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## Using backscattering data

H. Kettle

# Using satellite-derived backscattering coefficients in addition to chlorophyll data to constrain a simple marine biogeochemical model

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## Abstract

Biogeochemical models of the ocean carbon cycle are frequently validated by, or tuned to, satellite chlorophyll data. However, ocean carbon cycle models are required to accurately model the movement of carbon, not chlorophyll and due to the high variability of the carbon to chlorophyll ratio in phytoplankton, chlorophyll is not a robust proxy for carbon. Using inherent optical property (IOP) inversion algorithms it is now possible to also derive the amount of light backscattered by the upper ocean ( $b_b$ ) which is related to the amount of particulate organic carbon (POC) present. Using empirical relationships between POC and  $b_b$ , a 1-d biogeochemical model is used to simulate  $b_b$  at 490 nm thus allowing the model to be compared with either remotely-sensed chlorophyll or  $b_b$  data. Here I test the hypothesis that using  $b_b$  in conjunction with chlorophyll data can help to constrain more model parameters than using chlorophyll alone. This is done by tuning the parameters of the biogeochemical model with a genetic algorithm, so that the model is fitted to either chlorophyll or to both chlorophyll and  $b_b$  data at three sites in the Atlantic with very different characteristics. There are several IOP algorithms available for estimating  $b_b$ . Four of these are investigated and three of them used for model tuning. The effect of the different  $b_b$  datasets on the behaviour of the tuned model is examined to ascertain whether the uncertainty in  $b_b$  is significant. The results show that the addition of  $b_b$  data can have a large effect on the modelled detritus and that differences in the IOP algorithms are not particularly significant.

## 1 Introduction

Quantifying the global carbon cycle is crucial for predicting our future climate. The oceans play an important role in the carbon cycle as they absorb CO<sub>2</sub> from the atmosphere enabling the transport of carbon to the deep ocean through physical and biological processes. Physical processes enable CO<sub>2</sub> rich waters from the ocean surface to sink downwards only resurfacing hundreds of years later. However, biological

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processes can actually remove carbon from the system by exporting particulate organic carbon (POC) to the sea-bed (a process termed as “export production”). Thus for climate change prediction it is crucial to quantify the amount of CO<sub>2</sub> that is transferred from the atmosphere to the ocean through the air-sea interface (the air-sea CO<sub>2</sub> flux) and the amount of carbon that is subsequently exported towards the seabed. Ideally, validation of ocean carbon cycle models would involve comparison of the simulated air-sea CO<sub>2</sub> flux and export production with measured data. Unfortunately these data are not available at the time and space scales necessary. However, chlorophyll concentrations inferred from satellite ocean colour data (Chl) are available globally at an adequate time-space resolution. Chl gives an indication of the amount of living phytoplankton in the ocean. This is useful since it is algal photosynthesis that removes CO<sub>2</sub> from the water allowing more CO<sub>2</sub> from the atmosphere to enter the ocean. Ideally, for carbon cycle modelling, we need to know the amount of carbon fixed by the phytoplankton but this is not directly related to the amount of chlorophyll since the carbon to chlorophyll ratio (C:Chl) within phytoplankton is highly dynamic (Geider et al., 1997). Therefore, chlorophyll is not a robust proxy for carbon unless there are also data on phytoplankton physiology (C:Chl). Thus it is perfectly possible to correctly predict chlorophyll concentrations without correctly predicting carbon concentrations.

However, satellite ocean colour data are simply measurements of the amount of sunlight (at certain wavelengths) that is scattered back out of the ocean (known as the water leaving radiance). Water leaving radiance can be used to estimate the inherent optical properties (IOPs) of the ocean surface waters – these include the absorption coefficient,  $a$  (m<sup>-1</sup>), and the backscattering coefficient,  $b_b$  (m<sup>-1</sup>). The total backscattering coefficient is the sum of the particulate backscattering coefficient ( $b_{bp}$ ) and the backscattering due to seawater ( $b_{bw}$ ). There are a number of algorithms available to calculate  $b_b$  or  $b_{bp}$  from the water leaving radiance, e.g., Loisel and Poteau (2006); Smyth et al. (2006), the QAA (Lee et al., 2002), and the GSM (Garver and Siegel, 1997; Maritorena et al., 2002; Siegel et al., 2002). Furthermore,  $b_{bp}$  derived from satellite data has been empirically related to the amount of POC in the surface wa-

ters (e.g. Loisel et al., 2001, 2002; Stramski et al., 1999). POC is a combination of the amount of carbon contained within living phytoplankton ( $C_p$ ) and biological detritus ( $C_D$ ). Other possible products from ocean colour data are the IOP  $a$  and the apparent optical property  $K_d$  (attenuation coefficient for downwelling light). However, in the open ocean variations in  $a$  and  $K_d$  will be strongly related to Chl so it is unlikely that there is significantly different information here to constrain the models much beyond simply using Chl.

Here, the potential to use satellite  $b_b$  data in addition to satellite Chl data to calibrate a simple 1-D open ocean biogeochemical model is investigated. The model consists of the Hadley Centre Ocean Carbon Cycle model (HadOCC; Palmer and Totterdell, 2001) coupled to the 1-D General Ocean Turbulence Model (GOTM, Burchard et al., 1999). HadOCC is a simple nutrient-phytoplankton-zooplankton-detritus (NPZD) plus carbonate chemistry model that is used in climate prediction models such as HadCM3. The model is applied to three sites in the Atlantic ocean that have very different physical and biological characteristics. The model parameters are tuned to coincident satellite Chl and  $b_b$  data using a genetic algorithm to search the parameter space. The hypothesis is that by using satellite  $b_b$  to validate the POC in global 3-D climate prediction models, the detrital and phytoplankton components of the model may be better constrained than when simply using Chl. Since there are several IOP algorithms available for estimating  $b_b$  the model is tuned to each of these different datasets to assess whether the uncertainty in the  $b_b$  data invalidates the hypothesis.

## 2 Sites

Three sites in the Atlantic are chosen due to the availability of observed data at these locations (see <http://www.noc.soton.ac.uk/animate>). They are: the Central Irminger Sea (CIS) at 60° N, 40° W, the Estacion Europea de Series Temporales del Oceano, Islas Canarias (ESTOC) at 29° N, 15.5° W and the Porcupine Abyssal Plain (PAP) at 49° N, 16° W. These sites have diverse characteristics, as demonstrated by SeaWiFS

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satellite measurements of their photosynthetically active radiation (PAR), chlorophyll concentrations and backscattering coefficients (Fig. 1) thereby providing a range of conditions on which to test the hypothesis.

