Optical remote sensing of chlorophyll $a$ in case 2 waters by use of an adaptive two-band algorithm with optimal error properties

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Two-band algorithms that use the ratio of reflectances at 672 and 704 nm have already proved successful for chlorophyll $a$ retrieval in a range of coastal and inland waters. An analysis of the effect of reflectance measurement errors on such algorithms is made. It provides important indications of the range of validity of these algorithms and motivates the development of an entirely new type of adaptive two-band algorithm for hyperspectral data, whereby the higher wavelength is chosen for each input spectrum individually. When one selects the wavelength at which reflectance is equal to the reflectance at the red chlorophyll $a$ absorption peak, chlorophyll $a$ retrieval becomes entirely insensitive to spectrally flat reflectance errors, which are typical of imperfect atmospheric correction, and is totally uncoupled from the retrieval or an estimation of backscatter. This new algorithm has been tested for Dutch inland and Belgian coastal waters. © 2001 Optical Society of America

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1. Introduction

There has been considerable success$^{1,2}$ in optical remote sensing of chlorophyll $a$ in case 1 waters where the variation of optical properties (absorption and scattering) is dominated by phytoplankton and associated material, and some consensus is emerging with regard to appropriate algorithms. In contrast, chlorophyll $a$ retrieval in case 2 waters, where the optical properties of inorganic suspended matter and colored dissolved organic matter (CDOM) must also be considered,$^3$ is still a matter of intense research activity, and few convincing examples are available of satellite-derived chlorophyll $a$ concentrations for such waters. However, the demand for detailed monitoring of chlorophyll $a$ concentrations in case 2 waters is high because of the need to manage inland and coastal eutrophication$^4,5$ and because of the importance of estuarine and coastal phytoplankton for atmospheric carbon dioxide$^6$ and hence possible climate change.

Because of the additional independent optically active constituents in case 2 waters the blue-green two-band ratio algorithms popular for case 1 waters are not appropriate and alternative approaches must be sought. In the case of Belgian coastal waters Fig. 1 illustrates the difficulties involved. For this sample in the 400–500-nm spectral range the absorption from tripton (particulate matter after removal of phytoplankton pigments) is generally greater than phytoplankton absorption, and the total particulate absorption coefficient shows an exponentially decreasing form for the 400–570-nm range, typical of tripton (detrital) absorption. Although there are departures from this detrital form at 440 and 470 nm associated with phytoplankton pigments, these signals are small. Considering that a satellite-based sensor sees only the effect of the total absorption coefficient (particulate plus dissolved matter plus pure water), it is clearly important to be able to dis-
tistinguish phytoplankton-related features at least in
the total particulate absorption spectrum. In the
case illustrated in Fig. 1, decomposition of any
satellite-derived total absorption coefficient into com-
ponents arising from phytoplankton and other ma-
terial will clearly be difficult without use of the 670-nm
chlorophyll a absorption feature. This is the focus of
this paper, although alternative approaches for chlo-
rophyll a retrieval exist in which fluorescence
or combined absorption and backscatter from phyto-
 plankton is also considered phenomena to be ex-
plotted.

Because of the greater number of independent op-
tically active constituents, a number of multiband
algorithms have been developed for case 2 waters. In such algorithms a system of equations for a num-
ber of bands (possibly all bands available from a given
sensor) is inverted to yield a solution set for typically
two or three optically active constituents, e.g., total
suspended matter concentration, chlorophyll a con-
centration, and CDOM absorption at a reference
wavelength. Alternatively, algorithms can be de-
veloped to determine only chlorophyll a concentra-
tion. For such an approach, provided the water is tur-
ed enough to produce a measurable signal in the near-
infrared (NIR), the chlorophyll a absorption feature
near 670 nm (Fig. 1) is particularly attractive since
this part of the spectrum minimizes interference from
tripton and CDOM absorption. A chlorophyll a re-
trieval algorithm for case 2 water was developed and
tested for airborne imagery, based on the ratio of
reflectances at 676 and 706 nm, and an approach in
which similar wavelengths are used, in combination
with backscatter estimated from reflectance at a
third NIR wavelength, has been used to retrieve chlo-
rophyll a successfully from above-water radiance
measurements for a wide range of coastal and inland
waters. Similarly in another study an empirical
relationship between the ratio of reflectances at 670
and 705 nm and chlorophyll a concentration was
found for both natural water and in an experiment
with cultured algae.

In this study a similar two-band red/NIR is
adopted. However, instead of using an algorithm
with two fixed bands, as is the case for nearly all
conventional algorithms, the wavelength of the sec-
ond band, away from the chlorophyll a absorption
feature, is allowed to vary. This extra degree of free-
dom allows adaptive optimization of the algorithm to
reduce errors in chlorophyll a retrieval associated
with imperfect atmospheric correction.

