Operational estimation of primary production at large geographical scales

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ABSTRACT

A protocol is developed for calculation of phytoplankton production from remotely-sensed data in the operational mode. The key element is an objective assignment, on a pixel-by-pixel basis, of the parameters required to implement a primary production model (parameters of the photosynthesis-response function and of the vertical distribution of pigment biomass). In a regional context, the assignment is made by searching the archived data on these parameters according to the (remotely-sensed) chlorophyll concentration and surface temperature. We refer to this approach as the Nearest-Neighbour Method. The procedure is justified on the basis of the known variation of bio-optical properties of phytoplankton with chlorophyll and temperature as well as through consideration of the seasonal variation of watercolumn stratification and its effect on the vertical pigment profile. We illustrate the method, and its justification, using data from the Northwest Atlantic Ocean. Using data from an oceanographic expedition not included in the archive, we find that the parameters estimated in this way are not significantly different from those obtained by direct measurement. We estimate the error associated with parameter assignment on the calculated phytoplankton production to be about 27%. Some potential limitations of the method are discussed.

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1. Introduction

The considerable body of work published during the past twenty years or so on the estimation of oceanic primary production using remotely-sensed visible spectral radiometry (ocean colour) has been motivated mainly by research questions. This mode of working is characteristic of a discipline in the relatively early stages of development. In oceanography generally, the trend of the times is to emphasise another mode of working, namely the operational one. The operational mode implies routine application of methods, established and proven in the research mode, to produce data streams intended for wide dissemination and practical application within an appropriate time limit tailored to the need. An excellent example, from another field, of operational application built on basic science is the routine collection of meteorological data at many sites and their incorporation into a weather forecast. By virtue of its synoptic view, remote sensing (earth observation) is a cost-effective method for data acquisition in the operational mode.

Remote sensing in the operational mode is distinguished from that in the research mode as follows. In the research mode, we produce the basic

scientific results, demonstrate that they can underpin a new technology, develop the appropriate procedures, and subsequently show by strategic applications that the technology may support a cost-effective contribution to knowledge with resultant benefit to mankind. The protocols applied may vary from demonstration project to demonstration project, according to the particular needs of the study. The protocols may also involve subjective steps, requiring intervention of a skilled person, with consequent delays in the release of the results. In the operational mode, we apply robust procedures on a regular basis to produce routine results that can be used directly in practical applications. In such cases, an *objective* procedure is clearly necessary. For the operational mode, the protocols are considered to be fixed, not adjustable.

Here, we consider the issues arising in the transition from research-mode to operational-mode estimation of primary production by remote sensing. Taking the Northwest Atlantic Ocean as an example, we propose an objective protocol for operational use. An ecophysiological justification of the approach is given. Finally, research and operational approaches are compared and contrasted for the same region.

2. Background

The issues underlying calculation of oceanic primary production using visible spectral radiometry (ocean colour) have been reviewed

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in Platt & Sathyendranath (1999). Given the synoptic view afforded by remotely-sensed imagery, the problem falls into two parts: the development of a local algorithm and its implementation on a large number of grid points (pixels).

By local algorithm, we mean a procedure to convert pigment biomass into primary production, where it is understood that all information essential to implement the procedure is available for the particular space-time point concerned: this is the idea of localness. The minimum information includes the pigment biomass and irradiance at the surface, an equation to describe the photosynthetic response to available light (the photosynthesis-light curve), the local magnitudes of the two parameters for this curve (the photosynthesis parameters), an equation to describe the vertical structure of the pigment biomass, and the local magnitudes of the parameters of that equation. In sum, the information required is considerable. But if everything is available, it is possible to make a robust calculation of daily, watercolumn primary production. In the context of this paper (operational oceanography), the local algorithm may be considered to be a solved problem. A choice can be made among various possibilities according to the degree of approximation that is acceptable and the computing time available. The local algorithm used here has been validated (Kyewalyanga et al., 1992, 1997; Platt & Sathyendranath, 1988).

But matters are far from being resolved for the task of implementing the local algorithm on many grid points over a large region. Generally speaking, although pigment biomass and surface irradiance (the independent variables) may be available for all grid points, the necessary parameters (photosynthetic response, vertical structure)

will not be: they are inaccessible to remote sensing. If the calculation is to be made, the parameters must be assigned at every grid point. In developing suitable protocols to accomplish this lies the difficulty of the calculation.

The possibilities are reviewed in Platt & Sathyendranath (1999). In the research mode, a commonly-used extrapolation procedure is to make a partition of the ocean into a suite of biogeochemical provinces and to use the partition as a basis for assignment of parameters. This approach has worked well for calculation of production at the global scale (Longhurst et al., 1995), where the resolution of the result was 1°×1°.

3. Extrapolation in the operational mode

In operational remote sensing, where the region of interest may be much smaller than global scale, a spatial resolution of 1°×1° may often be considered to be too coarse. The Longhurst partition of the global ocean comprises some 57 provinces. Where the interest is centred on only part of a single ocean basin, the number of provinces involved at this scale might be less than ten, perhaps too few for a high-resolution study. Thus, for routine use in defined areas, as opposed to research demonstration of capability, we may need to examine alternatives to the formal classification of Longhurst (Longhurst et al., 1995; Longhurst 1998).

To take a concrete example, we consider the Northwest Atlantic Ocean (Fig. 1). For this region (comprising some 1.8 million in-water pixels at a nominal pixel resolution of 1.5 km), we have constructed
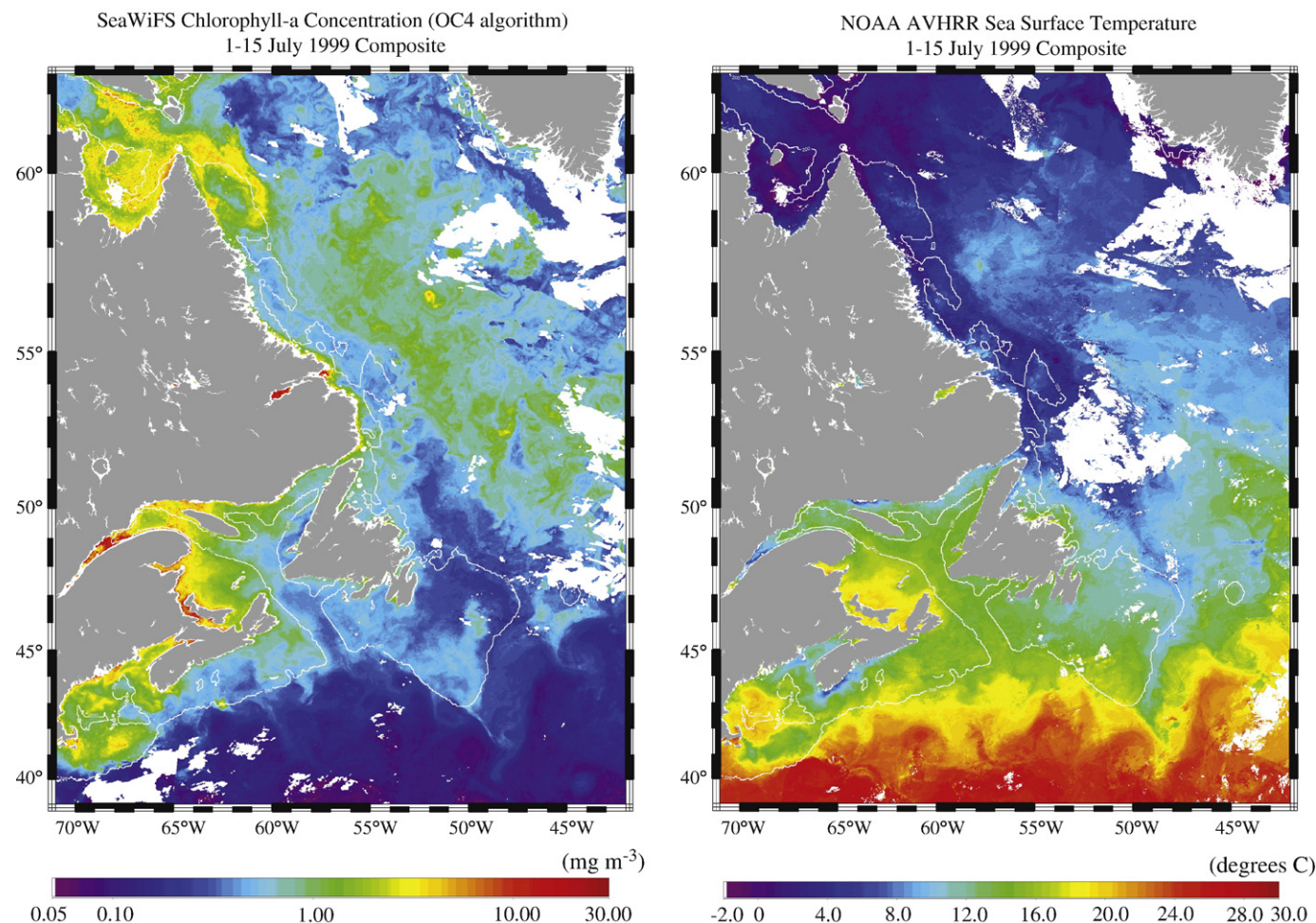