### 3 Satellite data

5 The ocean colour data were downloaded from <ftp://oceans.gsfc.nasa.gov/SeaWiFS/Binned/8Day/>. These datafiles contain binned normalised water leaving radiances,  $nLw$  (at wavelengths 412, 443, 490, 510, 555 and 670 nm and chlorophyll-*a* data (from the OC4v4 algorithm), averaged over 8 days intervals. The remote sensing reflectance ( $R_{rs}$ ) is computed from  $nLw$  using

$$10 \quad R_{rs}(\lambda) = \frac{nLw(\lambda)}{F0(\lambda)} \quad (1)$$

where  $F0(\lambda)$  are 173.00, 190.15, 196.47, 188.16, 183.01, 151.14.

### 4 Methods

#### 4.1 Deriving the particulate backscattering coefficient, $b_{bp}$

15  $b_{bp}$  can be derived from  $nLw$  or  $R_{rs}$  using a variety of Inherent Optical Property (IOP) inversion algorithms. Here  $b_{bp}$  at 490nm (required for relating to POC) is obtained using the following four IOP algorithms:

LP (Loisel and Poteau, 2006; Loisel and Stramski, 2000; Loisel et al., 2001). This algorithm gives  $b_b$  (total backscattering coefficient) at 410, 440, 490, 510 and 550 nm.  $b_b(490)$  is then converted to  $b_{bp}(490)$  using

$$20 \quad b_{bp}(490) = b_b(490) - b_{bw} \quad (2)$$

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where  $b_{bw}=0.001581378 \text{ m}^{-1}$  is the backscattering coefficient due to water.

GSM (The Garver–Siegel–Maritorena semi-analytical algorithm; Garver and Siegel, 1997; Maritorena et al., 2002; Siegel et al., 2002). This algorithm gives  $b_{bp}(443)$  which, for use in this work, is converted to  $b_{bp}(490)$  using

$$b_{bp}(490) = b_{bp}(443) \left( \frac{490}{443} \right)^{-\gamma} \quad (3)$$

where

$$\gamma = -0.855 \log(\text{Chl}) + 1.259. \quad (4)$$

(Loisel et al., 2006).

PML (Plymouth Marine Laboratory; Smyth et al., 2006). This gives  $b_{bp}$  at 412, 443, 490, 510, 555 and 670 nm.

QAA (The Quasi-Analytical Algorithm, Lee et al., 2002). This gives  $b_{bp}$  at 410, 440, 490, 510, 555 and 670 nm.

Where the solar zenith angle is a necessary input (e.g., for LP and PML) it is set to  $0^\circ$ . The code for computing the LP and QAA algorithms was obtained from <http://www.ioccg.org/groups/software.html> and the algorithms were driven by eight-day averages of  $nLw$  or  $R_{rs}$  (Eq. 1) from SeaWiFS. The results of the GSM (v4) algorithm for  $b_{bp}(443)$  (using SeaWiFS 5.2) were downloaded from <http://www.science.oregonstate.edu/ocean.productivity/inputBbpGsmData.php>. And finally, the PML algorithm results were provided by Tim Smyth.

The different IOP algorithms can give quite different values of  $b_{bp}(490)$  as shown in Figs. 2 and 3. In Fig. 3 it is clear that the QAA and LP results agree very well (Fig. 3c) but there is considerably less agreement between the other algorithms, with

the largest discrepancies between PML and GSM (Fig. 3e). However, the intention here is not to compare these algorithms but rather to investigate whether the  $b_b$  data from the different algorithms are similar enough to each other to constrain the ocean biogeochemical model in a consistent way.

## 4.2 Biogeochemical model

The biogeochemical model used here is the NPZD Hadley Centre Ocean Carbon Cycle model (HadOCC; Palmer and Totterdell, 2001) coupled to the 1-D General Ocean Turbulence Model (GOTM, Burchard et al., 1999) (henceforth denoted GOTM-HadOCC). For further details and model equations please refer to Kettle and Merchant (2008).

The difference in the model used here is the calculation of C:Chl, for which the mainly physically-based equation of Cloern et al. (1995) is used rather than that of Geider et al. (1997) which is largely determined by biological parameter values (further details are given in Sect. 4.2). In the application here underwater light and photosynthesis are modelled using 6 wavebands, with the downwelling attenuation coefficient modelled according to Morel and Maritorena (2001) and the absorption of light by phytoplankton from Bricaud et al. (1998) (see Kettle and Merchant, 2008 for more detail). The remineralisation of detritus ( $D$ ) back to nutrient (not described by Kettle and Merchant, 2008) is computed as follows: below 100 m the amount of detritus remineralised is  $\frac{\gamma}{\text{depth}}D$  (see Table 1 for  $\gamma$ ); above 100 m is it fixed at  $0.1D$  ( $\text{mmol N m}^{-3} \text{d}^{-1}$ ). The model is driven with ERA-40 reanalysis meteorological data from ECMWF at 6 hourly resolution and the physical model (GOTM) is tuned to reproduce the observed temperatures in the ANIMATE dataset (see Kettle and Merchant, 2008). At CIS the shortage of satellite data caused by its high latitude means it was necessary to tune the model to 2 years of data (2003–2004), but at ESTOC and PAP the model is only tuned to 2003 data due to computation time constraints.

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## 4.2.1 Model set-up

The initial profiles of inorganic nutrient are taken from the Levitus climatology (Levitus et al., 1993) and concentrations of phytoplankton and zooplankton are both initialised at  $0.01 \text{ mmol N m}^{-3}$  and detritus is started at zero. Initial conditions for dissolved inorganic carbon (DIC) and alkalinity are  $2058 \mu\text{mol l}^{-1}$  and  $2396 \mu\text{mol l}^{-1}$ , respectively, representing typical global values. Since for parameter optimization the model must be runs thousands of times, the vertical grid is reduced to 25 layers with geometrical zooming towards the surface (surface layer has thickness 5cm going to thicknesses of 900 m at abyssal depths). GOTM-HadOCC requires some “spin-up” time to remove sensitivity to the initial conditions so the model is run for 12 months before the results are compared with the satellite data. The driving data for the spin-up year is simply a copy of the 2003 data.

