERIS/ENVISAT orbit. In order to show the central tendencies of the distributions we divided the full range (in log₁₀ scale) into 100 segments, found the median of the first sensor points in each segment and the median of the

corresponding second sensor points in each segment. These median bracket points are a good approximation of the central tendency until the values diverge at about 0.001 (-3 in \log_{10} units). It is obvious that there is a lot of scatter in Rrs estimates of the same day and same pixel. When these different Rrs values are used in sensitive inversion algorithms, we can assume very different outputs for the derived IOPs for the same day and location. Fig. 2 shows that differences of an order of magnitude and larger are common in Rrs, especially at lower Rrs levels which are expected at higher levels of absorption, i.e. primarily in the coastal zones. While the median bracket points of all the sensor pairs are close to the one-to-one line until they diverge at low *Rrs412* values, the median MERIS *Rrs412* values are significantly below those of SeaWiFS in 2004 and especially of those of MODISA in 2012. The differences between MERIS and MODIS increased from 2004 to 2012. At the $log_{10}(Rrs412)$ value of about -2.5 MERIS Rrs412 is only about 60% of the corresponding MODISA value of 2012 match-ups (Fig. 3). While Rrs412 of MODISA is close to that of



Fig. 2. Inter-sensor comparison of satellite-derived remote sensing reflectance at 412 nm (*Rrs412*). Blue dots show same day match-ups between Level-3 global 9-km mapped datasets, red line is the one-to-one line, yellow line is the least squares linear regression. Small red circles are the median bracket points that were generated by dividing the full horizontal range (in log10 units) into 100 equal sections and finding median values for the abscissa variable and the corresponding points of the ordinate variable. (A) MODISA versus SeaWiFS in 2004; (B) MERIS versus SeaWiFS in 2004; (C) MERIS versus MODISA in 2004; (D) MERIS versus MODISA in 2012. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 3. Ratio of the corresponding *Rrs412* value estimated by different satellite sensors. The plots show the median bracket points of the satellite to satellite match-ups at daily Level-3 images over the year of 2004 for MODISA versus SeaWiFS and MERIS versus SeaWiFS and for year 2012 for MERIS versus MODISA. The heavy black line of *Rrs412/Rrs412*=1 corresponds to the ideal case of no intersensor bias.

SeaWiFS, the median MODISA Rrs412 is still only about 90% of the corresponding SeaWiFS value over a wide range (Fig. 3). While the analysis shown here uses only the 412 nm band, quite similar differences were observed for all other bands (not shown). An advantage of band ratio algorithms is that a large part of these differences are correlated between Rrs bands and therefore cancels out when band ratios are used. When using semi-analytic algorithms that are sensitive to the actual Rrs values we can expect large errors in most products due to the differences in the estimated satellite Rrs values. In contrast, estimates of the coefficient of total absorption a490 are robust (see below) and were predicted well with the standard QAA. Our conclusion from this rather limited exercise is that when using satellite Rrs values in sensitive inversion schemes like QAA, we need either remove the bias between sensors or adjust the coefficients for each sensor. We cannot expect compatible output from different satellite sensors when applying models with generic coefficients to satellite Rrs values with systematic and random bias.

3.2. Optimizing the QAA model for individual satellite sensors

We applied the standard QAA model (http://www.ioccg.org/ groups/Software_OCA/QAA_v5.pdf) to satellite Rrs data corresponding to the match-ups with in situ data (Fig. 4, left columns). For all four sensors we observed that satellite predictions of *a*490 by the standard QAA model corresponded very well to in situ measurements. However, the QAA-estimated bbp490 was significantly overestimated and the QAA-estimated aph440 was significantly underestimated compared to in situ data. For OCTS we did not have temporally overlapping in situ bbp490 data but the aph440 underestimation was similar to other sensors and therefore we assume the same relationship. After applying empirical tuning to the QAA coefficients and subsequent empirical adjustment, we derived empirically optimized models to estimate the selected IOPs, based on in situ match-ups (Fig. 4, right columns). As a490 was already estimated well by the standard QAA model, there was no improvement for a490. In fact, applying the final algorithm resulted in insignificant deterioration in Bias (from 0 to -1) but slight improvement in R^2 and *delta* (Table 3, top rows). For all other selected IOPs the optimization process increased R^2 , reduced scatter (delta) and drastically reduced bias compared to in situ match-ups. After applying the linear adjustment to remove the remaining linear bias the final RMA regressions have the slope of 1.0 and intercept of 0.0 (Fig. 4, right columns).