Fig. 1. Remotely-sensed composite images of chlorophyll and sea-surface temperature for the Northwest Atlantic Ocean. Pairs of images such as these, produced every two weeks, form the basis of a time series characterising the State of the Marine Ecosystem in the Atlantic Zone of Canada.

time series of the available, full-resolution fields of pigment biomass from the SeaWiFS mission, composited at the biweekly and weekly time scales. Taken together with the sea-surface temperature fields retrieved also by remote sensing at the same scales of time and space, the series is referred to as the State of the Marine Ecosystem for the Canadian Atlantic Zone. The purpose of the time series is to provide information that could be used to address a variety of scientific questions and develop understanding that could be used as the basis of scientific advice for ocean management, including fisheries management. Applications of the series so far have dealt with ground fish (Platt et al., 2003), with shrimps (Fuentes-Yaco et al., 2007; Koeller et al., 2007), with the relation between physical forcing of the ocean and phytoplankton distribution (Platt et al., 2005), and with the development of ecological indicators for the pelagic ocean (Platt & Sathyendranath, 2008-this issue).

It was considered that the value of the project would be enhanced if the scope of the time series were expanded to include the field of primary production computed on the same scales using the remotely-sensed fields of pigment biomass and temperature as inputs. Whereas several authors have computed primary production from remotely-sensed data on ocean colour, to our knowledge, the routine calculation for a particular area, with a view to establishing and applying a highly-resolved time series, has not been attempted.

Before we embark on operational estimation of primary production, one of the factors that must be weighed is the existing body of knowledge about the phytoplankton (vertical profiles of chlorophyll, photosynthetic performance) for the region under consideration. In the case of the Atlantic Zone of Canada, more than fifteen hundred stations are available in the archive for which photosynthesis parameters and vertical structure of chlorophyll were measured. This is a relatively large number of stations compared with what might be expected in other regions. We start from the premise that the archive of these parameters will provide the basis for the extrapolation procedure.

To select a protocol for assignment of parameters, the following options may be considered (Platt & Sathyendranth, 1999).

(1) According to some objective function of a continuous variable such as depth, latitude or sea-surface temperature.
(2) According to dynamic partition of region into suite of biogeochemical provinces wherein parameters are piecewise constant or piecewise continuous (Longhurst et al., 1995; Platt & Sathyendranath, 1988; Sathyendranath et al., 1995).
(3) According to a match between given remotely-sensed fields (chlorophyll, surface temperature) and information in archives of ship observations for the same region.

To choose between these options, or any combination of them, we should acknowledge that the region is complex and highly dynamic, with cold water from the Labrador Current and warm water from the Gulf Stream in close proximity. For such complex conditions, objective functions that would assign all the parameters we need in all seasons are still in the development stage. Thus, we set aside the first option for the time being.

Although the second option is based on the idea of a *dynamic* partition into provinces, the initial implementation used a static template for the boundaries of the provinces. For example, the early, global-scale partition of Longhurst et al. (1995), not intended for operational purposes, uses fixed rectilinear boundaries. For the Atlantic seaboard of Canada, where the seasonal signals of physical forcing and ecosystem response are very strong, a static partition will not suffice for operational use, especially when the spatial resolution is much finer than the $1° \times 1°$ used at the global scale by Longhurst. We have made progress in finding a viable, dynamic partition of our region into provinces, where the qualifier "dynamic" implies that the boundaries of the provinces are free to vary from composite image to composite image (Devred et al., 2005a, 2007; Platt et al., 2005), and

we have demonstrated the seasonal movement of the boundaries, but at present this approach is not ready for routine use. Because we require a protocol that responds to seasonal dynamics, we reject the second option in its present state of development.

Thus, we resort to the third option, assigning the parameters according to matches between the image data and the archived station data. We refer to the approach, which we now describe, as the Nearest-Neighbour Method.

4. Nearest-Neighbour Method

The rationale for the approach is that the magnitudes of the photosynthesis parameters observed at a particular time and place would be determined by a suite of factors including the kinds and size of the cells present in the phytoplankton assemblage, their growth history, including light environment, the nutrient regime, temperature, degree of vertical mixing and so on. The combined effect of all the variables will be encoded in the parameter magnitudes (Parenthetically, we note that these variables will also help to set the local chlorophyll biomass.). We suppose that the parameter magnitudes (set by the aggregate of all these properties, characteristic of a particular time and place) could be estimated to the first order from archived data on the parameters from the same area, arranged according to the environmental context in which they were collected. Of course, an important element of environmental context is that arising from the seasonal cycle of stratification and species succession. The former is associated with the annual cycle of surface temperature and the latter also with changes in the autotrophic biomass (chlorophyll concentration).

Fortunately, both these properties are accessible to remote sensing. Thus the possibility is open that important environmental properties useful for aiding parameter assignment are available routinely on synoptic scales. This is the basis of the Nearest-Neighbour Method for parameter assignment: we use the remotely-sensed information about a given space-time point as an entrée into the regional archive of parameters. Having been guided to a particular place in the archive, we examine an arbitrary number (say, ten) of the nearest neighbours of the archived point before making an assignment of parameters for that pixel. The procedure is developed formally as follows.

For any pixel in the images, we know the biomass B' and the surface temperature T'. We also know the water depth z' and the day number t'. The primes indicate properties of the image pixels. In the archived data, over and above the properties already mentioned for the images, we know the parameters α^B and P_m^B of the photosynthesis-light curve, and the parameters z_m, ρ and σ of the chlorophyll profile when it is fitted to a standard shape (Sathyendranath et al., 1995). We must then consider the intersection between these data sets (Fig. 2).

We can represent each pixel in the remotely-sensed image by a vector with the elements B', T', z', t'. Similarly, we can represent each point in the archive by a vector with elements B, T, α^B, P_m^B, z_m, σ, ρ, z, t. Then, we match as closely as possible (Fig. 3) the corresponding elements of the two vectors (B, B', T, T'). For the point (B, T) in the archive with the closest match to (B', T'), we take the values of parameters α^B, P_m^B, z_m, σ, and ρ: we assume that these represent first estimates of the required parameters for the pixel concerned. A technical issue is that, before looking for the closest match between (B', T') and (B, T), we must transform the values of B, B', T and T' such that they have similar ranges and are given equal weight in calculation of the Euclidean distance between the two points.