## 4.2.2 Computing Chl within GOTM-HadOCC

Chlorophyll concentration ( $\text{mg m}^{-3}$ ) is computed using

$$\text{Chl} = \frac{M_C(\text{C:N})_P}{\text{C:Chl}} \text{Phyto} \quad (5)$$

where Phyto is the concentration of nitrogen in the phytoplankton compartment,  $M_C$  is the molar mass of carbon ( $12.01 \text{ g mol}^{-1}$ ), and  $(\text{C:N})_P$  is the molar C:N ratio in phytoplankton ( $6.625 \text{ mol C (mol N)}^{-1}$ ). The C:Chl (mass) ratio, is computed using physical variables and the nutrient limitation on growth ( $N_{\text{lim}}$ ) according to Cloern et al. (1995):

$$\text{C:Chl} = \left( 0.003 + 0.0154e^{(0.05T_M - 0.059(I_M))} N_{\text{lim}} \right)^{-1} \quad (6)$$

where  $T_M$  is the temperature of the mixed layer ( $^{\circ}\text{C}$ ) and  $I_M$  is the mean daily irradiance in the mixed layer ( $\text{mol photons m}^{-2} \text{ d}^{-1}$ ) (the expression is inverted as Cloern et al.,

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1995 use Chl:C). The nutrient limitation on growth is given by:

$$N_{\text{lim}} = \frac{N}{K_N + N} \quad (7)$$

where  $N$  is inorganic nutrient (nitrogen) and  $K_N$  is the growth saturation parameter (see Table 1).

### 5 4.2.3 Computing $b_{bp}(490)$ within GOTM-HadOCC

The scattering of underwater light is affected by the amount of POC in the water. In GOTM-HadOCC, POC is calculated by adding together the carbon in the phytoplankton and detrital compartments:

$$\text{POC} = M_C((\text{C:N})_P \text{Phyto} + (\text{C:N})_D \text{Det}) \quad (8)$$

10 where Det is the nitrogen concentration ( $\text{mmol N m}^{-3}$ ) in the detritus compartment and  $(\text{C:N})_D$  is the C:N ratio in detritus (set to 7.5). POC is then used to simulate  $b_{bp}(490)$  through the following series of equations.

The scattering coefficient due to POC,  $b_{\text{POC}}(490)$ , is estimated from POC using a simple linear relationship:

$$15 \quad b_{\text{POC}}(490) = \frac{\text{POC}}{400} \quad (9)$$

(Loisel et al., 2002; Claustre et al., 1999). This is converted to the backscattering coefficient due to POC by

$$b_{b\text{POC}}(490) = 0.0096 b_{\text{POC}}(490) \text{Chl}^{-0.253} \quad (10)$$

(Twardowski et al., 2001). The total particulate backscattering coefficient is then assumed to be the sum of  $b_{b\text{POC}}$  and a background value ( $b_{b\text{BG}}$ ) which is unrelated to biological activity and set to  $0.17 \times 10^{-3} \text{ m}^{-1}$  (Fujii et al., 2007), such that:

$$20 \quad b_{bp}(490) = b_{b\text{POC}}(490) + b_{b\text{BG}}. \quad (11)$$

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Thus the minimum value for  $b_{bp}(490)$  predicted by GOTM-HadOCC is  $0.17 \times 10^{-3}$  which is just slightly higher than the minima shown by the satellite data for the three sites (Fig. 2).

#### 4.2.4 Optical weighting

5 In order to compare depth-resolved model variables with the equivalent remote sensing variable, the vertical profile must be weighted according to its contribution to the light leaving the water. Since the light must travel down through the water and back out again, the dimishing factor is  $\exp(-2K_d(z))$  (assuming the attenuation of upwelling irradiance is equal to the downwelling irradiance attenuation) where  $K_d$  is the attenuation coefficient for downwelling light. Thus for a variable  $X$  its remotely sensed equivalent,  
10  $X_{rs}$  is computed here using:

$$X_{rs} = \frac{\int_0^{z_{90}} X(z)g(z)dz}{\int_0^{z_{90}} g(z)dz} \quad (12)$$

where

$$g(z) = \exp\left(-2 \int_0^{z_{90}} K_d(z')dz'\right)$$

15 (Gordon and Clark, 1980), where  $K_d$  is spectrally averaged and  $z_{90}$  is the first attenuation depth (the depth above which 90% of the light received by the satellite sensor originates).

#### 4.3 Tuning model parameters

Eleven of the model parameters are tuned, based on a recent sensitivity analysis of  
20 the model by Scott et al. (2008). Table 1 shows the tuning parameters and their range of possible values. Given the similarity between the LP and QAA  $b_b(490)$  datasets it

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was deemed unnecessary to tune the model to both datasets and so the QAA dataset was omitted from the following work. Thus GOTM-HadOCC is tuned at each site to the following four datasets:

C Chlorophyll

5 L Chlorophyll and  $b_b(490)$  from LP

G Chlorophyll and  $b_b(490)$  from GSM

P Chlorophyll and  $b_b(490)$  from PML

For a given parameter set, GOTM-HadOCC outputs  $\text{Chl}_{rs}$  and  $b_{brs}$  which are then compared to the observed dataset using the cost function:

$$10 \text{ cost} = \sum_{j=1}^J \frac{1}{N\sigma_j^2} \sum_{n=1}^N (\text{obs}_{jn} - \text{mod}_{jn})^2 \quad (13)$$

where  $N$  is the number of observations,  $j$  is the data type (i.e., Chl or  $b_b$ ),  $J$  is the number of datatypes (i.e., 1 or 2),  $\sigma_j^2$  is the variance of the observed data and  $\text{mod}_j$  is an 8 day moving average of the 6-hourly model output. When there is more than one type of observation, i.e., both Chl and  $b_b$ , they each have the same number of data points.

### 4.3.1 Optimisation using a genetic algorithm

To search through the parameter space to find the optimum parameter set (i.e., the one which minimizes the cost function – Eq. 13), a genetic algorithm (GA) is employed (following Schartau and Oschlies, 2003). This is simply a search/optimization technique based on Darwin's theory of natural selection (for an good introduction to GAs see Goldberg, 1989). The basic idea is that a set of model parameters is viewed as an "individual" whose fitness is determined by  $\frac{1}{\text{cost}}$ . A number of individuals make up a "population" within which the individuals "reproduce" to make a population of new

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individuals (the next generation). Whether or not attributes from a certain individual are transferred to the next generation depends on whether the individual is allowed to reproduce, which in turn depends on its fitness. Individuals with high fitness levels are more likely to reproduce than those with low fitness (survival of the fittest). The offspring from two individuals is a new individual (parameter set) with characteristics from each parent. To bring in new information, mutation may be used to make small modifications to some of the children. Thus, the procedure produces successive generations of parameter sets that give models whose output is a better match to the observed data, eventually converging to the parameter set that gives the best possible model fit.