In this paper the theoretical background to this
adaptive two-band approach to chlorophyll a re-
trieval is described. Particular attention is paid to
the effect of errors in reflectance measurements be-
cause, although often neglected, such an error anal-
ysis is vital to ensuring that resources are not
wasted chasing an ultimately impossible goal. The
method is then tested by using a data set of spectral
reflectances and chlorophyll a concentrations mea-
sured in Dutch inland waters and in Belgian coastal
waters. Finally, perspectives are discussed for ap-
lication of the method to future hyperspectral
satellite-based sensors.

2. Theory

A. Steps for Chlorophyll a Retrieval

The estimation of chlorophyll a concentration from
satellite measurements of upwelling spectral radi-
ance by using an analytical approach can typically be
accomplished in four steps:

1. Atmospheric correction consists of calculating
the atmospheric effects to yield above-water up-
wellling radiance (i.e., water-leaving radiance plus
sunlight and skylight reflected at the air–sea inter-
facedownwelling irradiance from at-sensor ra-
diace. This step is far from easy and could
generate considerable errors. However, significant
progress has been made in modeling atmospheric ef-
fects, including consideration of turbid water ef-
fects on the NIR range used for correction of
scattering from aerosols and fairly reliable up-
wellling radiances can now be derived from satellite
sensors.

2. Air–sea interface correction consists of calcu-
lying subsurface irradiance reflectance from the
above-water upwelling radiance and downwelling ir-
radiance by removing the reflection of sunlight and
skylight at the air–sea interface, accounting for
transmission and refraction of light through the in-
terface and for the ratio of radiance to radiation.
This step is relatively simple, although there is un-
certainty regarding the angular distribution of
upwellling radiance.

3. Bio-optical modeling consists of estimating the
phytoplankton absorption coefficient at a designated
wavelength from subsurface irradiance reflectance.
This step seems to represent the greatest obstacle at
present to chlorophyll a retrieval in case 2 waters and
is the focus of this study.

4. Finally, conversion of the phytoplankton ab-
sorption coefficient into chlorophyll a concentra-
tion can introduce significant errors in chlorophyll a re-
trieval inasmuch as the chlorophyll-specific phyto-
 plankton absorption coefficient can vary as a function

Fig. 1. Example of an absorption spectrum for Belgian near-shore coastal waters for total particulates (upper, thick solid curve) and its components arising from tripton (lower, thin solid curve) and phytoplankton (dashed curve).
of a number of factors, including phytoplankton species composition and the trophic state. Moreover this conversion factor depends on the precise meaning of the phytoplankton absorption coefficient and of the measurement method used for chlorophyll a concentration (pigment extraction and analysis). An in-depth analysis of such matters is beyond the scope of this study. In this study this step is effectively combined with bio-optical modeling to obtain chlorophyll a directly from the bio-optical model.

B. Description of General Two-Band Red/Near-Infrared Algorithm

As a basis for this study we used the well-established family of models that expresses subsurface irradiance reflectance $R$ as a function of the total absorption coefficient $a$ and the total backscatter coefficient $b_b$:

$$R(\lambda) = f \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}, \quad (1)$$

where $\lambda$ is the wavelength and $f$ is an empirical factor, which depends on the incident light field and the volume-scattering function of the water. Although considerable variation in the numerical value of $f$ has been reported, over limited spectral ranges the wavelength dependence of $f$ is limited and in this study is considered negligible. Note that similar expressions exist for remote-sensing reflectance, although with a different numerical value and dependence on solar zenith angle for $f$. As seen in Eq. (24), this empirical factor disappears from the new adaptive algorithm described here, which is thus equally applicable to subsurface irradiance or remote-sensing reflectances.

Two wavelengths are used to deduce chlorophyll a concentration from reflectance. The first wavelength $\lambda_1$ is located within the region of the red chlorophyll a absorption peak, and the second wavelength $\lambda_2$ is located within the 700–740-nm range. The following assumptions with regard to inherent optical properties are used in the theoretical development of this model:

1. The total absorption coefficient at $\lambda_1$ is dominated by absorption from pure water $a_{w1}$ and phytoplankton pigments $a_{phy1}$ with negligible contributions from CDOM and tripton:

$$a(\lambda_1) = a_{w1} + a_{phy1}. \quad (2)$$

2. The total absorption coefficient at wavelength $\lambda_2$ is dominated by absorption from pure water $a_{w2}$ alone, and contributions from phytoplankton pigments, CDOM, and tripton can be neglected:

$$a(\lambda_2) = a_{w2}. \quad (3)$$

(3) The backscatter coefficient is assumed to be independent of wavelength over the limited red/NIR spectral range considered here:

$$b_b(\lambda_1) = b_b(\lambda_2) = b_{b0}. \quad (4)$$

Thus, when Eqs. (1)–(4) are used, the ratio $\gamma$ of reflectances at $\lambda_2$ and $\lambda_1$ denoted by $R_2$ and $R_1$ can be expressed as

$$\gamma = \frac{R_2}{R_1} = \frac{a_{w1} + a_{phy1} + b_{b0}}{a_{w2} + b_{b0}}. \quad (5)$$