The strategy for the protocol, then, is, for any given pixel, to enter the archive with the values of biomass and surface temperature for that pixel and find the archive station with the closest coordinates of biomass and surface temperature (Fig. 2). The chlorophyll profile and photosynthesis parameters for that archive station are the first-order estimates of the parameters for that pixel.
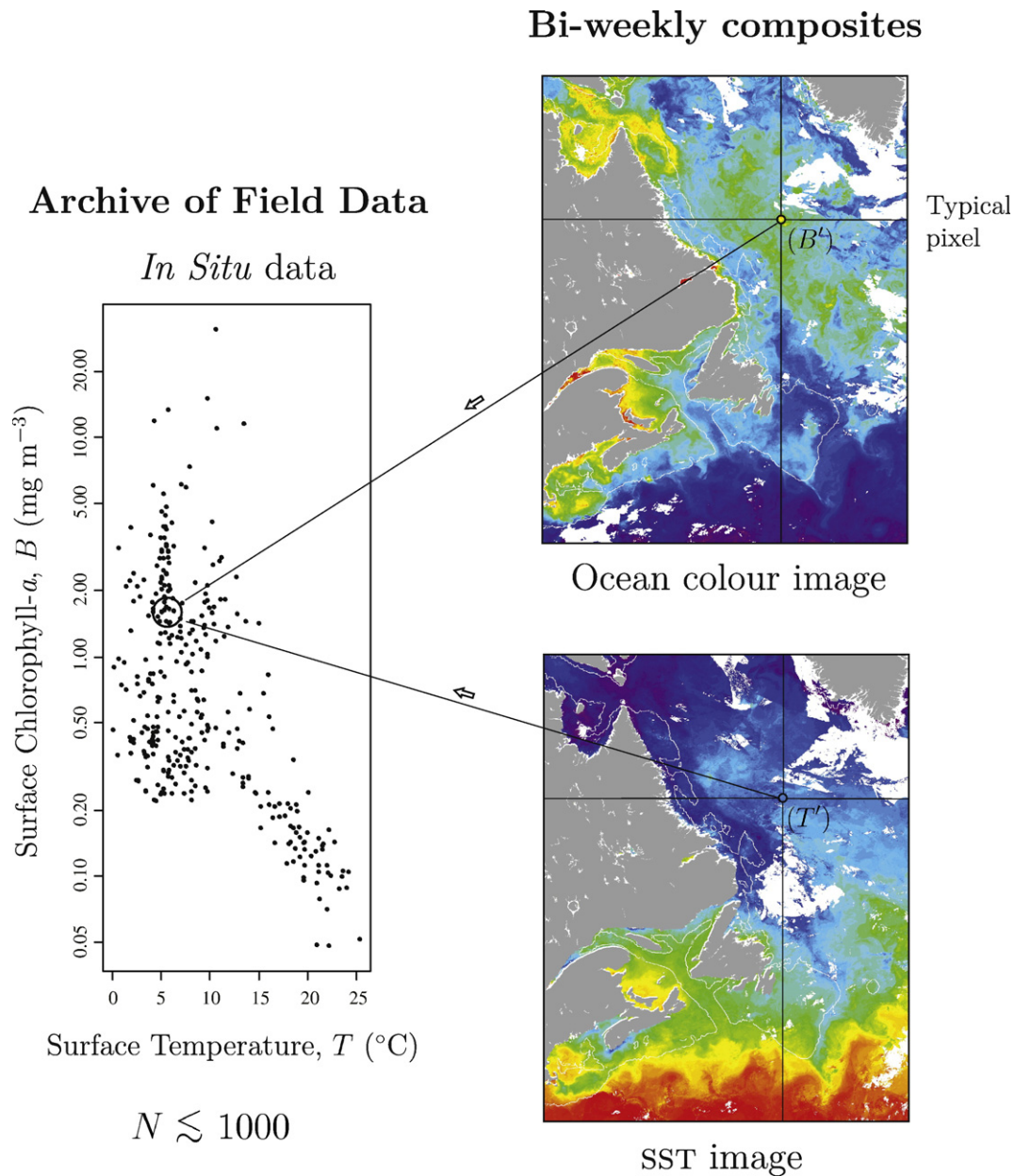
Bi-weekly composites

Typical pixel

(B^{L})

Ocean colour image

(T')

SST image

Fig. 2. The protocol used for parameter assignment in calculation of primary production for the Atlantic Zone. For every pixel in the remotely-sensed images, we determine the chlorophyll and the sea-surface temperature, then enter the archive of *in situ* data with these values of chlorophyll and temperature. For the station that most closely matches these coordinates, we select the parameters we need as the ones that were measured on that station.
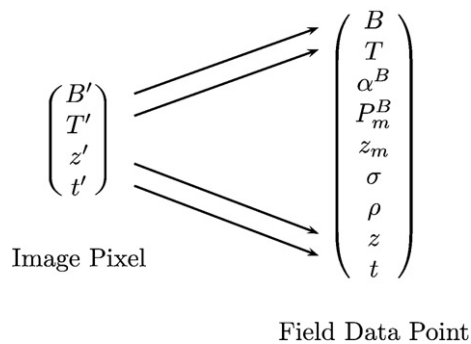

Fig. 3. The intersection of the data from the image pixel and the archive data. Chlorophyll, temperature, day number and water depth are common to the two sets. When the two sets are matched according to the common coordinates of chlorophyll, temperature and time, the photosynthesis and profile parameters from the archive set are assigned to the image pixel.

Let $\mathbf{x}$ be the vector of parameters required to calculate primary production on a given pixel.

$$\mathbf{x} = \left(\alpha^{B}, P_{m}^{B}, z_{m}, \sigma, \rho\right). \tag{1}$$

Our approach is to map from the images into archive and then to the parameter vector:

$$(B', T') \rightarrow (B, T) \rightarrow (B, T, \mathbf{x}). \tag{2}$$

In the archive, we search in the local neighbourhood of (B, T) for the information required.

Certain refinements can now be made. Instead of taking the parameters from only the single archive point with the closest coordinates in the biomass-temperature plane, we can also incorporate information from a number (ten, say) of the nearest neighbours to (B', T'), and calculate the average parameter values over this set (Fig. 4). In calculating the average, we take into further consideration that the
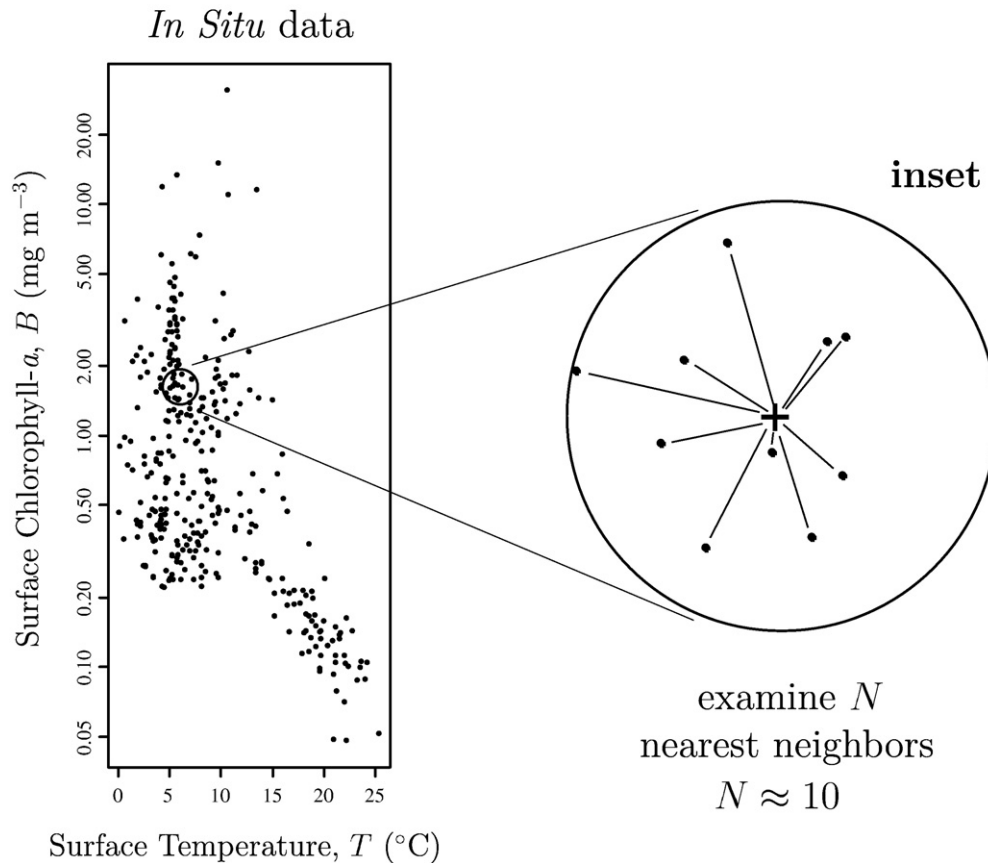
Archive of Field Data

In Situ data

Fig. 4. Once the image coordinates have been matched in the archive data, the nearest-neighbour points in the archived data are also searched, and the required parameters averaged over these stations (weighted as shown in Fig. 5).

archive station and the image may have been taken in different seasons (t and t' may not match), so we can weight the utility of the archived station according to $t - t'$, the difference in day number between it and the image, constructing a weighted average of the parameters over the nearest-neighbour set (Fig. 5). This is the procedure that is in use in our laboratory. Further refinements may be possible based on water depth and geographical location, but these have not yet been explored. Other procedures, perhaps based on other principles, may emerge in the future.

The advantage of the method presented is that it exploits fully the intersection between the image data and the archive data, using information from both the ocean-colour and the sea-surface-tem-

Fig. 5. Weighting function for the parameters revealed in the nearest-neighbour search. If the archived field data has the same day number as the image pixel, it is given maximum weight. The greater the difference in the day numbers of the field data and the image pixel, the smaller the weight assigned to that point when the parameters for the nearest neighbours are averaged.

perature images. It is also an objective procedure. An example of the result is shown in Fig. 6, produced using the same satellite-derived inputs as displayed in Fig. 1. The forcing field for this calculation is spectrally-resolved irradiance calculated from the model of Bird (1984) and corrected for cloud effects using data from SeaWiFS on total photosynthetically-active irradiance.