Here a micro-genetic algorithm ( $\mu$ GA) coded and published by Carroll (1996) and made freely available at <http://cuaerospace.com/carroll/ga.html> is used. Details of the  $\mu$ GA are given by Krishnakumar (1989). The  $\mu$ GA is based on the same operations as a general GA but it does not contain mutation and gives greater influence on elitism principles thereby assuring that the best individual (parameter set) is transferred to the next generation. As soon as all the individuals of one generation show less than 5% difference between each other, a new random population is generated (although the best individual is retained).

Here each parameter in the set of 11 tuneable parameters (Table 1) is represented by a 6 digit binary string thus enabling each parameter to take 64 possible values (the resulting parameter increments are given in Table 1). The string for each individual (i.e. parameter set) is thus 66 ( $11 \times 6$ ) digits long and the population is chosen to comprise of 11 individuals. The optimization is run for 2000 generations ( $11 \times 2000$  model runs) to ensure convergence.

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## 5 Results and discussion

### 5.1 Model fit to data

At each site GOTM-HadOCC is tuned in turn to the C, L, G and P datasets (defined in Sect. 4.3). In most cases the GA has achieved the optimum fitness after  $\sim 1000$  generations. It is possible that the same degree of fitness can be achieved by a number of different parameter sets, however, in all cases here there is only one optimum parameter set for each dataset at each site. Figs. 4 and 5 show the model outputs of  $\text{Chl}_{rs}$  and  $b_{b_{rs}}$  (from here on simply referred to as Chl and  $b_b$ ) when run with the optimised parameter sets, compared with the appropriate satellite data. The fits are remarkably good given GOTM-HadOCC is only 1-D with no accounting for advection. Broadly speaking, tuning also to  $b_b$  data increases the magnitude of both modelled Chl and  $b_b$  (Figs. 4 and 5). Table 2 gives the RMSEs for the different model fits. In general, and as expected, adding in  $b_b$  data causes an increase in Chl error. Somewhat surprisingly Table 2 shows that in some cases the  $b_b$  RMSE is actually smaller when the model is not tuned to  $b_b$  (e.g., at CIS and PAP tuning to dataset P gives a larger  $b_b$  RMSE than tuning to dataset C; at ESTOC tuning to L and P are worst than tuning to C). This is to do with the way the errors are calculated whereby the models tuned to dataset C are compared with the mean of the observed  $b_b$  datasets, whereas the models tuned to a particular  $b_b$  dataset are then compared with that dataset. The combined RMSE results show that GOTM-HadOCC produces the best fit to dataset G which implies that the SeaWiFS chlorophyll data and the GSM  $b_b$  data are related in a way that is the most consistent with the mechanisms contained within GOTM-HadOCC.

### 5.2 Optimised parameter values

Table 3 shows the optimum parameter values for each dataset at each site. Since the GA evaluates a very large amount of parameter sets and cost functions (22 000 for each site and dataset) these can be used to gain insight into how well each parameter

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is constrained. By examining the cost function for every value of a particular parameter generated it is possible to see the sensitivity of the cost function to that parameter (given that the other parameters may take any value). For each of the 64 values of any given parameter the associated minimum cost function indicates the best combination of the other parameters. Thus, plotting the possible values for a given parameter against the minimum of the cost functions generated for that parameter value indicates how well that parameter is constrained. Figure 6 shows this with values binned into 15 intervals over the parameter range (to smooth excessive scatter) and crosses to indicate the optimal parameter values. If the optimization problem is well posed and the parameters are uncorrelated, all the subplots would show sharp symmetric parabolas and the parameters would be fully constrained (Schartau and Oschlies, 2003). However, from Fig. 6 it is clear that most of the parameters are not well constrained which is unsurprising given that data on nutrient and zooplankton are not used, and that the parameter values will heavily interact with each other.

Some of the parameters are not constrained to one value but instead there appears to be a range of values which give similarly low costs but beyond which the cost function increases rapidly, e.g.,  $\phi$  (at CIS and ESTOC),  $\mu_1$  (at CIS),  $g_{\max}$  (at CIS) and  $m_0$  (at PAP). Other parameters are constrained to the upper or lower limit of their ranges, e.g.,  $R$  (at CIS and ESTOC),  $m_0$  (at CIS and ESTOC),  $\mu_2$  (at CIS),  $V$  (at CIS) and  $K_N$  (at PAP). For some parameters the slopes of the cost function are greater when  $b_b$  data are included implying that the  $b_b$  data are helping to constrain parameters but this is not always the case. Due to the inability of the data to strongly constrain model parameters, it is important to realise that the parameters of the tuned models can not be reliably used to infer properties of the system, for instance, the presence of a particular species of phytoplankton.

### 5.3 Model behaviour

Given that the optimal parameter values may show a range of values for the different tuning datasets, it is more informative to examine the actual model outputs to ascertain

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the real effect of including  $b_b$  data. Figure 7 shows the modelled nutrient, phytoplankton, zooplankton and detritus for each site for each optimised model. Results vary considerably between sites with all of the differently optimised models having very similar behaviour at CIS, very different behaviour at ESTOC and differences which depend on the model compartment examined at PAP. At ESTOC, it is clear that the satellite data are too noisy to sufficiently constrain the model behaviour. At all of the sites, however, the models tuned to datasets G and L show very similar behaviour implying that the  $b_b$  data from these 2 algorithms are not significantly different. At CIS and PAP the models tuned to dataset P (dotted lines) have outputs which are generally similar to those for L and G with the notable exception of the complete extinction of zooplankton at PAP! At CIS the model tuned to dataset C (the chlorophyll only dataset) shows slightly less phytoplankton (and subsequently less nutrient uptake), and zooplankton and detritus than the models that are also tuned to  $b_b$ . At PAP, the model tuned to dataset C shows similar concentrations of nutrient and phytoplankton but significantly less detritus (the zooplankton compartment is clearly not well constrained by the satellite data).

Interestingly at ESTOC the phytoplankton compartment shows a wide range of values which implies the model is simulating very different phytoplankton physiology (C:Chl ratios) since the chlorophyll concentrations are similar (Fig. 4). Figure 8 shows C:Chl ratios in the mixed layer depth for each site. At CIS they are virtually identical for the different models; at PAP there are large differences when the model is tuned to dataset P and small differences between the other models in the latter half of the year. At ESTOC, however, there are very large differences in C:Chl between the models. This indicates that correctly simulating Chl at this location with GOTM-HadOCC will not necessarily result in the correct estimation of carbon fixation. Furthermore, the fairly large differences between the models tuned to datasets with  $b_b$  included indicates that at this location (where there is no strong seasonal cycle), the differences in the  $b_b$  values from different IOP algorithms is significant. This is supported by the values for mean column primary production predicted by the models which are tuned to the datasets that include  $b_b$  data (Table 4) – at ESTOC the values vary by up to 191%,

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at CIS by up to 24% and at PAP by up to 54%.