This can easily be inverted to give

$$a_{phy1} = \gamma(a_{w2} + b_{b0}) - a_{w1} - b_{b0}. \quad (6)$$

Then, supposing that the chlorophyll a specific phytoplankton absorption coefficient at $\lambda_1$, $a_{phy1^a}$, as defined by

$$a_{phy1^a} = \frac{a_{phy1}}{C}, \quad (7)$$

is known, the chlorophyll a concentration $C$ can be simply found from

$$C = \frac{a_{phy1^a}}{a_{phy1}} = \frac{1}{a_{phy1}} \left[ \gamma(a_{w2} + b_{b0}) - a_{w1} - b_{b0} \right]. \quad (8)$$

With the choices of $\lambda_1 = 672$ nm and $\lambda_2 = 704$ nm, Eq. (8) is exactly equivalent to Eq. (5) of Ref. 14, which is referred to as G99, although in Eq. (6) of that paper an additional empirical calibration as exponent of the final term $-b_b$ in Eq. (8) is introduced.

An important and well-known advantage of this type of algorithm is that, by taking a ratio of reflectances, the problems associated with the evaluation of $f$ have been removed. However, an estimation of $b_b$ is still required for evaluation of Eq. (8). This is performed in G99 by use of a third wavelength, further into the NIR (776 nm), and inversion of Eq. (1) by use of an estimate of $f$ based on an empirical relation involving the average cosine of downward irradiance. Thus

$$b_{b0} = \frac{a_{w3} R_3}{f - R_3}. \quad (9)$$

This procedure exposes the algorithm to some degree to errors associated with the calculation of $f$. A second more important weakness of Eq. (8), when applied to satellite-derived reflectance data, is that the estimation of chlorophyll a concentration will be affected by wavelength-independent reflectance errors through the ratio $\gamma$. The purpose of this study is to analyze the two-band algorithm’s sensitivity to reflectance errors and hence determine the optimal choice of wavelengths for chlorophyll a retrieval.
C. Theoretical Analysis of Reflectance Errors

An imperfect removal of aerosol-path radiance in the case of satellite measurements and air–sea interface correction for all above-water measurements will give an offset error to \( R \), which can be significant but is spectrally fairly flat. Thus, denoting the measurement error as \( R' \) and the true (error-free) reflectance as \( R' \), the measured reflectance \( R'' \) is given by

\[
R'' = R' + R'_e,
\]

where \( R'_e \) is the retrieval error.

In this section our purpose is to estimate the effect of such reflectance errors on the chlorophyll \( a \) retrieved from Eq. (8). Thus the reflectance ratio, backscatter coefficient, and retrieved chlorophyll \( a \) concentration in the presence of reflectance measurement errors are defined by setting \( (R_1, R_2, R_3) = (R_1', R_2', R_3') \) in Eqs. (5), (8), and (9):

\[
\gamma'' = \frac{R_2''}{R_1''}, \quad b_{\text{bb}}'' = \frac{a_{\text{bb}}R_3''}{f - R_3''}, \quad C'' = \frac{1}{a_{\text{phy}1'}} [\gamma''(a_{\text{bb}} + b_{\text{bb}}'') - a_{\text{bb}} - b_{\text{bb}}''],
\]

and similar expressions (with superscript \( m \) replaced by the superscript \( t \)) for the true (error-free) reflectance ratio \( \gamma' \), the backscatter coefficient \( b_{\text{bb}}' \), and the chlorophyll \( a \) concentration \( C' \) are defined by setting \( (R_1, R_2, R_3) = (R_1', R_2', R_3') \). Then the error in the estimation of reflectance ratio \( \gamma' \), the backscatter coefficient \( b_{\text{bb}}' \), and the chlorophyll \( a \) retrieval error \( C' \), as defined by the difference between the measured and the error-free estimations, can be evaluated at first order as follows:

\[
b_{\text{bb}} = a_{\text{bb}}R_3 - a_{\text{bb}} - b_{\text{bb}}
\]

Equation (18) for the error in chlorophyll \( a \) retrieval has a number of important implications for the choice of wavelengths \( \lambda_1 \) and \( \lambda_2 \). Considering the first factor, it can be seen that \( \lambda_1 \) should be chosen to maximize \( a_{\text{phy}1'} \). (This rather obvious condition is important enough to fix \( \lambda_1 \).) Also, as noted in a previous study,\(^{13}\) choosing \( \lambda_2 \) so that \( R_2 \) is as large as possible, while keeping \( \lambda_1 \) and \( \lambda_2 \) as close as possible spectrally, is preferred. However, one can achieve a more effective reduction of error by considering the probable spectral correlation of reflectance errors. Two types of reflectance error are considered here:

(a) Reflectance errors arising from imperfect atmospheric correction (especially removal of aerosol-path radiance) are strongly correlated spectrally and over the narrow red/NIR range considered here can be considered as spectrally fairly flat (see Table 1 of Ref. 21). Thus, substituting

\[
R_1' = R_2' = R_3' = R
\]

into Eq. (18) gives to first order (dropping the \( t \) superscript from the notation)

\[
C' = \frac{1}{a_{\text{phy}1'}} f_{\text{bb}}(1 - \gamma) \left( \frac{1}{R_1R_2} - \frac{1}{R_3(f - R_3)} \right) R'.
\]

Thus, when \( \lambda_2 \) is chosen as the wavelength where \( R_1 = R_2 \) and thus \( \gamma = 1 \), the consequent error in chlorophyll \( a \) retrieval is exactly zero, \( C' = 0 \), i.e., for such a choice of \( \lambda_2 \) spectrally flat reflectance errors will
generate absolutely no error in the chlorophyll $a$ concentration.

(b) Reflectance errors associated with sensor noise are typically uncorrelated in the spectral sense and will vary in time. Thus the error term $C^e$ is best estimated by taking the least favorable case where $R_1^e$ and $R_2^e$ are of opposite sign and $R_3^e$ has the same sign as $R_1^e$ or $R_2^e$, depending on whether $\gamma$ is less than or greater than one. In this case Eq. (18) gives to first order in $R^e/R$

$$
|C^e| = \frac{1}{a_{\text{phy}1}} f_b b_0 \left[ \frac{|R_2^e| + |\gamma| |R_1^e|}{R_1^e R_2^e} \right] + \frac{|R_3^e|}{R_3^e (f - R_3^e)}. \tag{21}
$$

Although in Eq. (21) the obvious requirement is suggested that all three bands be chosen for wavelengths at which relative noise-equivalent reflectance $R^e/R$ is low, such considerations are usually specified in the sensor design and, in general, will have little effect on the design of algorithms. In this case of spectrally uncorrelated error, as seen below, the absolute error in chlorophyll $a$ retrieval $C^e$ is strongly dependent on backscatter (high backscatter is favorable) but almost independent of $C$ itself (the only dependence is by $R_1$), and thus the relative error $C^e/C$ is expected to be greatest for low $C$.

D. New Adaptive Two-Band Algorithm

The preceding analysis motivates development of a new adaptive two-band chlorophyll $a$ retrieval algorithm. Taking advantage of the hyperspectral reflectance data that will be available on future satellite sensors [e.g., the technology-proving compact high-resolution Imaging Spectrometer (CHRIS) to be launched in 2001] and is already available for airborne sensors [e.g., the Compact Airborne Spectrographic Imager (CASI), the Environmental Probe System (EPSA), and the Airborne Prism Experiment (APEX)], it is possible to set wavelength $\lambda_3$ for each input spectrum individually. The new algorithm developed here makes the choice $\lambda_3 = \lambda_2^e$, where $\lambda_2^e$ is the critical wavelength, found by use of a simple search algorithm, for which

$$
R(\lambda_2^e) = R_1. \tag{22}
$$

This is illustrated in Fig. 2. With such a choice, $\gamma = 1$, and defining the residual pure water as absorption coefficient $a_{w} = a_{w/2} - a_{w1}$, Eq. (8) reduces to

$$
C = a_w/\alpha_{\text{phy}1}. \tag{24}
$$

This can be understood simply by taking into consideration that, if the reflectances at two wavelengths are equal, and it is assumed that the backscatter coefficients are equal, the total absorption coefficients are equal at the two wavelengths. Thus, using assumptions (2) and (3), the phytoplankton absorption coefficient at $\lambda_1$ is simply equal to the difference in pure-water absorption coefficients and one can calculate the chlorophyll $a$ concentration by dividing by the specific phytoplankton absorption coefficient. This new algorithm, referred to as Chlorophyll $a$ retrieval using an adaptive two-band algorithm (CRAT), shares the advantages of the more conventional fixed two-band red/NIR reflectance ratio algorithms but with two important extra properties:

1. Equation (24) for chlorophyll $a$ retrieval requires no estimation of the backscatter coefficient or the reflectance scaling factor $f$. Moreover, with this approach chlorophyll $a$ retrieval is even independent of the underlying form [Eq. (1)] assumed for reflectance as the function of $a$ and $b_0$, because for other forms such as the simpler $R = fb_0/a$ or a more complex second- or higher-order expansion in terms of $b_0/(a + b_0)$, the same reasoning applies, leading to Eq. (24).