5. Ecophysiological justification

5.1. Photosynthesis parameters

It is becoming clear that robust global-scale patterns exist in the distribution of phytoplankton, with respect to biomass, size of the cells, taxa concerned and their physiological performance. The gradients are related to gradients in environmental conditions. Very generally, cooler well-mixed water rich in nutrients implies larger cells, usually diatoms, higher biomass and lower biomass-specific rates of primary production as indexed by the photosynthetic parameters P_m^B and α^B. At intermediate temperatures and nutrient concentrations, nanophytoplankton, in particular prymnesiophytes, dominate and photosynthetic parameters tend to be higher. Warm, highly stable and oligotrophic water implies smaller cells, usually the cyanobacterial genera *Prochlorococcus* and *Synechococcus*, lower biomass and less strong photosynthetic performance (Bouman et al., 2005).

In the region of our interest, the Northwest Atlantic Ocean, the same broad patterns are found (Fig. 7). We estimated the percent contribution of large cells to chlorophyll-*a* biomass for samples
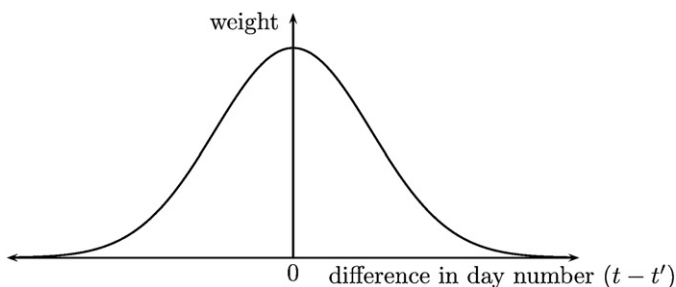
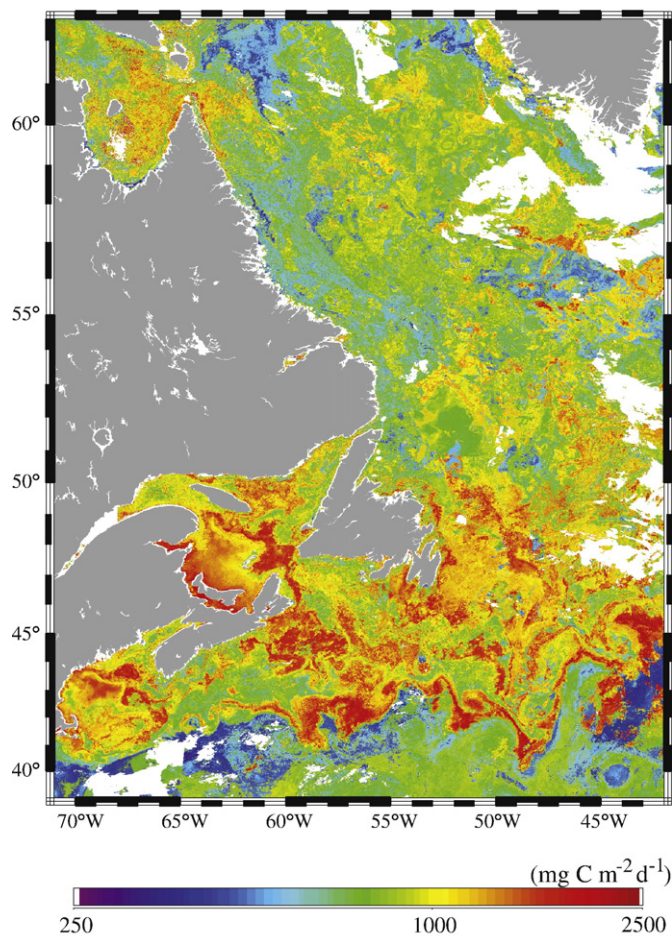## SeaWiFS Primary Production
1–15 July, 1999

Fig. 6. An example of a field of primary production calculated according to the protocol described in this article. Input images shown in Fig. 1.

collected in the Northwest Atlantic using the pigment index proposed by Bricaud et al. (2004):

$$D_\mu = 100 \times \frac{1.41D_f + 1.41D_p}{1.41D_f + 1.41D_p + 1.27D_h + 0.35D_b + 0.60D_a + 1.01D_c + 0.86D_z},$$

(3)

where D_f and D_p represent the concentrations of fucoxanthin and peridinin, both of which are diagnostic pigments of diatoms and dinoflagellates, respectively. They are typically associated with the microphytoplankton size class. The quantities D_h, D_b and D_a denote the concentrations of 19′ hexanoyloxyfucoxanthin, 19′ butanoyloxyfucoxanthin and alloxanthin, respectively. These are three carotenoids associated with the nanophytoplankton size class. Chlorophyll-*b* (D_c) and zeaxanthin (D_z) are pigments associated with chlorophytes and cyanobacteria, which are generally found in the pico-phytoplankton size class. The coefficients that multiply the concentrations are the typical ratios of chlorophyll-*a* to each diagnostic pigment.

For the Scotian Shelf, a negative correlation is found between D_μ and temperature (Fig. 7a). The data further reveal that large cells are also predominant at high chlorophyll concentrations (>3 mg m^{-3}), consistent with the view that diatoms are responsible for the Spring bloom on the Scotian Shelf (Fig. 7b). For the Labrador Sea, however, weak correlations between the pigment index and environmental covariates are observed (Fig. 7a, b). This probably arises from the presence of *Phaeocystis*, a prymnesiophyte, which has fucoxanthin as a dominant accessory pigment. Since fucoxanthin is used in Eq. (1) as

an indicator of the presence of large cells, in particular diatoms, the presence of *Phaeocystis* may lead to an overestimate in the relative contribution of diatoms, and hence large cells, to pigment biomass. The specific absorption coefficient of phytoplankton at 440 nm ($a^*(440)$) (absorption per unit concentration of chlorophyll-*a*), which is strongly influenced by both cell size and pigment composition, can also be used as an indicator of size and taxonomic structure (Bouman et al., 2003; Bricaud et al., 2004). In the Labrador Sea and on the Scotian Shelf there is an increase in $a^*(440)$, and therefore a decrease in the relative contribution of large cells to pigment biomass, with increasing temperature and biomass (Fig. 8).

Photosynthetic performance is also strongly correlated with environmental conditions indexed by the two variables routinely accessible by remote sensing: sea-surface temperature and chlorophyll. When the *P–I* parameters P_m^B and α^B are plotted against temperature, clear positive correlations are observed (Fig. 9). These relationships between the *P–I* parameters and temperature have been observed in other studies of temperate marine ecosystems and are caused by, in part, the influence of physical forcing on phytoplankton community structure (size and taxonomic composition). Negative correlations between the *P–I* parameters and biomass are also apparent (Fig. 9), although they are less pronounced, owing to the weak relationship between chlorophyll concentration and the environmental conditions regulating species succession and photophysiology. In the Northwest Atlantic, low biomass occurs both in the winter and summer months. The former is a result of light limitation due to a combination of low irradiance at the sea surface
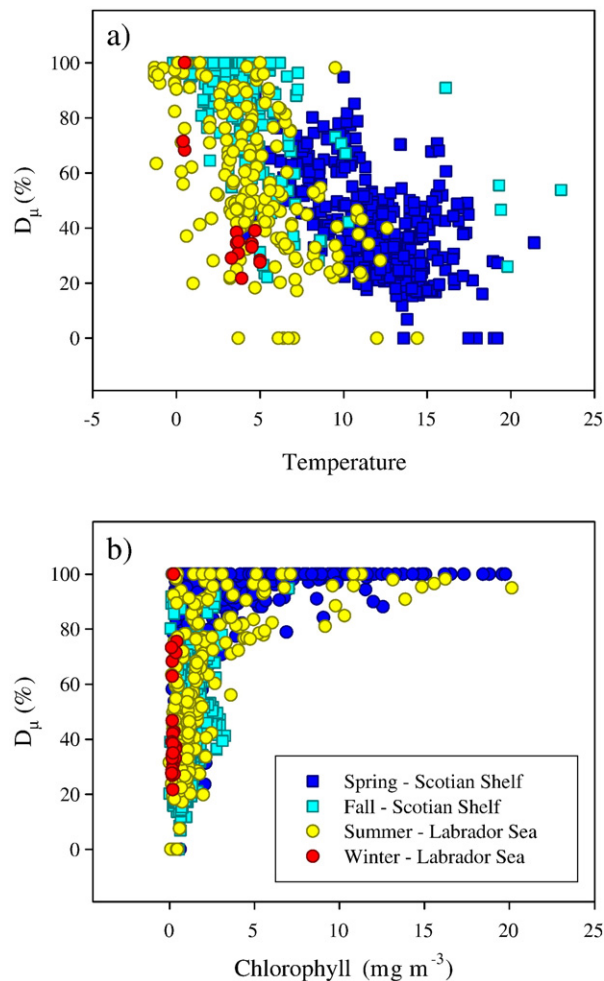