Importantly for climate prediction, the air-sea flux of  $\text{CO}_2$  does not alter significantly between the differently optimised models as shown in Table 4. This is because the air-sea  $\text{CO}_2$  flux is largely controlled by physical not biological processes at these locations (particularly ESTOC) and the biological process is the uptake of DIC by phytoplankton which are largely constrained by Chl not  $b_b$  at CIS and PAP. The other important variable for climate prediction is the export of detrital material to the sea bed (export production). This is a balance between the rate at which the material sinks and the rate at which it is remineralised back to nutrient. In order to compare the effect of the different parameter sets on export production, the amount of detritus below 200 m on the last day of the simulation is used. The choice of depth level is arbitrary since the physics of the models at each site are the same. Note this not exactly export production as some of the material may not make it to the sea bed. Table 4 shows that the amount of detrital carbon below 200 m is highly variable even for models that have very similar surface behaviour (e.g., models tuned to datasets L and G at CIS). This is because it is highly sensitive to the remineralisation rate,  $\gamma$  which is not well constrained since its effects are seen beneath the depth to which the satellite sensor can retrieve information.

## 6 Conclusions

It has been shown here that satellite Chl and  $b_b$  data are not sufficient to fully constrain ocean carbon cycle model parameters. However, at two of the locations chosen (CIS and PAP) using the Chl and  $b_b$  datasets together *is* sufficient to constrain modelled outputs of nutrient, phytoplankton and detritus (but not always zooplankton). Moreover, including  $b_b$  data rather than simply using Chl can significantly alter the modelled detritus. The differences in  $b_b$  resulting from different IOP inversion algorithms do not appear to be a significant as the models tuned to the different datasets show fairly consistent behaviour. The change in modelled detritus caused by tuning to  $b_b$  data is important for climate prediction modelling since it is the detrital compartment that

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relates to the amount of carbon that is exported to the seabed and therefore effectively removed from the system. However, modelled export production is determined by the parameters for the detrital sinking rate ( $V$ ) and remineralisation ( $\gamma$ ). Constraining  $\gamma$  is difficult using satellite data as its effects are seen deeper in the water column. Therefore, satellite  $b_b$  data are not sufficient to constrain export production in ocean carbon cycle models but they can help to improve modelling of detritus in the mixed layer which is a step in the right direction.

*Acknowledgements.* Many thanks to D. Carroll for making his genetic algorithm code freely available. Also thanks to T. Smyth for providing IOP data. Also thanks to the providers of the ANIMATE dataset (EU project: EVR1-CT-2001-40014) and the ERA-40 ECMWF dataset (British Atmospheric Data Centre). This work was funded by a personal fellowship from the UK Natural Environment Research Council.

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**Table 1.** Parameters of the NPZD model. Note the fixed parameters are shown in Table 2 in Kettle and Merchant (2008) with the exception that  $F_{th}$  is set to  $0.01 \text{ mmol N m}^{-3}$  at all sites.

Parameter for variation	symbol	units	lower bound	upper bound	interval
Half saturation constant of N uptake	$K_N$	$\text{mmol N m}^{-3}$	0.01	0.85	0.0133
Max. photosynthetic rate	$P_m$	$\text{d}^{-1}$	0.1	5.1	0.0808
yield	$\phi$	$\text{mol C mol quanta}^{-1}$	0.01	0.12	0.0018
Respiration rate	$R$	$\text{d}^{-1}$	0.005	0.095	0.0014
Conc. dependent specific mortality	$m_0$	$\text{d}^{-1}(\text{mmol N m}^{-3})^{-1}$	0.008	0.25	0.0038
Constant specific mortality (zoo.)	$\mu_1$	$\text{d}^{-1}$	0.03	0.2	0.0027
Zoo-dependent specific mortality	$\mu_2$	$\text{d}^{-1}(\text{mmol N m}^{-3})^{-1}$	0.03	0.57	0.0086
Half saturation constant for Z grazing	$K_f$	$\text{mmol N m}^{-3}$	0.4	1.0	0.0095
max Z grazing rate	$g_{max}$	$\text{d}^{-1}$	0.06	2.0	0.0308
Detrital sinking rate	$V$	$\text{m d}^{-1}$	3.0	32.0	0.4603
Deep remineralisation rate	$\gamma$	$\text{d}^{-1}$	3.8	13.36	0.1518

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**Table 2.** RMS errors between the tuned-model output and the satellite data. Note  $b_b$  output from models tuned to dataset C are compared with the mean of the 3  $b_b$  datasets whereas the others are compared with the  $b_b$  dataset they were tuned to. The combined error is computed by scaling the two RMSEs by the mean for the 4 tuning datasets and then adding the two scaled error values. The number of observed data points is shown in brackets (note CIS covers 2 years).

Dataset	C	L	G	P
RMSE with observed Chl ( $\text{mg m}^{-3}$ )				
CIS	0.177	0.194	0.190	0.205
EST	0.0245	0.0256	0.0256	0.0260
PAP	0.134	0.136	0.148	0.164
RMSE with observed $b_b$ ( $10^{-4} \text{ m}^{-1}$ )				
CIS	13.383	9.991	8.113	21.018
EST	2.412	2.880	2.110	3.208
PAP	11.46	9.241	7.139	16.323
Combined error (dimensionless)				
CIS	1.94 (54)	1.77 (48)	1.61 (51)	2.67 (44)
EST	1.86 (45)	2.10 (43)	1.80 (45)	2.24 (38)
PAP	1.96 (38)	1.77 (33)	1.66 (36)	2.60 (28)

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**Table 3.** Optimised model parameter sets for each tuning dataset at each site.