2. As illustrated in Fig. 2, any spectrally flat error that offsets the measured reflectance will have no influence on wavelength $\lambda_2$ and hence no influence on chlorophyll $a$ retrieval.

This algorithm is represented graphically in Fig. 3, which shows the residual pure-water absorption coefficient as a function of wavelength as well as the corresponding chlorophyll $a$ concentration according to Eq. (24). Thus, for a range of possible retrieval
wavelengths given by $704 \, \text{nm} \leq \lambda_2 \leq 740 \, \text{nm}$ (avoiding the $740$–$760$-nm range because of the temperature dependence of the pure-water absorption coefficient\cite{32}), the corresponding CRAT chlorophyll $a$ retrieval range is given by $12.0 \, \text{mg} \, \text{m}^{-3} \leq C \leq 117.6 \, \text{mg} \, \text{m}^{-3}$. If higher chlorophyll $a$ concentrations are to be retrieved, suitable reflectance data are available, the same concept could be applied also to the wavelength range for $\lambda_2 \geq 825$ nm (see Fig. 3) provided absorption of bacteriochlorophylls can be excluded. For lower chlorophyll $a$ concentrations CRAT is, however, less appropriate because the critical wavelength $\lambda_2^c$, if it exists, will lie within the range $672 \, \text{nm} \leq \lambda_2 \leq 704 \, \text{nm}$ and the assumption that $a_{\omega 2}$ is not affected by phytoplankton absorption is no longer valid. Although a correction term could be envisaged, for example, replacing the denominator of Eq. (24) by $a_{\text{phy}1} = a_{\text{phy}2}^*$, where $a_{\text{phy}2}^*$ is the chlorophyll-specific phytoplankton absorption coefficient at $\lambda_2$, such an approach may be hazardous if $a_{\text{phy}2}^*$ is poorly known or if the sensor bandwidth is significant. Thus, in this study, we performed chlorophyll $a$ retrieval for $\lambda_2^c \leq 704 \, \text{nm}$ by reverting to the fixed two-band algorithm [Eq. (8)] with $\lambda_2 = 704 \, \text{nm}$ and with $b_{\omega 0}$ estimated from a third wavelength, $\lambda_3 = 776 \, \text{nm}$. In a similar way, for $\lambda_2^c \geq 740 \, \text{nm}$ the algorithm reverts to the fixed two-band algorithm [Eq. (8)] with $\lambda_2 = 740 \, \text{nm}$ and $b_{\omega 0}$ estimated from a third wavelength, $\lambda_3 = 776 \, \text{nm}$.

The performance of this new algorithm and the associated fixed-band algorithms are considered in Section 3 where both numerically simulated reflectance data and reflectance spectra measured from a ship are used.

3. Numerical Simulations

A. Simulation Methods

The effect of both types of reflectance error discussed in Section 2 for chlorophyll $a$ retrieval when Eq. (8) is used can be illustrated by a model simulation, whereby a simple forward model is used to generate subsurface irradiance reflectances for specified input pairs of $b_{\omega 0}$ and $C$. These reflectances are then perturbed by a reflectance error of atmospheric correction and sensor noise types, respectively, and the resulting measured reflectances are inverted to give retrieved chlorophyll $a$. In the forward model, the reflectance model [Eq. (1)] is used with the assumptions that the inherent optical properties conform to Eqs. (2)–(4) and that phytoplankton absorption can be represented in the form of Eq. (7). The reflectance errors are added to forward model generated reflectances as in Eqs. (10)–(12), and the resulting reflectance ratio and backscatter coefficient from Eqs. (13) and (14) are input to Eq. (8) to give the resulting retrieved chlorophyll $a$. Typical parameters\cite{14,30} of $f = 0.275$ and $a_{\text{phy}1} = 0.018 \, \text{m}^2 \, \text{mg}^{-1}$ were used with input backscatter coefficients, $b_{\omega 0} = 0.1 \, \text{m}^{-1}$ and $b_{\omega 2} = 1.0 \, \text{m}^{-1}$, and input chlorophyll $a$ concentrations ranging from low ($C = 1.0 \, \text{mg} \, \text{m}^{-3}$) to high ($C = 215 \, \text{mg} \, \text{m}^{-3}$) to cover conditions likely to be encountered in coastal and inland waters. For $b_{\omega 0} = 0.1 \, \text{m}^{-1}$ only $C < 100.0 \, \text{mg} \, \text{m}^{-3}$ is shown because the backscatter from phytoplankton and phytoplankton-deriven trip-\cite{33} will render this backscatter coefficient unrealistic at higher concentrations. To illustrate how the error properties vary with choice of wavelength, simulations have been performed with a $672:704$-nm algorithm, as in G99 (and similar to the $665:705$-nm bands available from MERIS), and with a $667:748$-nm algorithm (corresponding to MODIS bands).