3.3. Optimizing the QAA model to reduce differences between satellite sensors

As shown in Fig. 4, we can tune the QAA model and significantly improve the predictions compared to in situ observations. However, in order to create consistent time series from multiple sensors we need algorithms that not only agree with in situ data but also minimize differences between each other. This can be formalized as 2 tasks: (1) minimize the differences with in situ data: and (2) minimize the differences between the corresponding products of different sensors. Ideally, with adequate number and distribution of in situ match-ups over the full range of possible values, task 2 would automatically follow from task 1. However, in reality the distribution of in situ match-ups is limited, highly nonuniform and most probably is not representative of the full range of variability not just along the magnitude axis but also in terms of other contributing factors, such as time of the year, distance from coast, location along the north-south and/or east-west axes, etc. Therefore, using algorithms derived solely from minimizing the differences with a limited and inadequately distributed set of in situ match-ups does not guarantee to get similar satellite estimates from different sensors and will most probably lead to systematic differences between the products of different sensors. This expectation was confirmed by our analysis. The statistical differences between sensors may actually increase using the algorithms tuned to in situ data compared to the standard algorithms. We therefore implemented a complex optimization procedure to minimize not only the differences between in situ and satellite data but also the differences between the modeled data of individual satellite sensors.

In Section 2.3 we described how we created satellite to satellite match-up datasets that have a relatively small number of welldistributed points covering nearly the full range of *Rrs412*. In our complex minimization process we included the following datasets: 19 in situ match-ups with MODISA, 12 in situ match-ups with MERIS, 46 in situ match-ups with SeaWiFS, 34 MODISA vs. SeaWiFS match-ups, 37 MERIS vs. SeaWiFS match-ups and 31 MERIS vs. MODISA match-ups. That is a total of 77 in situ matchups and 102 satellite to satellite match-ups. For each match-up we evaluated the difference of 4 variables: a490, bb490, aph440 and adg440 which make 716 pairs of comparison to be minimized. As output, we obtained the optimal values of 30 coefficients in QAA, i.e. 10 for each of the three overlapping sensors (SeaWiFS, MODISA and MERIS, Table 1). As OCTS did not have simultaneous measurements by other sensors, this analysis could not be applied to OCTS and we used the coefficient values obtained from comparisons with in situ match-ups only (Fig. 4A). The linear adjustment coefficients (intercept and slope) are used to remove the remaining linear bias in log₁₀ space and are separate for each sensor and IOP variable (Table 2). After applying these operations, the final RMA regressions have a slope 1.0 and an intercept of 0.0 (Figs. 5-7). The performance of the standard QAA and the empirically optimized QAA are compared in Table 3.

3.4. Time series of the merged multi-sensor IOPs

We applied the QaaCalFit algorithms (Tables 1 and 2) to the daily Level-3 *Rrs* datasets of the four sensors (OCTS, SeaWiFS, MODISA and MERIS). Merged daily QaaCalFit datasets of *a490*, *adg440*, *aph440* and *bbp490* were created by averaging the corresponding valid values of the individual sensors. The merged daily QaaCalFit datasets were then composited into monthly datasets by averaging the valid daily values over a month. While we calculated the time series for all four IOPs, we will concentrate on *adg440* and *aph440* which are of most interest in the context of understanding the status of the ecosystem. We will not discuss the



Fig. 4. Satellite match-ups (blue dots) after applying the standard QAA (left columns) and after the optimized and adjusted QAA (right columns). The red line is the one-toone line, yellow line shows the standard linear regression, and blue line shows the reduced major axis regression. (A) aph440 and adg440 for OCTS; (B) bbp490 and aph440 for SeaWiFS; (C) bbp490 and aph440 for MODISA; (D) bbp490 and aph440 for MERIS. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

 Table 1

 Optimized QAA coefficients in QaaCalFit compared to the standard QAA model.