Fig. 7. The relative contribution of large cells to phytoplankton community structure, indexed as the property D_μ given in Eq. (3), as functions of (a) temperature; and (b) chlorophyll concentration in different regions of the Northwest Atlantic Ocean.
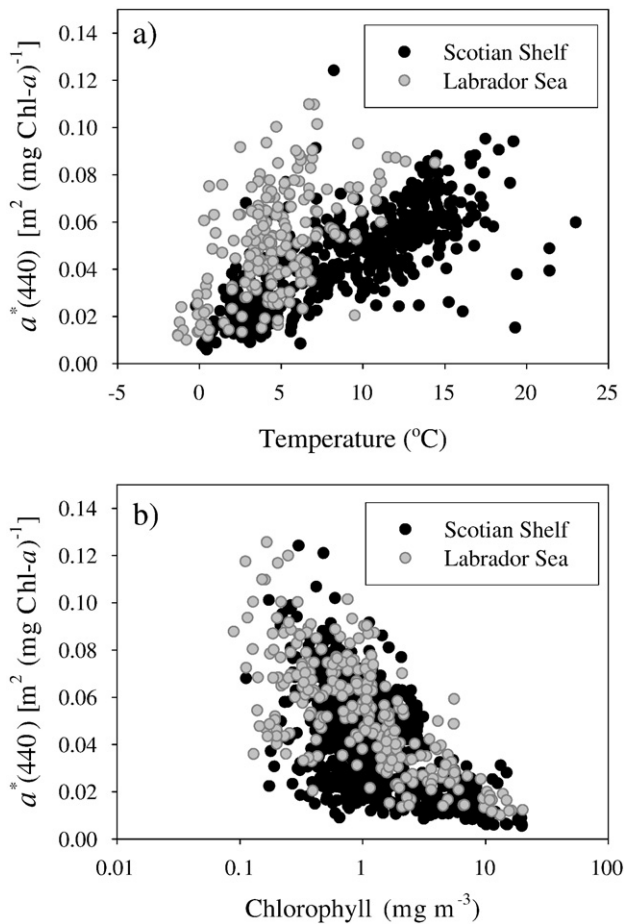
Fig. 8. The specific absorption of phytoplankton at 440 nm as functions of (a) temperature; and (b) chlorophyll concentration in different regions of the Northwest Atlantic Ocean.

and deep mixing, whereas the latter is caused by depletion of nutrients in the surface ocean following the onset of stratification. Thus low biomass may occur under very different sets of environmental conditions, which in turn would be manifested differently in both the structure of the phytoplankton communities and their physiological status. However, at high biomass concentration, we observe that diatoms always dominate and that P–I parameters are consistently low. Multiple linear regression analysis reveals that temperature alone can explain a significant fraction of the variability in P^B_m ($r^2 = 0.56$, $N = 477$) and that adding the $\log_{10}$ of chlorophyll ($\log_{10}$Chl) as a further independent variable does not significantly increase the explained variance ($r^2 = 0.57$, $N = 472$). However, in the case of the light-limited parameter, α^B, using both temperature and $\log_{10}$Chl concentration as independent variables explains a markedly higher percentage of the total variance ($r^2 = 0.43$, $N = 464$), then either variable alone (temperature, $r^2 = 0.37$, $N = 469$; log(Chl), $r^2 = 0.22$, $N = 464$).

The generalities discussed in this section suggest that the combined use of biomass (chlorophyll concentration) and temperature, both accessible to remote sensing, should provide a plausible approach to assignment of the photosynthesis parameters. They provide an excellent realisation of the notion that the magnitudes of the photosynthesis parameters contain latent information on environmental conditions, especially in so far as they affect community structure manifest both in the size and taxonomic affiliation of the cells.

5.2. Parameters of chlorophyll profile

The vertical structure of the chlorophyll field is required to calculate primary production of the watercolumn. It cannot be recovered directly

from remote sensing. One way to cope with the problem is to describe all profiles with the same general mathematical function and then to specify the particular profile at a given time and place through assignment of particular parameters to that profile within the same general equation. This is the approach of Platt et al. (1988) who used as the general function a shifted Gaussian with four parameters. This approach has been able to represent a very broad range of profiles as observed throughout the world's oceans. Profiles collected from particular stations can be fitted to the shifted Gaussian and the resultant four parameters provide an economical way to describe the vertical distribution of the autotrophic biomass at that station. An archive of such parameters can be accumulated over the region of interest in different seasons. Note that, in remote-sensing applications, the satellite data provide information on the magnitude of the chlorophyll biomass in the near-surface waters, such that the profile parameters required can be reduced to three, representing only the shape of the vertical profile (Sathyendranath et al., 1995).

At most locations in the ocean, the vertical distribution of chlorophyll is a seasonally-varying structure. It is closely related to the seasonal development of stratification, which in turn depends on the resultant of two opposing trends: the tendency for the ocean to stratify under solar heating (strongest in summer) and the tendency for mixing induced by wind to erode stratification (strongest in winter). Because these opposing trends are each seasonally-dependent, each being strongest at a different season, the resultant itself (watercolumn stratification) also has a strong seasonal cycle. Of course, the solar heating cycle varies in phase according to latitude, so that the stratification cycle varies with latitude as well as with season.

In a region of interest with a wide range in latitude, the seasonal cycle will proceed with a different phase in different parts of the region, which complicates the issue of assigning parameters of the profile based on seasonality: seasonality is not the same everywhere at the same time. A requirement thus arises to quantify the seasonality for any pixel in any image.

To meet this requirement we rely on remote sensing of surface temperature and consider the seasonal evolution of temperature at any location (pixel). If T is the surface temperature, its (climatological) variation throughout the year will be bounded by a seasonal maximum T_{max} and a minimum T_{min}. The annual range is clearly the difference $(\Delta T)_i = (T_{max})_i - (T_{min})_i$, where the index i labels the pixel.

Now, we seek an index $x_i(t)$ to represent the extent to which, at time t the surface temperature has progressed along its seasonal cycle. Explicitly, if $T_i(t)$ is an observation of temperature at pixel i at an arbitrary time t, with $T_{min} \leq T \leq T_{max}$, then

$$T_i(t) = (T_{min})_i + x_i(t)(\Delta T)_i, \qquad (4)$$

where $x_i(t)$ lies in the range $0 \leq x_i(t) \leq 1$. We call $x_i(t)$ the *Seasonal Advancement Index*, or more concisely the *Seasonality Index*. It can be defined with respect to a single pixel or through aggregation over any number of pixels. Small values of $x_i(t)$ correspond to winter conditions (low stratification) at time t, high values to summer conditions (stable stratification). The magnitude of the seasonality index should reflect the strength of the stratification at pixel i and time t.

We expect that $x_i(t)$ should correlate with the magnitudes of the parameters of the vertical chlorophyll profile at location i as they change with season. We further expect that any measure of the degree of stratification, for example the buoyancy frequency, should correlate with $x_i(t)$. The seasonality index $x_i(t)$ reflects the reality that, according to latitude and other factors, seasonal dynamics are compressed in time to a greater or lesser extent. In a given year, the magnitude of $x_i(t)$ on a given day number should reveal whether, at location i, the season is advanced or retarded or normal.