	$K_N$	$P_m$	$\phi$	$R$	$m_0$	$\mu_1$	$\mu_2$	$K_f$	$g_{max}$	$V$	$\gamma$	fitness
CIS												
C	0.7167	1.2219	0.0397	0.0107	0.2500	0.0786	0.5700	0.6571	1.4149	3.9206	7.1384	1.88
L	0.8500	0.5756	0.0886	0.0050	0.2500	0.0435	0.5443	0.92381	1.1070	3.0000	3.8000	0.70
G	0.8500	0.5756	0.0921	0.0050	0.2500	0.0543	0.5700	0.6952	0.9222	3.0000	13.3600	0.91
P	0.8500	0.7371	0.0903	0.0050	0.2500	0.0813	0.5700	1.0000	1.5381	3.0000	3.8000	0.40
EST												
C	0.8500	0.6563	0.1130	0.0050	0.0080	0.2000	0.2014	0.5333	1.7844	4.8413	3.8000	1.86
L	0.0100	4.5344	0.1200	0.0150	0.0118	0.1433	0.4500	0.9048	0.6759	19.5714	3.8000	0.70
G	0.0100	4.6152	0.1130	0.0279	0.0080	0.1163	0.5700	0.8381	1.2302	31.5397	4.8622	0.65
P	0.8500	5.1000	0.0641	0.0050	0.0118	0.1163	0.0729	0.9810	1.9384	3.0000	3.8000	0.70
PAP												
C	0.6900	3.1610	0.0100	0.0193	0.1578	0.0597	0.0300	0.5524	0.6451	7.6032	13.3600	2.12
L	0.8233	4.5344	0.0135	0.0164	0.2423	0.0867	0.0900	0.4000	0.5527	3.0000	13.3600	0.89
G	0.8500	0.6563	0.0571	0.0621	0.2231	0.0408	0.2529	0.5333	0.3987	3.0000	12.9048	0.83
P	0.8500	2.4338	0.0152	0.0164	0.2193	0.1838	0.3643	0.4857	1.9692	3.0000	4.1035	0.47

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**Table 4.** Comparing results from the differently optimised models for the mean  $\text{CO}_2$  flux ( $\text{mol C m}^{-2} \text{a}^{-1}$ ) into the ocean, the mean primary production for the water column ( $\text{mg C m}^{-2} \text{d}^{-1}$ ) and the amount of detrital carbon below 200 m ( $\text{g C m}^{-2}$ ).

Tuning Data:	C	L	G	P
Site	Air-sea $\text{CO}_2$ flux			
CIS	14.90	15.00	14.93	15.08
EST	0.65	0.75	0.70	0.63
PAP	3.87	3.81	3.85	3.98
	Mean column primary production			
CIS	152.4	181.0	182.5	224.5
EST	92.4	40.9	65.8	119.4
PAP	62.3	86.7	134.2	95.7
	Detrital carbon below 200 m			
CIS	0.42	2.12	0.09	2.62
EST	1.95	2.55	1.56	1.06
PAP	0.08	0.01	0.01	0.47

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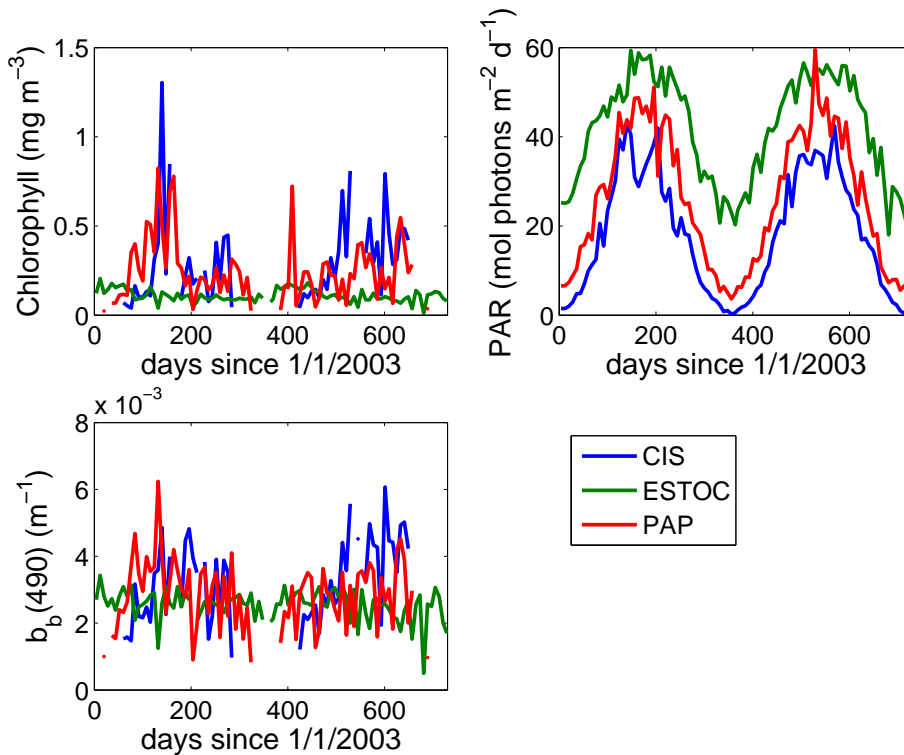
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**Fig. 1.** Comparing PAR (SeaWiFS), chlorophyll (SeaWiFS) and  $b_b(490)$  (LP algorithm) at the three different sites in the Atlantic.

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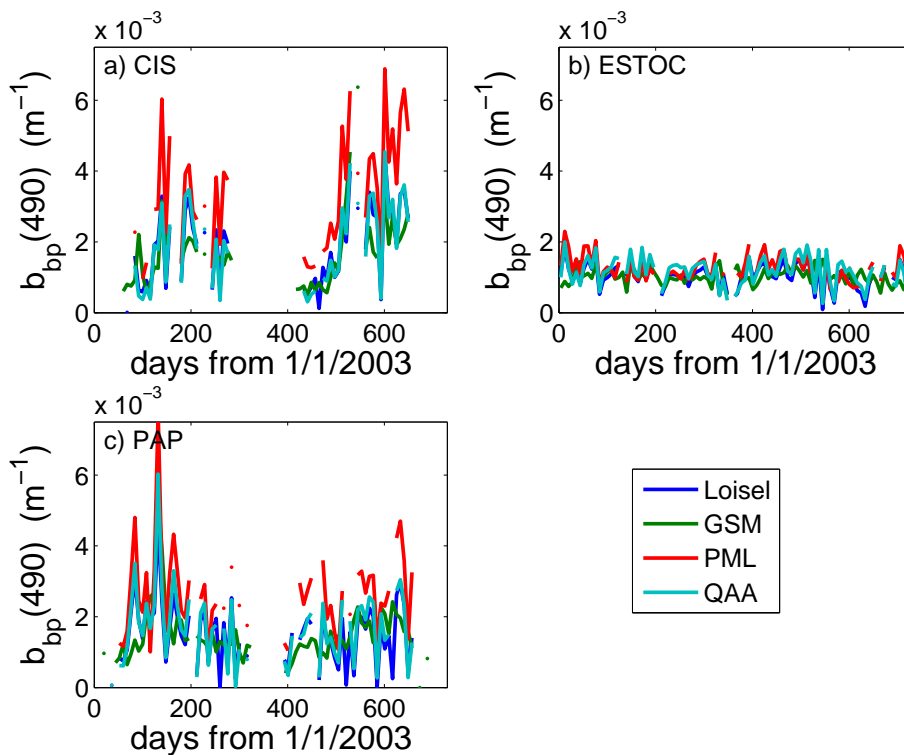


Fig. 2. Satellite-derived  $b_{bp}(490)$  at each site using 4 different IOP inversion algorithms.