| QAA OCTS | 2 50.326 | 1 35.549 | 1.2 - 35.692 | 0.9 0.001 | 0.015 0.015 | 0.74 0.461 | 0.2 0.117 | 0.8 0.805 | 0.002 0.081 | 0.6 0.678 |
|-------------|-------------|-------------|-----------------|--------------|----------------|---------------|--------------|--------------|----------------|--------------|
| SeaWiFS | 3.588 | 2.287 | 2.651 | 0.067 | 0.051 | -2.574 | 0.727 | 0.354 | 0.004 | -0.538 |
| MODIS | 1.730 | 0.178 | -1.618 | 1.485 | 0.045 | -1.691 | 2.207 | 0.053 | -0.014 | 0.424 |
| MERIS | 1.086 | -0.157 | 0.125 | 1.861 | 0.036 | - 1.189 | 1.452 | -0.012 | 0.007 | 0.688 |

time series of bbp490 as the inter-sensor compatibility produced by the current version of QaaCalFit is not satisfactory (Table 3). *bbp490* has the lowest R^2 (Sat/Sat)=0.425 when applied to the 2004 match-up datasets between MODISA/SeaWiFS and MERIS/ SeaWiFS and the 2012 dataset between MERIS/MODISA. The lower

| Table | 2 |
|-------|---|
|-------|---|

Linear adjustment coefficients of the QaaCalFit model.

| Sensor | Variable | Intercept | Slope | |
|---------|----------|-----------|-------|--|
| OCTS | a490 | 0.121 | 1.087 | |
| | bbp490 | | | |
| | aph440 | -0.197 | 0.936 | |
| | adg440 | -0.329 | 0.743 | |
| SeaWiFS | a490 | -0.136 | 0.930 | |
| | bbp490 | -0.668 | 0.663 | |
| | aph440 | -0.399 | 0.824 | |
| | adg440 | -0.634 | 0.653 | |
| MODISA | a490 | 0.059 | 1.072 | |
| | bbp490 | 0.022 | 0.984 | |
| | aph440 | -0.471 | 0.782 | |
| | adg440 | -0.418 | 0.782 | |
| MERIS | a490 | -0.520 | 0.721 | |
| | bbp490 | -0.838 | 0.484 | |
| | aph440 | -0.492 | 0.820 | |
| | adg440 | -1.046 | 0.492 | |
| | | | | |

N=77, R2=0.310, Y=-0.090+0.838 * X N=77, R2=0.566, Y=0.000+1.000 * X -1.5 -1.5 -1.75 -1.75 -2 -2 -2.25 -2.25 All sensors bbp490 All sensors bbp490 -2.5 -2.5 -2.75 -2.75 -3 -3 -3.25 -3.25 -3.5 -3.5 Predicted -3.75 -3.75 OneToOne **RMA** line -4 -4 -3.75-3.5 -3.25 -3 -2.75-2.5 -2.25 -2 -1.75-1.5 -3.75-3.5 -3.25 -3 -2.75-2.5 -2.25 -2 -1.75-1.5 -4 In situ bbp490 In situ bbp490 N=102, R2=0.425, Y=0.000+1.000 * X N=102, R2=0.398, Y=0.531+1.210 * X -1.5 -1.5 -1.75 -1.75**MODISA-MERIS bbp490 MODISA-MERIS bbp490** -2 -2 -2.25 -2.25 -2.5 -2.5 -2.75 -2.75 -3 -3 -3.25 -3.25 -3.5 -3.5 Predicted -3.75 -3.75 OneToOne RMA line -4 -4 -4 -3.75-3.5 -3.25 -3 -2.75-2.5 -2.25 -2 -1.75-1.5 -3.75-3.5 -3.25 -3 -2.75-2.5 -2.25 -2 -1.75-1.5 -4 SeaWiFS-MODISA bbp490 SeaWiFS-MODISA bbp490