For describing error behavior it is sufficient here to consider a central wavelength approach with a delta-function sensor response. Pure-water absorption coefficients are taken from Ref. 34, giving $(a_{\omega 1}, a_{\omega 2}) = (0.415 \, \text{m}^{-1}, 0.630 \, \text{m}^{-1})$ for $(\lambda_1, \lambda_2) = (672 \, \text{nm}, 704 \, \text{nm})$ and $(a_{\omega 1}, a_{\omega 2}) = (0.408 \, \text{m}^{-1}, 2.72 \, \text{m}^{-1})$ for $(\lambda_1, \lambda_2) = (667 \, \text{nm}, 748 \, \text{nm})$. In all cases backscatter is estimated from $\lambda_3 = 776 \, \text{nm}$ where $a_{\omega 2} = 2.71 \, \text{m}^{-1}$.

For atmospheric-correction-type errors both positive and negative near-white errors are simulated with $R^0$, which are supposed to vary linearly from $R_1^* = \pm 0.010$ to $R_3^* = \pm 0.008$ (chosen from experience and theoretical estimates for Belgian coastal waters). For sensor-noise-type errors the values $R_1^* = R_3^* = 0.0005$ and $R_2^* = -0.0005$ were used (typical of the MERIS specification\cite{35}).

B. Simulation Results

The results of simulations of the performance of Eq. (8) for atmospheric-correction-type errors and for sensor-noise-type errors are shown in Figs. 4 and 5, respectively.

Figure 4 shows that atmospheric-correction-type errors of the magnitude considered will cause noticeable chlorophyll $a$ retrieval errors for the conventional fixed two-band algorithms. The greatest errors occur in conditions of low backscatter, because $C^*$ is inversely proportional to the backscatter coefficient through the reflectances appearing in Eq. (20). Results for the $667:748$-nm algorithm were similar to the $672:704$-nm algorithm for the high backscatter
coefficient (since reflectance errors are then less significant compared with the total signal) and are not shown. However, for lower backscatter a considerable difference is found and a key implication of Fig. 4 is that for each pair of wavelengths used in this kind of two-band reflectance-ratio algorithm there exists a critical value of chlorophyll \( a \) concentration for which spectrally flat reflectance errors produce a zero chlorophyll \( a \) retrieval error. In Fig. 4 this is shown by the intersection point of the curves for different backscattering with the perfect retrieval (dotted) line, as seen most clearly in the 667:748-nm algorithm. This occurs when \( \gamma = 1 \), which corresponds to a critical chlorophyll \( a \) concentration of \( C = 11.9 \) mg/m\(^3\) for the 672:704-nm wavelength pair and \( C = 128.4 \) mg/m\(^3\) for the 667:748-nm algorithm. A first conclusion from this is that if the target chlorophyll \( a \) concentration range is from 1 to 100 mg/m\(^3\), the 672:704-nm choice is preferred to the pair with the second wavelength farther into the NIR as regards resistance to spectrally flat reflectance errors. Second, it is clear that this critical chlorophyll \( a \) concentration is a simple function of wavelength, and the intersection point in Fig. 4 will slide along the perfect retrieval line when \( \lambda_2 \) is varied. This observation motivated development of the new adaptive two-band chlorophyll \( a \) algorithm [Eq. (24)] whereby the second wavelength is chosen independently for each spectrum considered such that the retrieved chlorophyll \( a \) is equal to the critical chlorophyll \( a \) value.

Figure 5 shows that sensor-noise-type errors of the magnitude considered will cause considerable chlorophyll \( a \) retrieval errors in clear water but correspondingly lower errors for more turbid waters because of the inverse proportionality of \( C^e \) to the backscatter coefficient. The 667:748-nm wavelength pair again produces larger errors compared with the 672:704-nm pair because the lower reflectance \( R_2 \) is proportionally more greatly affected by the absolute magnitude of the reflectance error.

The same simulations have been performed for the CRAT algorithm. For the atmospheric-correction-type errors (Fig. 6) the CRAT algorithm gives, by design, a very low error for the chlorophyll \( a \) concen-
trations within the range of application of Eq. (24), i.e., for which \( \gamma_t \) can be found in the 704–740-nm range. For lower chlorophyll \( a \) concentrations results are identical to the fixed 672-nm:704-nm algorithm, whereas for higher chlorophyll \( a \) concentrations the performance is similar to the two-band 667:748-nm algorithm (which is preferable to 672:704 nm for such very high concentrations). For the sensor-noise-type errors the performance throughout is similar to the 672:704-nm algorithm shown in Fig. 5 and is therefore not shown again. For low backscatter conditions the reflectance throughout the red/NIR range is of the same order as the sensor noise, and chlorophyll \( a \) retrieval with any algorithm is subject to large errors.