We have examined data from the Atlantic Zone in the context of seasonal advancement. In particular, for the five-year period beginning at the start of the SeaWiFS data series, the seasonal advancement
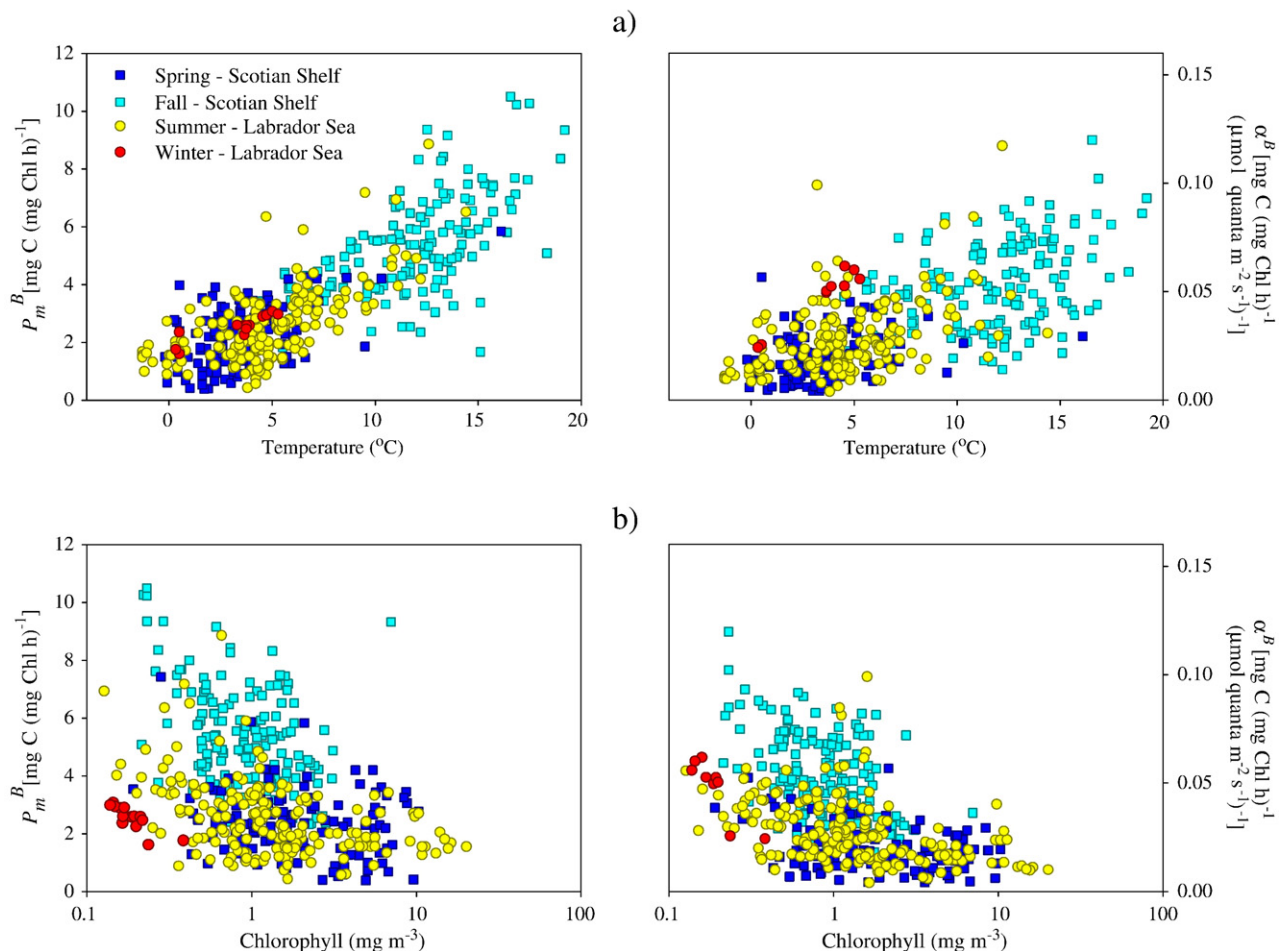
a)

b)

Fig. 9. The parameters of photosynthetic response as functions of (a) temperature; and (b) chlorophyll concentration in different regions of the Northwest Atlantic Ocean.

index varies smoothly with the mixed-layer depth (Fig. 10a,b). There is a hysteresis in this relationship (Fig. 11) such that the rate of decrease in mixed-layer depth in the heating season is more rapid than the rate of increase in the cooling period. Similar results are obtained for the degree of stratification (buoyancy frequency), with less-pronounced hysteresis (Fig. 12). The seasonal advancement index does indeed have the property of normalising the annual cycle of SST at different latitudes (Fig. 13): it is more successful in this regard for the heating season than for the cooling season.

These results are consistent with the view that we can estimate vertical structure in the watercolumn, and therefore in the pigment field, using an objective index of seasonality. Temperature itself is an approximation to seasonality, but the significance of a particular temperature at a particular time will vary somewhat depending on location. Temperature may be used as a first-order proxy for vertical structure. Some function of the local temperature, to better indicate local seasonality, would be an improvement. On the other hand, absolute temperature (together with pigment biomass) is the appropriate predictive indicator (as discussed above) for the photosynthesis-response parameters. Hence, the most simple procedure would involve using pigment biomass and temperature as predictor variables for both sets of parameters (photosynthesis response and vertical structure), and this is the basis of our standard methodology.

6. Error analysis

The extrapolation procedure (parameter assignment) is a key issue in operational primary production. Ideally, the method used will meet the following criteria: (a) reproducibility and objectivity; (b) weak dependence on scale in that rank-preserving transformations (such as logarithms) do not lead to large changes in the results; (c) locality, in that local assignments are not affected by distant parts of the image; (d) plausibility, in that the method should produce results that are credible and physically realistic, given what we know of the system; and (e) only weakly dependent on changes in sampling. In selecting the method applied here, we have attempted to satisfy these criteria. In this section, we examine in more detail the errors in the output from a variety of sources, including parameter assignment.

The local algorithm (spectral, non-uniform biomass profile) that underlies calculation of primary production has been validated (Kyewalyanga et al., 1992, 1997; Platt & Sathyendranath, 1988). The errors associated with the computation of primary production using remotely-sensed chlorophyll fields and parameter assignment according to archived data with a partition into provinces have been discussed (Platt & Sathyendranath, 1993; Platt et al., 1995). It was concluded that such estimates of primary production might entail a random error of some 50%, the bulk of the error arising from biomass retrieval, assumed to be not better than 35% (Gordon et al., 1983). To the extent that some pixels may be located in waters that fall into the optically-complex category, the added difficulty in chlorophyll retrieval would tend to inflate the error in estimated primary production. The potential error resulting from aggregation of the archived parameter data into provinces was taken to be about 7%, based on the standard error, relative to the mean, of the parameters within particular provinces and seasons (Platt et al., 1995).
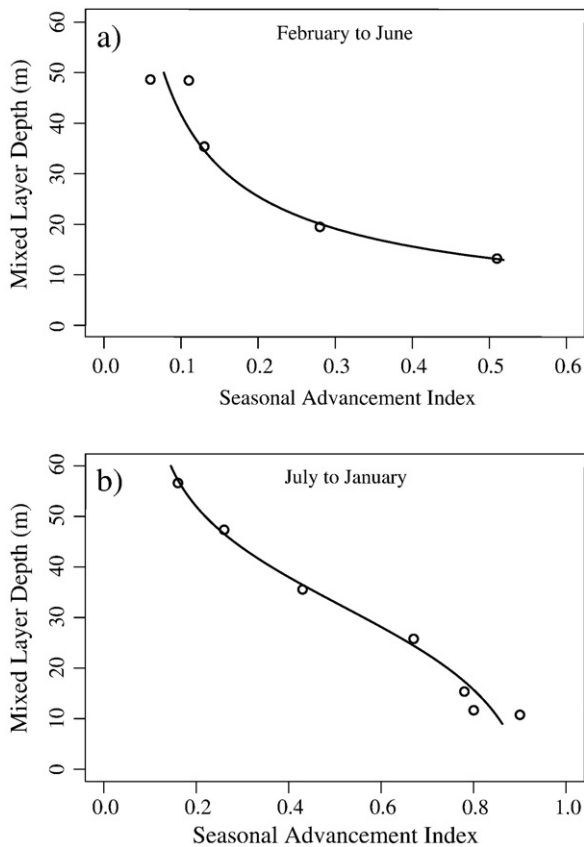
Fig. 10. The variation of mixed-layer depth with degree of seasonal advancement (see Eq. (4) during (a) the heating season; and (b) the cooling season in the Northwest Atlantic Ocean.

Fig. 12. (a) The evolution with time of Brunt–Väissälä frequency, a measure of strength of stratification, and seasonal advancement index (see Eq. (4)); and (b) the relation between seasonal advancement index and Brunt–Väissälä frequency showing the limited hysteresis.

For the Nearest-Neighbour Method, the error involved in assignment of the parameters can be assessed by using station data not contained in the archive. We have used data from an oceanographic cruise to the continental shelf of Nova Scotia (May, 2004) for which some thirty stations are available (Fig. 14a). All the parameters of the chlorophyll profile and the two photosynthesis parameters were measured on all stations, as were the surface temperature and surface chlorophyll. Using an archive of data not containing these thirty stations, otherwise containing 1638 observations of α^B, 1041 values of P_m^B (observations not deeper than 20 m) and 1585 sets of profile parameters, and starting with the surface temperature and chlor-

ophyll, we estimated all required parameters for each station using the nearest-neighbour method. We then compared the estimated parameters with the observed ones on a pairwise basis. The estimated sets were not significantly different (0.05 significance level) from the observed sets (Table 1, Fig. 15). Overall, these results are encouraging for the method of parameter assignment.