skill of the algorithms to estimate bbp490 compared to the absorption coefficients is a consequence of their different role in the *Rrs* spectrum. While $bbp(\lambda)$ is closely related to the magnitude of Rrs spectrum and is therefore more affected by residual errors in atmospheric correction (e.g. Hu et al., 2013), the total absorption coefficient (and $aph(\lambda)$ and $adg(\lambda)$) are more related to the shape of the Rrs spectrum with much of the noise in magnitude being canceled out. The time series of a490 are also of less interest as they are similar to the sum of *adg440* and *aph440*. The mean annual cycles of *adg440* and *aph440*, averaged over 16 years (1996–2012). appear to be surprisingly similar (Fig. 8). The annual maximum of both adg440 and aph440 in the offshore regions occurs in the winter (mostly in January). In the transition zone the annual cycles of adg440 and aph440 are more variable, particularly that of adg440 which often has maxima in the spring. In the coastal zone both adg440 and aph440 peak in spring to summer (March to May). The ratio adg440 to aph440 (Fig. 8) shows an annual cycle that is quite similar to the annual cycle of *adg440*: the maximum in winter in the offshore regions, in spring in the transition zone and in springsummer in the coastal zone. There is a clear trend of decreasing adg440 and the ratio of adg440 to aph440 from north to south. The

ratio of adg440 to aph440 is mostly below 1 offshore, around 1 in the transition zone (over 1 in the north and below 1 in the south)

Predicted

OneToOne

Predicted

OneToOne

and above 1 in the coastal zone.

Fig. 5. Combined (SeaWiFS, MODISA, MERIS) match-ups (blue dots) of bbp490 between satellite estimates and in situ (top row) and between individual satellites (bottom row). Left column shows output from the standard QAA model, right column has output from the optimized QaaCalFit. The satellite to satellite matchups have combined MODISA vs. SeaWiFS, MERIS vs. SeaWiFS and MERIS vs. MODISA. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 6. Combined (OCTS, SeaWiFS, MODISA, MERIS) match-ups (blue dots) of aph440 between satellite estimates and in situ (top row) and between individual satellites (bottom row). Left column shows output from the standard QAA model, right column has output from the optimized QaaCalFit. The satellite to satellite match-ups have combined MODISA vs. SeaWiFS, MERIS vs. SeaWiFS and MERIS vs. MODISA. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

For each of the 12 areas (Fig. 1B) we created time series using spatially averaged monthly QaaCalFit datasets (Fig. 9A–C). In addition to the strong annual cycle, some areas showed patterns of multi-year variability. A common feature for the Central and Southern California transition and coastal zones (areas 2, 3, 5, 6) was a general increasing trend from 1998 until 2012 and a subsequent drop in 2012. This pattern was evident in all three IOPs (*adg440*, *aph440* and *bbp490*) and also in the *adg440* to *aph440* ratio. The southern coastal areas (Northern and Southern Baja) did not show a similar increase. The 1997–1998 El Niño had a dramatic effect, especially in the south.

In order to remove the dominant effects of the annual cycle we calculated monthly anomalies by first calculating the long-term mean values of each month and then divided the monthly values of each pixel to the respective long-term mean value of the month. Time series were created by averaging the anomalies in each area. In some areas (e.g. Area 2) the time series of *aph440* anomaly seems to have a periodic component with a long period. Anomaly plots show trends but also a sharp decrease in 2012 in most areas.

To get a more detailed spatial pattern of the potential trends we evaluated *aph440* trends and their significance for each pixel of the mapped images using the nonparametric Sen slope estimator (Sen, 1968). The nonparametric Mann–Kendall test was used to evaluate the statistical significance of the trend according to Salmi et al. (2002). Significant trend (at 99% confidence level) of

increasing aph440 in the coastal and transition zones of Central and Southern California and of decreasing aph440 in the transition and offshore areas of the Southern Baja areas were detected (Fig. 10A). Similar analysis was performed for the monthly anomalies of wind speed (1987-2011) that showed increasing winds along the coast and also offshore at about 50° N (Fig. 10B). Although we have not validated the QaaCalFit algorithm for the North Pacific Gyre outside the California Current we extended the evaluated area west to the Hawaiian Islands. The observed pattern of a significant decreasing trend in *aph440* anomalies is clearly visible in the North Pacific gyre waters and is consistent with the earlier reports on "expanding ocean deserts" (Behrenfeld et al., 2006; Polovina et al., 2008; Kahru et al., 2012). However, we must note that while the linear trend may be statistically significant, it may not be the best approximation to the observed variability (as shown by the anomaly plots). The drop in 2012 in many areas is of special interest as it may be signaling an important change in the environment but can also be an artifact of the satellite data.