C. Field Observations—Method

The new algorithm has been tested with data from the IJssel Lagoon (Dutch inland water) already presented in G99 (114 samples) and from two cruises in Belgian coastal waters (28 samples) by the research vessel Belgica on 15–17 April 1998 and 17–19 April 2000. The coastal water cruises were carried out during blooms of *Phaeocystis globosa*, although some diatoms were also present.

Near-surface water samples were taken and analyzed for chlorophyll \( a \) concentration, after removal of pheo pigments, by the Dutch standard method NEN 6520 (spectrophotometric analysis after pigment extraction with hot ethanol). For comparison, in Belgian coastal waters a second set of chlorophyll \( a \) measurements was made by using the method of Lorenzen. The rms of the difference and of the relative difference between these two data sets (20 values) were 3.6 mg m\(^{-3}\) and 30.2%, respectively. For coherence with the IJssel Lagoon data set only the data where the Dutch standard method was used are presented here.

Simultaneously with the water samples, radiance spectra were collected above water with a PR-650 SpectraColorimeter (manufactured by Photo Research) as described more fully in Ref. 14. Subsurface irradiance reflectance is calculated from a set of four measurements (upwelling radiance from the water, sky radiance, and upwelling radiance from an exposed reference Lambertian plaque and upwelling radiance from the same plaque but shaded from direct sunlight). To assess temporal fluctuations arising from surface waves and illumination conditions, three spectral scans were made for each set of measurements. Patchy clouds during both coastal water cruises caused highly variable illumination conditions at many stations. The average of the three scans was used for subsequent chlorophyll \( a \) retrieval. The reflectance spectra were then processed with the CRAT algorithm.

D. Field Observation Results

The results of the comparison between chlorophyll \( a \) concentration measured in situ from water samples against concentration deduced from above-water radiance measurements are presented in Fig. 7. Calibration of the phytoplankton absorption coefficient retrieved with the CRAT algorithm against the in situ chlorophyll \( a \) concentration led to the calibration constants of \( a_{\text{phy}1} = 0.0198 \text{ m}^2 \text{ mg}^{-1} \) and \( a_{\text{phy}1} = 0.0205 \text{ m}^2 \text{ mg}^{-1} \) for the Belgian coastal water and the IJssel lagoon data sets, respectively. These values are surprisingly close.

Figure 7 shows that the method is promising for remote sensing of chlorophyll \( a \) concentration in these waters. The absolute and relative rms errors in chlorophyll \( a \) retrieval were 4.5 mg m\(^{-3}\) and 35% for the Belgian coastal water data and 12.7 mg m\(^{-3}\) and 39% for the IJssel lagoon data. In general, greater scatter is seen for lower concentrations, where CRAT reverts to a fixed two-band algorithm. This conforms to the results of the theoretical error analysis.

Such algorithm accuracy is similar to that of the fixed-wavelength algorithm described in Refs. 14 and 38, and until hyperspectral satellite data become available the advantages of the adaptive approach in limiting the effect of atmospheric correction errors will remain largely theoretical. However, for shipborne-radiance measurements near-white errors can be expected to result from imperfect air–sea interface correction. Thus, tests were made by application of the CRAT algorithm to each of the triplet spectra measured at the high chlorophyll \( a \) Belgian coastal water stations. In nine of eleven cases the range of the three chlorophyll \( a \) estimates was smaller for CRAT than for the fixed 672:704-nm algorithm. The main differences between the three measurements being in the sky-radiance reflection error rather than in the composition of the water being observed suggests that CRAT is less sensitive to such errors, although we note that the sky-radiance reflection error for this data set seems not to be a significant source of chlorophyll \( a \) retrieval error.

For comparison, we made further tests on the IJssel lagoon data set by using the eutrophic waters component of the MODIS semianalytical chlorophyll \( a \) algorithm defined in Eq. (12) of Ref. 28.
Results were poor, with little correlation between measured and retrieved chlorophyll $a$ and a relative rms error of more than 100%, which is not surprising since such algorithms are not designed to work for such extreme case 2 waters.

4. Discussion

For case 2 waters with strong absorption from tripton or CDOM the main hope for retrieval of chlorophyll $a$ concentration from satellite-based optical sensors lies in exploiting the signal provided by the chlorophyll $a$ red absorption peak near 670 nm. Two-band algorithms based on a ratio of reflectances near 672 and 704 nm have already proved successful for highly turbid coastal and inland waters. A theoretical analysis of how errors in reflectance measurements affect chlorophyll $a$ retrievals has been made in this study for a two-band red/NIR reflectance-ratio algorithm with a general choice of wavelengths. This analysis provides a number of important conclusions:

(a) Errors are greatest in conditions of low backscatter. In contrast to algorithms in which blue-green spectral bands are used, where nonalgae particulate absorption is highly detrimental, particulate backscatter, whether of organic or inorganic origin, improves red/NIR chlorophyll $a$ retrieval by increasing the available signal-to-noise ratio (Fig. 4.11 of Ref. 39).