A more stringent test is to compare observed parameters with those estimated using the nearest-neighbour method where the inputs are not the observed temperature and chlorophyll but those captured by remote sensing. We prepared composite images of temperature (AVHRR) and chlorophyll (SeaWiFS) for the period May 1 to 15, 2004, covering the
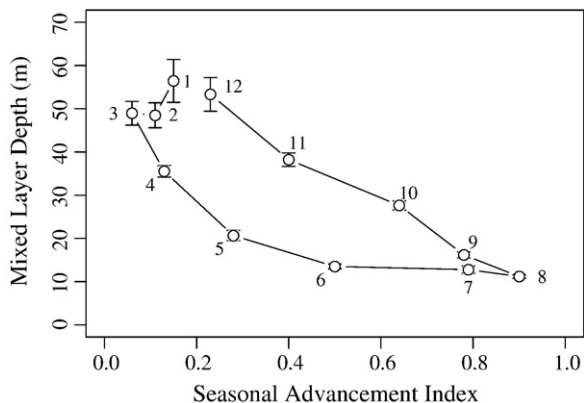

Fig. 11. The variation of mixed-layer depth with degree of seasonal advancement (see Eq. (4) in the Northwest Atlantic Ocean showing the hysteresis between the heating and cooling seasons. Numbers refer to months.
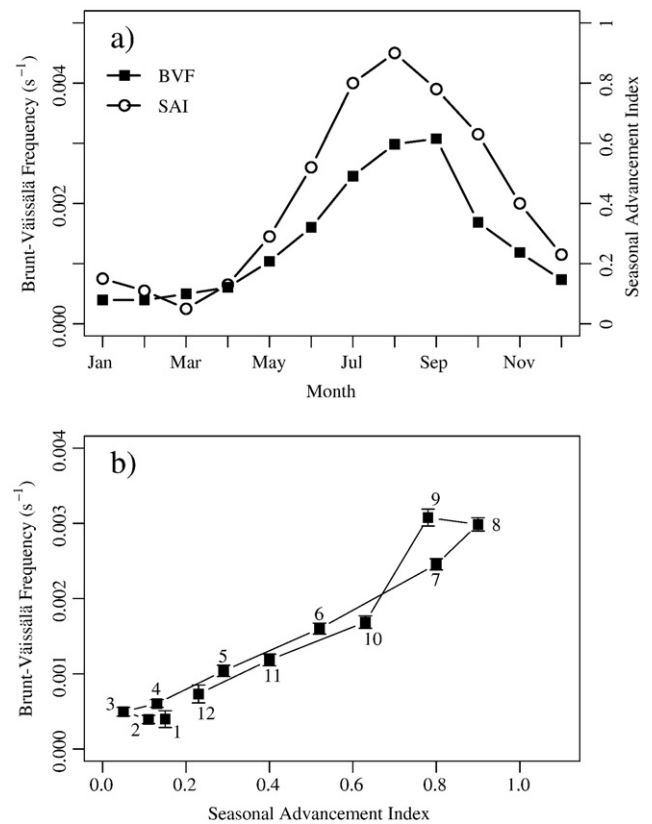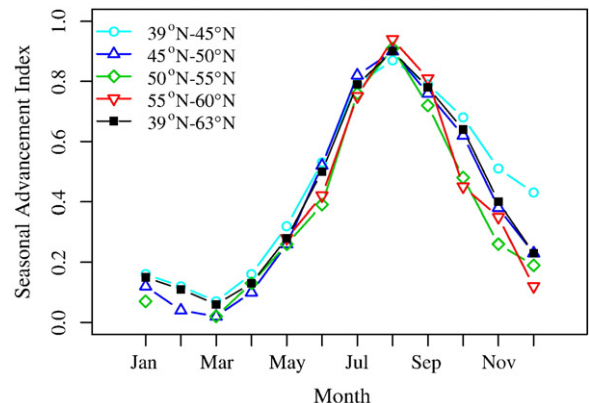

Fig. 13. The time course of seasonal advancement index (see Eq. (4) in different latitudinal bands of the Northwest Atlantic Ocean, showing how this index serves to normalise the seasonal cycles at different latitudes.
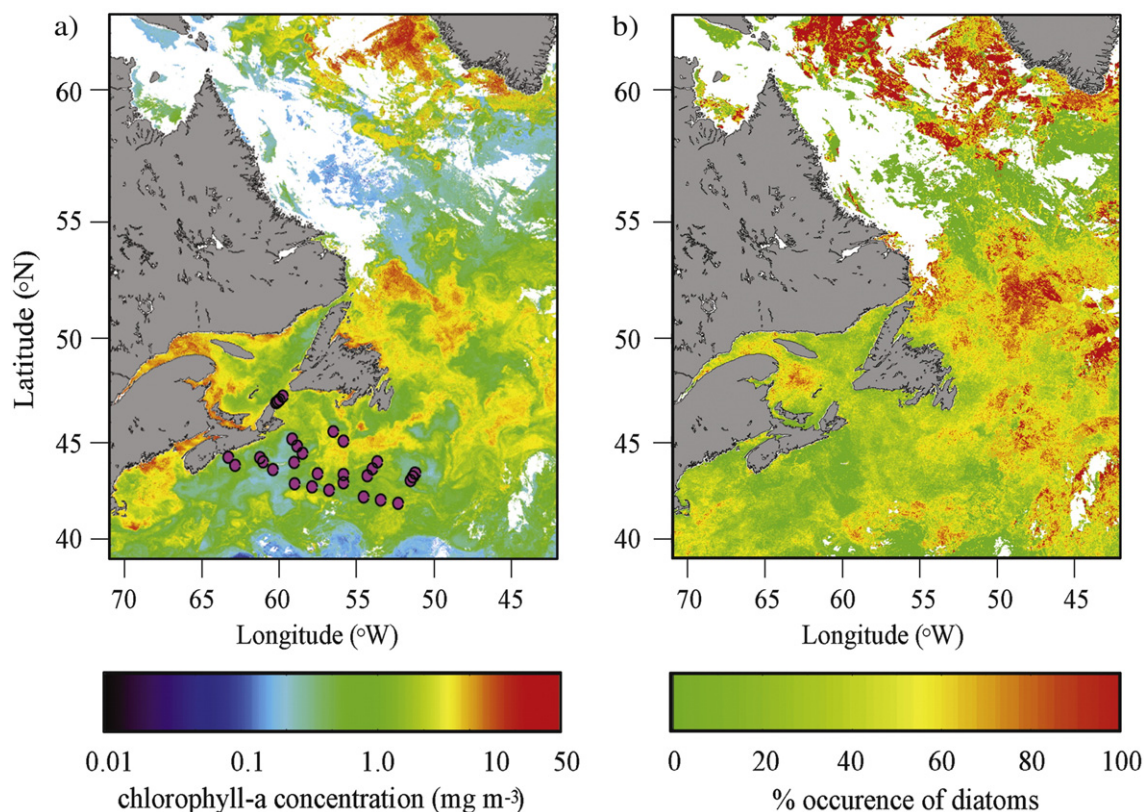
Fig. 14. The Northwest Atlantic Ocean in the first half of May 2004, (a) showing the chlorophyll distribution and also the location of the thirty oceanographic sampling stations mentioned in the text; and (b) the probability of diatom dominance, as determined using the algorithm derived for that purpose by Sathyendranath et al. (2004).

duration of the cruise. For pixels corresponding to the station positions, temperature and chlorophyll were digitised. Using these as inputs, parameters were estimated by the Nearest-Neighbour Method, and compared with observed parameters as before. In this case also (Table 1, Fig. 15), the estimated parameter sets were not significantly different from the observed ones (0.05 confidence level).

Another way to evaluate the parameter assignment is through its influence on the estimation of primary production. For all thirty stations we established as the reference values of primary production those calculated with a spectral model (Platt & Sathyendranath, 1988) using the observed photosynthesis parameters, observed biomass profile and clear-sky irradiance computed according to Bird (1984). We then estimated all required parameters by the nearest-neighbour method using as inputs the observed surface temperature and chlorophyll for each station. Primary production was calculated for all stations using these parameters and the same irradiance forcing as for the reference calculation. The differences between these estimates

and the reference values could be ascribed only to the errors associated with parameter assignment. No other source of variance was present. We found that the mean relative difference (regardless of sign) between the estimates and the reference values was 27.0%. This is our best estimate of the relative error in the estimation of primary production arising from parameter assignment by the nearest-neighbour method. Generally, these estimates of primary production were low (under-estimated) compared with the reference values.