4. Discussion

In order to be able to produce climate data records (National Research Council, 2004) it is critical to merge data from multiple satellite sensors and extend the time series beyond the limited



Fig. 7. Combined (OCTS, SeaWiFS, MODISA, MERIS) match-ups (blue dots) of adg440 between satellite estimates and in situ (top row) and between individual satellites (bottom row). Left column shows output from the standard QAA model, right column has output from the optimized QaaCalFit. The satellite to satellite matchups have combined MODISA vs. SeaWiFS, MERIS vs. SeaWiFS and MERIS vs. MODISA. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

lifetime of a single sensor. As an added benefit, merging data from multiple sensors has the potential to improve the coverage and decrease the sampling errors (IOCCG and Ocean-Colour Data Merging, 2007). However, merging data from multiple sensors also adds additional problems and can potentially introduce artificial trends and abrupt changes associated with a shift in available sensors (Gregg and Casey, 2010). GlobColour project of the European Space Agency is using multiple methods to merge water-leaving radiances or Chla from three sensors (SeaWiFS, MERIS, and MODISA) (Maritorena et al., 2010). While the large scale Chla distributions produced by the major ocean color missions were generally consistent over a wide range of conditions (Morel et al., 2007; Djavidnia et al., 2010), systematic and significant biases are found in the time series of individual sensors. Gregg and Conkright (2001) pioneered the blending of satellite Chla data with in situ data and Gregg et al. (2009) introduced a method called the Empirical Satellite Radiance-In situ Data (ESRID) that is using in situ data to reduce the discrepancy between different sensors. Kahru et al. (2012) modified ESRID by using local, high-resolution Level-2 match-ups and added a step of minimizing the deviations between satellite sensors. These previous attempts at merging in situ and satellite used Chla as the target variable. While available in situ datasets of Chla contain thousands of records, the number of comparable, high-quality datasets of IOPs is typically orders of magnitude smaller (Werdell

and Bailey, 2005). The advantage of estimating Chla using band ratio models is their robustness to random errors but the disadvantage is their significant bias when the adg440 to aph440 ratio changes. Estimating IOPs from satellite Rrs is fundamentally a better approach but the disadvantage is that the semi-analytic models used in the inversion process are sensitive to errors in the Rrs data (less so for a490). In our analysis we explicitly acknowledge the inconsistency between the Rrs products of different sensors. The tuning of coefficients of a particular model framework is similar to developing the GSM semianalytic model (Maritorena et al., 2002; Maritorena and Siegel, 2005) but OAA does not require fixed spectral shapes, as does GSM. The novelty of our analysis is that we minimize not just the differences with in situ data but also the differences between the outputs of the different satellite sensors. We produced a merged time series of several IOPs using four ocean color sensors within the framework of QAA with tunable coefficients. We restricted our analysis to the California Current, producing a regional model called QaaCalFit. Similar analysis could be applied to global datasets using, for example, the NOMAD dataset (Werdell and Bailey, 2005). It is clear that the number of our in situ match-ups is too small and is probably not well distributed to be representative of the real distribution of IOPs regarding a number of factors.

By using the time series of merged ocean color satellite data we were able to show significant changes in the California Current

Table 3

A comparison of the performance of the standard QAA model versus the optimized QaaCalFit model as applied to match-ups with in situ measurements (Sat/Insitu) and between different satellite sensors (Sat/Sat). R^2 =coefficient of determination, delta=estimate of scatter, *Bias*=estimate of bias. Bold numbers show improvement of QaaCalFit over QAA.