(b) The absolute errors in chlorophyll $a$ retrieval caused by spectrally uncorrelated reflectance measurement errors, e.g., resulting from sensor noise, are only weakly dependent on chlorophyll $a$ concentration itself, and hence the relative error $C' / C$ becomes most significant at low (e.g., $C < 10$ mg/m$^3$) chlorophyll $a$ levels.

(c) For reflectance errors that are spectrally flat over the red/NIR range, as is approximately so for the important case of imperfect atmospheric correction, the effect on chlorophyll $a$ retrieval depends strongly on the choice of wavelength. Thus a 672:704-nm algorithm performs best in this respect for medium ($C \sim 10$ mg/m$^3$) concentrations, whereas for the wider-spaced MODIS bands (667 nm:748 nm) good performance is achieved only at very high concentrations ($C \sim 100$ mg/m$^3$).

Conclusion (c) has led to development of a completely new type of algorithm, whereby the second, higher wavelength used for retrieval is chosen distinctly for each spectrum to be processed. Thus, when this second wavelength is chosen so that reflectance there is equal to the reflectance at the first chlorophyll $a$ absorption wavelength, the resulting retrieval becomes entirely insensitive to spectrally flat reflectance errors, giving optimal performance for a wide range of concentrations. A second advantage is that for such a choice of wavelengths chlorophyll $a$ retrieval becomes completely independent of backscatter retrieval, as noted in a previous study,10 and independent of any empirical scaling factor depending on illumination conditions and bidirectional reflectance effects.

Tests in which in situ measurements of above-water radiances and near-surface chlorophyll $a$ concentration are used in difficult conditions (high tripton and CDOM absorption, highly variable illumination) show that this new algorithm is promising. As suggested by the theoretical error analyses, results are best for medium-high concentrations ($C > 10$ mg/m$^3$). Because it is these higher concentrations that are of most interest for marine managers concerned with eutrophication issues, the algorithm should prove particularly useful once satellite-based sensors with sufficient spectral resolution become available, e.g., CHRIS and follow-on missions.

It is interesting to compare the present approach to chlorophyll $a$ retrieval with the discussion of band sensitivity in Ref. 16. The criterion for choice of $\lambda_1$ used here is similar in both studies and is related to optimizing sensitivity to phytoplankton absorption as expressed by maximization of $-\partial R_1 / \partial C$. However, in that paper $\lambda_2$ is chosen to take advantage of phytoplankton backscatter by maximization of $\partial R_2 / \partial C$ where $b_{\text{bio}}$ is expressed as a function of $C$ as well as including backscatter from inorganic particles. An increase in $C$ thus has a combined effect on the ratio $\gamma$ by increased absorption at $\lambda_1$ and increased backscatter at $\lambda_2$. However, with such an approach retrieval of chlorophyll $a$ (not described explicitly in that reference) is then coupled to retrieval of a backscatter coefficient (or a related quantity such as total suspended matter or inorganic suspended matter) and requires knowledge of the chlorophyll-specific phytoplankton-backscatter coefficient. We avoided these two problems by targeting only the absorption properties of phytoplankton. Moreover in the present study not just spectrally uncorrelated reflectance errors are considered, but also atmospheric-correction-type errors are considered, whose effect can be significantly reduced by exploitation of the fact that such errors are spectrally rather flat over the red/NIR range considered.

The rather simple formulation of the new algorithm, defined by Eqs. (22)–(24), clearly indicates the most crucial measurements that are required for improvement:

(a) A prerequisite for application of the algorithm is the availability of reflectance data with sufficient spectral resolution in the 700–740-nm range and good wavelength accuracy to enable the critical wavelength $\lambda_2^*$, to be accurately located. In this respect the present generation of airborne imaging spectrometers may already be suitable, while future satellite-based sensors such as CHRIS and follow-on missions look promising. For concentrations higher than $\sim 120$ mg/m$^3$ as found in some inland waters the 830–900-nm spectral range will also be needed for optimal performance.

(b) As for any analytical algorithm based on chlorophyll $a$ absorption, retrieved concentrations are inversely proportional to the chlorophyll-specific...
phytoplankton-absorption coefficient. Any error in this calibration parameter will thus be transmitted directly to an error in the retrievals. At present the region or species dependence of this calibration parameter is poorly known.

(c) More attention may need to be paid to input data for the pure-water absorption coefficient in the red/NIR range, especially to determine the magnitude of any salinity- or temperature-dependent variations.32

In addition to future research in these directions, testing the algorithm for other case 2 water bodies is necessary to determine its robustness and clarify the range of conditions in which chlorophyll a retrievals are reliable.

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