However, in operational use, the parameter assignment would be implemented using as inputs the temperature and chlorophyll determined by remote sensing. We therefore made another set of estimates using parameters assigned in this way. The sources of variance between these estimates and the reference values were now two: errors arising from biomass retrieval and errors arising from parameter assignment. We found that the mean relative difference between these estimates and the reference values was 52.0%. Comparing this result with that of 27.0% when only errors associated with parameter assignment were present leads to the conclusion that the error associated with biomass retrieval is 25.0%. It is known that in the northwest Atlantic Ocean the SeaWiFS OC4 algorithm underestimates chlorophyll (Devred et al., 2005b; Fuentes-Yaco et al., 2005), and this bias could account for some of the underestimation of primary production using the operational procedure. Moreover, the remote-sensing inputs are based on two-week composite images, whereas the ship observations represent particular days.

The canonical expression for P_{ZT}, the daily, watercolumn production (Platt & Sathyendranath, 1993) is

$$P_{ZT} = \frac{BDP_m^B}{K} f(I_*^m), \qquad (5)$$

where B is the pigment biomass, D is the day length, K is the diffuse vertical attenuation coefficient for visible light and f is a dimensionless function of the normalised noon irradiance I_*^m. Eq. (5) is linear in the

Table 1
Probability p associated with paired t-tests between parameters measured at sea on the Scotian Shelf Spring 2004 and parameters estimated using the nearest-neighbour method with inputs either from field measurements or satellite measurements of chlorophyll and temperature

Parameters	Probability p	
	Field data	Satellite data
P_m^B (mg C (mg Chl)$^{-1}$ h^{-1})	0.052	0.31
α^B (mg C (mg Chl)$^{-1}$ h^{-1} (μmol quanta m^{-2} s^{-1})$^{-1}$)	0.48	0.77
z_m (m)	0.35	0.26
σ (m)	0.98	0.89
ρ (dimensionless)	0.89	0.56

When the probability p exceeds the chosen confidence level of 0.05, the null hypothesis cannot be rejected, thus the two sets of data are equivalent.
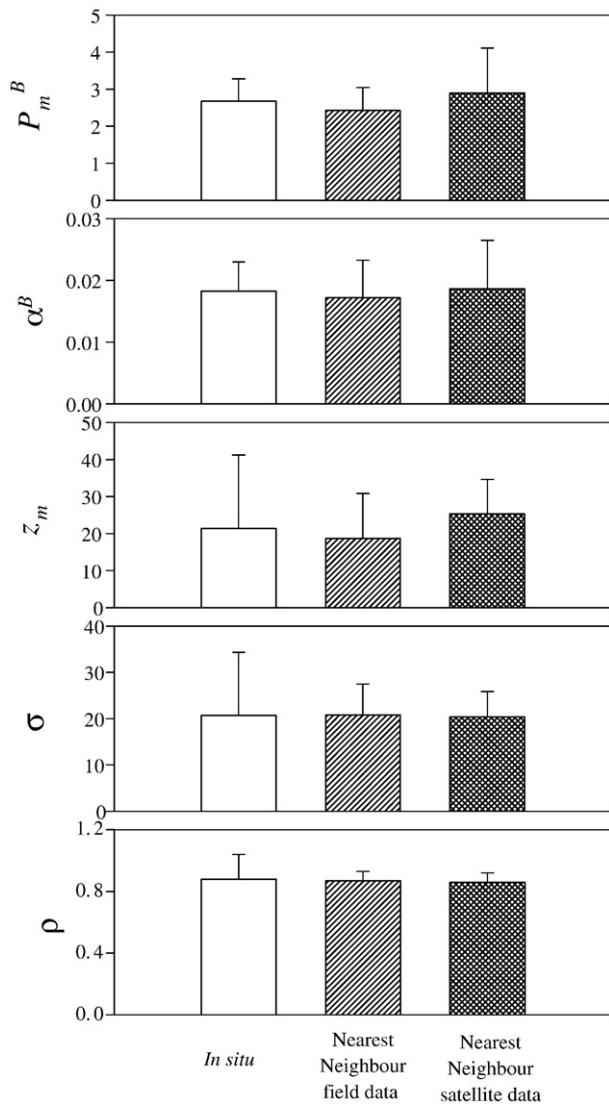
Fig. 15. Photosynthetic-response and pigment-biomass-profile parameters from the Scotian Shelf measured *in situ* during the cruise from April 28 to May 08 2004 or assigned by the nearest-neighbour method using as input either field data or data from satellite images (1–15 May 2004). Photosynthesis parameters were measured from photosynthetic-irradiance experiments and biomass profiles from profiles of extracted chlorophyll-*a*. The error bars represent the standard deviation. Units are P_m^B (mg C (mg Chl)$^{-1}$ h^{-1}); α^B (mg C (mg Chl)$^{-1}$ h^{-1} (μmol quanta m^{-2} s^{-1})$^{-1}$); z_m (m); σ (m); ρ (dimensionless).

biomass, such that errors in biomass retrieval will propagate directly to the daily, watercolumn production. This error will always be present. Note that an error in biomass will lead to an error of the same sense in K, since K is a function of biomass. This will tend to reduce the error in estimated production. However, the Nearest-Neighbour Method for parameter assignment invokes remotely-sensed biomass as an entrée to the parameter archive. Hence, any error in biomass retrieval will also affect parameter assignment to the extent that the archive is entered with an erroneous biomass.

Another issue concerns the uncertainty of the parameters as recovered by the method presented here. Depending on the particular values of chlorophyll and temperature associated with a given pixel in a given image, the closeness of the corresponding stations in the archive (the nearest neighbours) will be different. In principle, one might have more confidence in the outcome when the nearest neighbours were closely packed (in chlorophyll-temperature space) than when they were not. Thus, an index of uncertainty in the assigned parameters could be developed from the normalised sum of the Euclidean distances to the nearest neighbours.

7. Discussion

The operational method we have adopted for estimation of primary production from remotely-sensed visible spectral radiometry uses a simple procedure to assign the required parameters on a pixel-by-pixel basis. It is simple because the two predictor variables used (chlorophyll concentration and SST) are both accessible to remote sensing (although one can readily see that other input variables could be used on the same template). Given the simplicity, it is as well to be aware of the potential limitations.

One issue is that the procedure forces all stations into the same mould, regardless of their locations. In other words, it is insensitive to regional peculiarities in the environmental dependence of the parameters, such as are implicit in a partition of the domain of interest into a suite of provinces. It is at the same time a strength and a weakness of the method. It may be partially corrected by introducing the seasonality index as a predictor variable, thus bringing the seasonal cycles at different latitudes to a common (dimensionless) time scale. The problem is compounded in highly-complex regions such as the Canadian Atlantic seaboard, where strong temperature gradients and convoluted oceanographic boundaries lead to intense local variations in the community structure of phytoplankton (Fig. 14b).

Another issue relates to times of the year when the ecological dynamics are changing rapidly, for example during the waning phase of the Spring bloom of phytoplankton. At this time, the environmental influence on the parameters of photosynthetic response changes as nutrients become exhausted until the community structure characteristic of the Spring bloom is replaced by that characteristic of post-bloom conditions. During such times of rapid change, our simple procedure may lead to bias in the estimates of the photosynthesis parameters (Forget et al., 2007b).

Uneven archival data coverage, in both space and time, is also a problem. This means that when the archive is entered for a particular pair of values of chlorophyll and temperature, the area in (B, T) space occupied by the ten nearest neighbours over which the parameters are averaged will not be constant. In regions of (B, T) space that are undersampled, remote neighbours may be included in the averaging, leading to bias in the parameter estimates. Some relief from this limitation may be provided through the recent work of Forget et al. (2007a), in which a method is developed to estimate the parameters of photosynthesis response from data on *in situ* primary production.

Difficulties aside, the procedure outlined in this paper, is objective and operational. It can be implemented by non-specialists to produce fields of primary production on a routine basis. Moreover, the procedure could be applied easily to areas other than the Northwest Atlantic Ocean, provided suitable databases existed, another justification for the establishment of ecological time series in the ocean. In principle, the results could be issued in near real time and made available to interested parties for a variety of applications in science (for example in studies of the ocean carbon cycle) and management of the marine ecosystem (for example in the development of ecological indicators).

Acknowledgements

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