| Variable and match-up type | Measure | QAA | QaaCalFit |
|----------------------------|----------------|--------------|--------------|
| a490 Sat/Insitu | R ² | 0.741 | 0.754 |
| | Delta | 24.8 | 7.7 |
| | Bias | 0.0 | – 1.0 |
| a490 Sat/Sat | R ² | 0.897 | 0.920 |
| | Delta | 16.0 | 14.4 |
| | Bias | 0.2 | – 1.8 |
| bbp490 Sat/Insitu | R ² | 0.310 | 0.566 |
| | Delta | 189.0 | 7.7 |
| | Bias | 120.4 | 0.2 |
| bbp490 Sat/Sat | R ² | 0.398 | 0.425 |
| | Delta | 68.3 | 64.9 |
| | Bias | - 3.4 | – 6.5 |
| aph440 Sat/Insitu | R ² | 0.743 | 0.818 |
| | Delta | 88.9 | 10.7 |
| | Bias | 37.1 | 0.4 |
| aph440 Sat/Sat | R ² | 0.629 | 0.790 |
| | Delta | 56.6 | 41.3 |
| | Bias | - 6.4 | 1.3 |
| adg440 Sat/Insitu | R ² | 0.287 | 0.327 |
| | Delta | 91.0 | 22.5 |
| | Bias | 32.3 | - 4.2 |
| adg440 Sat/Sat | R ² | 0.893 | 0.915 |
| | Delta | 40.4 | 34.5 |
| | Bias | 15.6 | 15.9 |

during the last 16 years (1996-2012). Our merged time series is hence twice as long as a time series using SeaWiFS data alone (e.g. Yoder et al., 2010). We detected a statistically significant increase in the phytoplankton biomass as estimated by the proxy variable aph440 in the coastal and transition zones of the California Current, consistent with past reports (Kahru et al., 2012). However, the simple linear trend does not seem to be a good model to describe the observed variability. It is more likely that the apparent trend is caused by decadal variability (e.g. Martinez et al., 2009: Di Lorenzo and Ohman, 2013). After a period of general increase from 1998 to 2012, aph440 seems to have undergone a decline in 2012. This sharp decline in a number of IOPs in 2012 may be related to an unusual outbreak of salps (Salpa spp.) in the spring of 2012 (M. Ohman, personal communication, 2012) which was recorded as an unprecedented deposition of salp carcasses and fecal material at the seafloor at Station M, in the southern part of the Central California transition zone (Fig. 1A, area 2) (Sherman and Smith, 2012). It remains to be seen if the decline of 2012 will continue or was a temporary outlier. A factor complicating this analysis is that after the demise of the MERIS sensor in April, 2012 we have only one sensor (MODISA) that is being used in the merged time series. The trend of increasing phytoplankton biomass (Fig. 11A) in the California Current is consistent with our previous analysis (Kahru et al., 2012) that used Chla estimated from tuned band ratio algorithms, and is consistent with several independent decadal time series within California using in situ data. This increase in phytoplankton biomass could potentially be explained by the observed increase in upwelling-favorable winds and wind-driven coastal upwelling (García-Reyes and Largier, 2010) and/or by the modeled predictions (Rykaczewski and Dunne, 2010) showing increased nitrate



Fig. 8. Mean annual cycle of the merged multi-sensor *adg440*, *aph440* (left axis) and the ratio of *adg440* to *aph440* (right axis) for the grid of 12 areas (Fig. 1A). The horizontal black line shows where *adg440/aph440*=1.



Fig. 9. Time series of inherent optical properties detected by the merged multi-sensor (OCTS, SeaWiFS, MODISA, MERIS) data for the grid of 12 areas (Fig. 1A). (A) adg440, m⁻¹; (B) aph440, m⁻¹; (C) ratio of adg440/aph440.

supply in upwelled waters due to a concomitant increase in deep source waters entering the California Current resulting from decreased ventilation of the North Pacific. Indeed, time series of satellite-detected wind speed show increasing wind speed along the west coast of North America (Fig. 11B). It appears that along the California coast winds have increased mostly in the coastal and transition bands while increased phytoplankton biomass (*aph440*) occurs in a wider band into the offshore band. This is consistent with the effects of upwelling being spread offshore by filaments and eddies. The sign of the correlation between wind speed and phytoplankton biomass (Chla) depends on the factor most limiting phytoplankton growth: in light-limited areas the correlation is negative and in nutrient limited areas the correlation is positive (Kahru et al., 2010). It appears that increasing winds have limited the increase in aph440 in certain areas: south of Vancouver Island (Fig. 11, label 1) and in the northwest Pacific, at approximately 47° N; 135° W (Fig. 11, label 2). The time series of wind speed anomaly in the 4×3 area grid (Fig. 12) shows that the increasing trend has been strongest in the Baja California coastal region (both northern and southern) since about 1994 with a mean trend of over 0.56 m s⁻¹ per 10 years.