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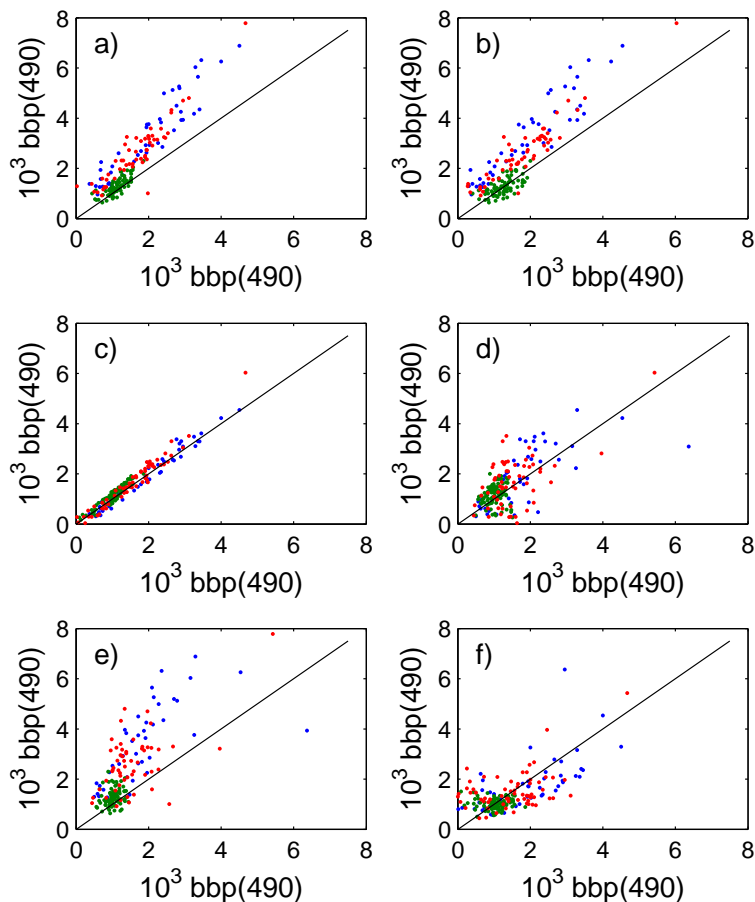
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**Fig. 3.** Comparing IOP inversion algorithms for  $b_{bp}(490)$  ( $\text{m}^{-1}$ ): **(a)** Loisel and PML, **(b)** QAA and PML, **(c)** Loisel and QAA, **(d)** GSM and QAA, **(e)** GSM and PML, **(f)** Loisel and GSM for CIS (blue), ESTOC (green) and PAP (red).

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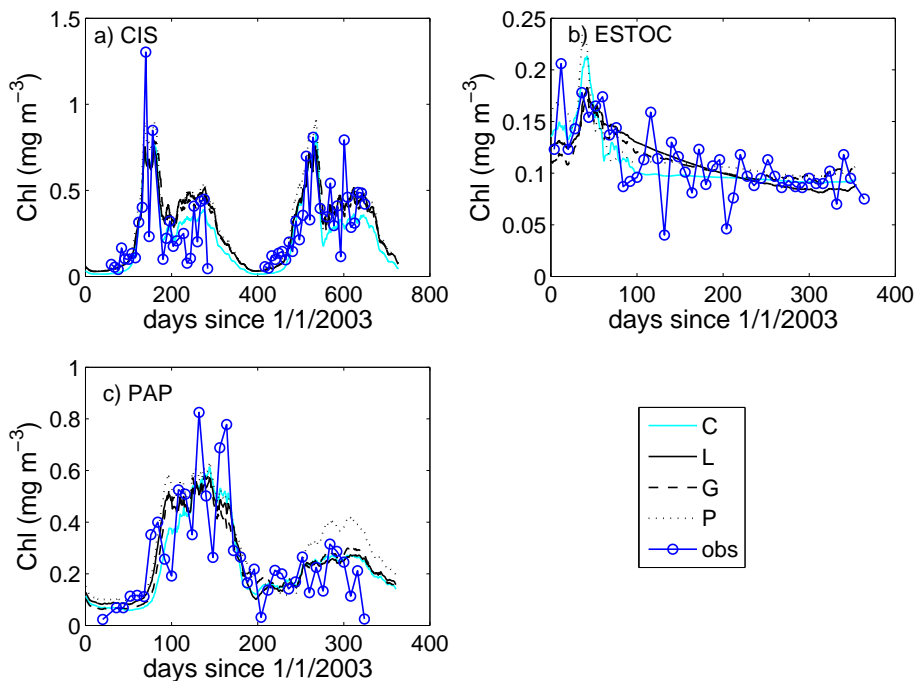
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**Fig. 4.** Comparing Chl from optimised models (8-day running means) with observed satellite data.