While this 16-year time series is long for satellite ocean color, it is certainly too short to separate interannual and multidecadal cycles from climate trends (Henson et al., 2010). The detection of any apparent trend in this relatively short time series is strongly affected by the timing of the start and end of the time series relative to the occurrence of the rare but extremely influential major El Niño events (Kahru and Mitchell, 2000, 2002). Since the launch of the first ocean color sensor (CZCS) in 1978 we have had two of these strong El Niño events (1982–1983 and 1997–1998) but only one during the era of modern ocean color.

The mean annual cycle for absorption shows clear evidence of an onshore-offshore gradient in seasonality. Near the coast (regions 3, 6, 9, 12) both *aph440* and *adg440* exhibit a strong spring peak (shifting from March to June moving from north to south) with a secondary autumn peak more apparent in the northern regions. Moving offshore, this seasonal cycle is dampened with a pronounced absorption minimum in August. Similar patterns were reported by Henson and Thomas (2007), who reported maximum variance in chlorophyll in spring/summer nearshore, shifting to autumn/winter offshore. Similarly, Kahru and Mitchell (2001) reported a dampening of magnitude and seasonality in CDOM



Fig. 10. Time series of *aph440* anomaly detected by the merged multi-sensor (OCTS, SeaWiFS, MODISA, MERIS) data for the grid of 12 areas (Fig. 1A). Anomaly has been calculated as the ratio of a current month value to the multi-year mean value of the particular month. Anomaly of 1 (black horizontal line) corresponds to the multi-year mean.



Fig. 11. (A) Linear trend in the monthly anomaly of *aph440* (1996–2012). (B) Linear trend in the monthly anomaly of wind speed (1987–2011, m/s/year). The grid of 12 selected areas in the California Current is overlaid. Areas where the trend is not significant at the 99% confidence level are shown as white. Labels 1 and 2 point to areas referenced in the text.

(derived from band-ratio algorithms) for the CCS. As described in Henson and Thomas (2007), this onshore-offshore and seasonal progression is likely caused by the seasonal offshore migration of eddy kinetic energy from the CCS coastal jet. Given this

interpretation, interannual changes in *adg440* and *aph440* would be directly or indirectly controlled by changes in the position and intensity of the California Current. Superimposed on this variability are changes caused by decadal oscillations such as ENSO, PDO, and



Fig. 12. Time series of monthly wind speed anomaly using the CCMP version 3.5 data for the grid of 12 areas (Fig. 1A). Anomaly has been calculated by subtracting the long-term mean value from the current monthly value for each pixel. Mean anomalies of the pixels were used to create time series for each area.

NPGO (e.g. Thomas et al., 2009). This would potentially lead to the rather complex interannual variability observed in this time series (Fig. 9).

While the length of our time series precludes definitive identification of trends driven by climate change, there are several interesting features that emerge. Examining changes in *aph440* (Fig. 11A), there is evidence for increasing phytoplankton biomass throughout the coastal waters of the CCS. This is somewhat different from similar analysis performed with band-ratio algorithms (Kahru et al., 2012) which showed an increase primarily in the central and southern CCS. There is also an increasing trend in the ratio of *adg440/aph440* (Fig. 9C). If we interpret increases in this ratio as increasing "contamination" of band-ratio chlorophyll estimates (Sauer et al., 2012), this would generally result in underestimation of low values and over-estimation of high values, potentially masking any underlying decadal trends. This reanalysis suggests that the previously reported decadal increase in biomass is coherent over most of the CCS from roughly 30–50° N (Fig. 11A).

Confirmation of increasing biomass extending into the Pacific Northwest is anecdotally supported by reports of increasing episodic blooms in that region (Du et al., 2011). The large latitudinal gradient also suggests that this decadal pattern is a response to either climate change or to multiple basin-scale oscillations, since ENSO, PDO, and NPGO generally show some latitudinal bias, with the ENSO and NPGO signal more apparent in the southern CCS and the PDO signal more apparent in the northern CCS. Fig. 11A also shows an increase in *aph440*

longitudinally at about 42–45° N. This is the approximate boundary identified by Huyer et al. (2005) as the transition from light limitation to nutrient limitation. This transition zone is probably sensitive to changes in both nutrients and mixed layer depth, driven by either climate change or basin-scale oscillations. Carr and Kearns (2003) also identified the northern CCS (40–48° N) as driven primarily by large-scale forcing, again suggesting that the apparent increased biomass in this region is responding to large-scale restructuring of the physical environment.

Development of semi-analytical algorithms has added benefits besides the potential improvement of chlorophyll retrievals based on IOPs rather than empirical relationships, since it provides the opportunity to assess other biochemical parameters linked to changes in IOPs. For example, McGaraghan and Kudela (2012) previously used OAA to derive a relationship between remotelysensed backscatter, fluorescence line height, and bio-available iron, while Palacios et al. (2009, 2012) derived synthetic salinity and water masses for the Pacific Northwest using outputs from semi-analytic inversion algorithms in statistical models. There has also been increasing interest in the development of phytoplankton functional type (PFT) models to derive more detailed information than bulk chlorophyll (Moisan et al., 2012). These efforts require both a better understanding of the errors associated with inversion algorithms such as QAA, and a careful analysis of the discrepancies between sensors and platforms. Here we provide the baseline knowledge for this assessment in the California Current System.

5. Conclusions

We demonstrated that the QAA inversion algorithm, which directly derives inherent optical properties (IOPs) from satellite remote sensing reflectance, can be regionally optimized to minimize error both within a region (the California Current System) and across multiple ocean color sensors (OCTS, SeaWiFS, MODISA, MERIS). IOPs provide direct estimates of changes in ocean color linked to underlying biogeochemical properties such as phytoplankton biomass and the concentration of colored dissolved organic matter. By retrieving these parameters directly, we minimize errors associated with traditional band-ratio algorithms, and separate the effects of CDM from changes in phytoplankton biomass (chlorophyll). This analysis is an important step towards creating Climate Data Records (CDRs), since we now have a consistent time series spanning 16 years and multiple sensors. The merged 16-year time series (November 1996–December 2012) show significant changes, corroborating the previous observations of increasing chlorophyll in much of the California Current System. These observed trends are consistent with predictions of largescale restructuring of the CCS in response to increased upwelling and/or changes in the source of upwelled waters associated with increasing nutrient concentrations. This analysis also suggests that the decadal positive increase in biomass may have been disrupted in 2012 for as yet unknown reasons. Further offshore, there is a contrasting trend of decreasing biomass in the oligotrophic subtropical Pacific, also consistent with previous observations. While direct estimates of IOPs from ocean color provide an opportunity to derive additional biogeochemical parameters beyond chlorophyll, uncertainties in our estimates of IOPs are still large and require further refinement. We demonstrate that we can minimize the inter-sensor differences in the produced IOPs, but it is still possible that artificial changes in the IOP time series are created by merging products across sensors. This is a serious issue for the development of CDRs. There is clear evidence for decadal changes in IOPs (and therefore underlying biogeochemical parameters) within the CCS, and that these changes are not simple linear trends. Identification of these underlying patterns, particularly separation of basin-scale oscillations from potential climate change, requires both CDRs and match-ups of high-quality in situ measurements of IOPs. To achieve this, we identify three key requirements. First, it is extremely important that the temporal shifts in sensor calibrations are continuously monitored and corrected (Franz et al., 2007). Second, we need access to more match-ups of high-quality in situ measurements of IOPs. Third, we need continued access to state-of-the-art ocean color sensors. MODISA is currently operating well beyond its originally planned lifetime and it remains to be seen if the same quality products can be retrieved from the VIIRS instrument launched on 2011. Without meeting these three requirements, it will be difficult to attribute the observed spatial and temporal changes in properties such as CDM and chlorophyll to specific processes, or to evaluate predictions for a changing coastal ocean.

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