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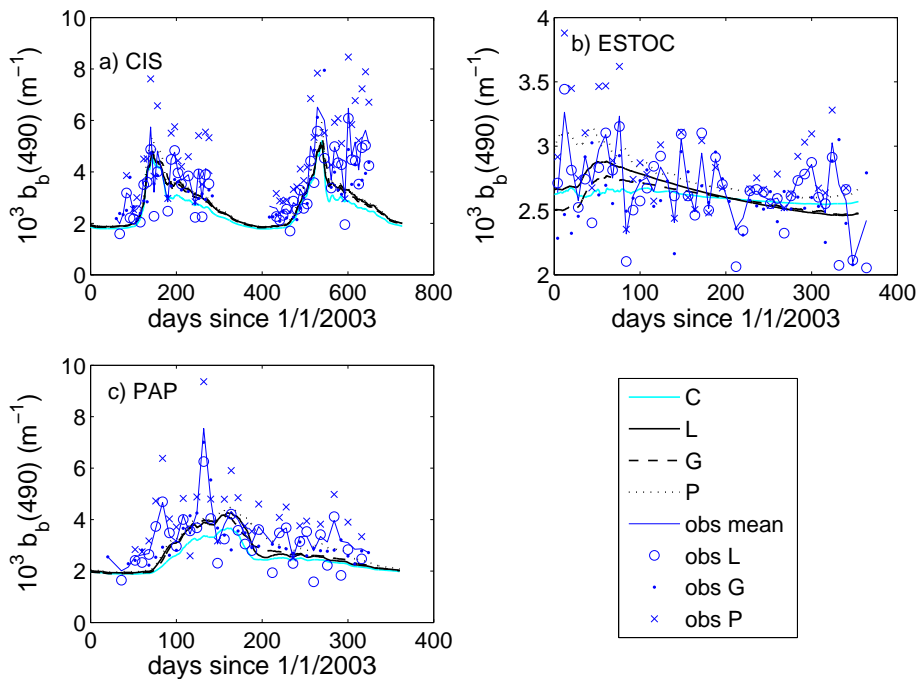
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**Fig. 5.** Comparing  $b_b(490)_{rs}$  from optimised models (8-day running means) with observed satellite data (average of all IOP algorithm results).

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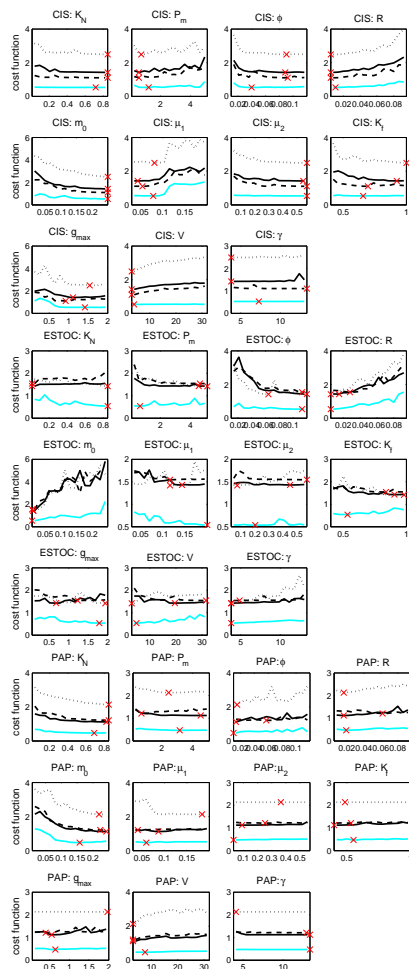
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**Fig. 6.** Possible parameter values plotted against the minimum of the computed cost functions (parameter range is divided into 15 equally spaced bins). The optimum parameter values are marked by crosses.

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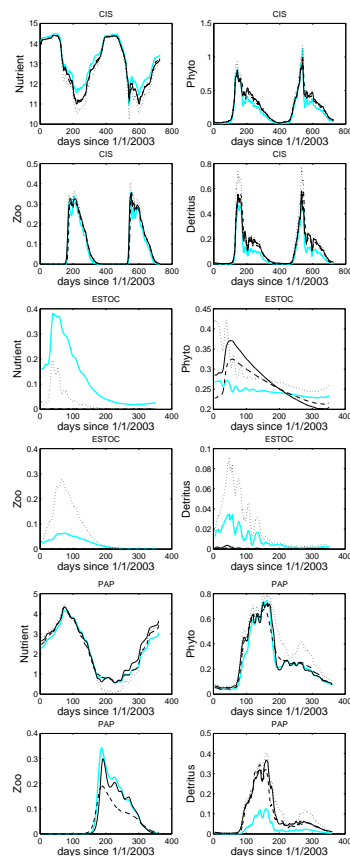
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**Fig. 7.** Modelled 8-day running means of mixed-layer nutrient, phytoplankton, zooplankton and detritus (all in  $\text{mmol N m}^{-3}$ ) produced by the optimised models at each site. Thick pale blue lines represent the model optimised to dataset C, black lines are for datasets L (solid), G (dashed) and P (dotted).

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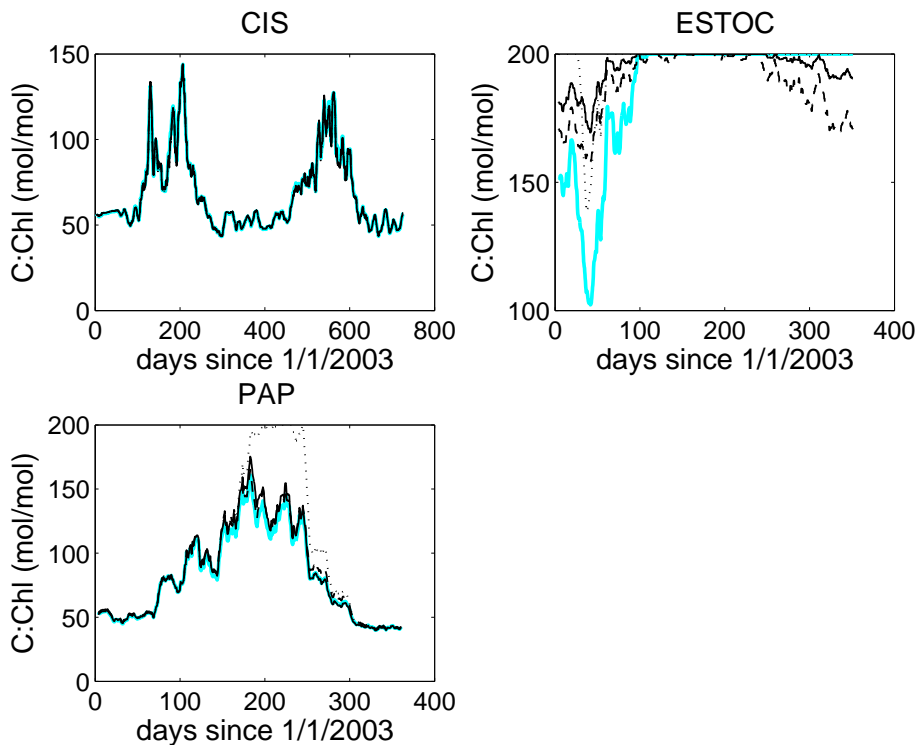
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**Fig. 8.** Modelled 8-day running means of mixed-layer C:Chl produced by the optimised models at each site. Thick pale blue lines represent the model optimised to dataset C, black lines are for datasets L (solid), G (dashed) and P (dotted).

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