

Average seasonal changes in chlorophyll *a* in Icelandic waters

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The standard algorithms used to derive sea surface chlorophyll *a* concentration from remotely sensed ocean colour data are based almost entirely on the measurements of surface water samples collected in open sea (case 1) waters which cover ~60% of the world's oceans, where strong correlations between reflectance and chlorophyll concentration have been found. However, satellite chlorophyll data for waters outside the defined case 1 areas, but derived using standard calibrations, are frequently used without reference to local *in situ* measurements and despite well-known factors likely to lead to inaccuracy. In Icelandic waters, multiannual averages of 8-d composites of SeaWiFS chlorophyll concentration accounted for just 20% of the variance in a multiannual dataset of *in situ* chlorophyll *a* measurements. Nevertheless, applying penalized regression spline methodology to model the spatial and temporal patterns of *in situ* measurements, using satellite chlorophyll as one of the predictor variables, improved the correlation considerably. Day number, representing seasonal variation, accounted for substantial deviation between SeaWiFS and *in situ* estimates of surface chlorophyll. The final model, using bottom depth and bearing to the sampling location as well as the two variables mentioned above, explained 49% of the variance in the fitting dataset.

Keywords: chlorophyll *a*, modelling, North Atlantic, remote sensing, seasonal, Subarctic.

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Introduction

Chlorophyll concentrations derived from the sea surface reflectance data gathered by satellite borne sensors have become widely accepted as measures of phytoplankton abundance in oceanic waters. Indeed for many ecological applications, no ground truth data sources are now available to supplement these data. Nevertheless, there are a number of well known unsolved problems with satellite collected data (Siegel *et al.*, 2005a; Werdell and Bailey, 2005; Alvain *et al.*, 2006; Lee and Hu, 2006) that sometimes are disregarded and may lead to considerable uncertainty, e.g. for the results of primary production estimates (Siegel *et al.*, 2005b). First, the observations apply to just a thin layer at the ocean surface, and subsurface chlorophyll concentrations remain undetected. Second, the standard algorithms for deriving chlorophyll concentration from spectral data are almost entirely based on concurrent reflectance and *in situ* measurements at open ocean sites, referred to as case 1 waters (O'Reilly *et al.*, 1998; Hooker and McClain, 2000). Considerable regional and seasonal deviations in satellite surface chlorophyll *a* have been noted when compared with measurements from near surface water samples (Dierssen and Smith, 2000; Burenkov *et al.*, 2001; Sathyendranath *et al.*, 2001; Gregg and Casey, 2004), especially from high latitudes and areas characterized as case 2 waters. The variable accuracy of calculated satellite chlorophyll estimates (Gregg and Casey, 2004), especially for case 2 areas, has been attributed to material of different colour in the water that

may be misinterpreted as chlorophyll (Mobley *et al.*, 2004). The definition applies especially to shallow and turbid waters over continental shelves, or otherwise influenced from land (Kirk, 1994), but also to boreal and Subarctic areas of the North Atlantic (Lee and Hu, 2006). Others have cited biological variation as a possible explanation because different phytoplankton communities vary in their absorption characteristics (Cota *et al.*, 2003; Sathyendranath *et al.*, 2004; Alvain *et al.*, 2006).

Simultaneous measurements of *in situ* chlorophyll *a* and ocean colour records from satellites (Gregg and Casey, 2004; Werdell and Bailey, 2005) are in some regions too few for detailed comparison (e.g. in Subarctic Atlantic waters). Therefore, blending methodologies have been applied to produce climatological models of the seasonal distribution of surface chlorophyll. For example, Clarke *et al.* (2006) used a penalized regression spline analysis to model *in situ* measurements of chlorophyll as a three dimensional function of day of the year, seabed depth, and multiannual average (1997–2002) of 8 d composites of SeaWiFS chlorophyll (CHL_{sat}). The model was applied to predict surface chlorophyll for any day of the year, and at any location in the domain, in this case the Northeastern Atlantic including the northern North Sea, 56–72°N and 30°W–20°E, and later extended (Speirs *et al.*, 2006) to the northern North Atlantic, 30–80°N and 80°W–85°E. The variable seabed depth was a proxy for the reflectance water type, i.e. case 1 water in open oceans or case 2 water over continental shelves.

The productive waters around Iceland and bordering the Arctic basin present a particular challenge for estimating the distribution of chlorophyll concentration from reflectance data. The continental shelf there is narrow with an anticyclonic coastal current driven by freshwater run off, which is occasionally loaded with glacial clay. Ocean currents of contrasting temperature and salinity flow along sections of the continental slope (Figure 1a): the warm saline North Atlantic Current (NAC) and the Irminger Current (IC) in the southwest, and the cold, less saline East Icelandic Current (EIC) in the northeast (Valdimarsson and Malmberg, 1999). As a result, the northern and southern Icelandic shelves have characteristically different water column stability and seasonal cycles of phytoplankton abundance (Gudmundsson, 1998). In general, the area may be characterized as case 2 waters, according to the definition of Lee and Hu (2006).

Clarke *et al.*'s (2006) Northeast Atlantic model (NEA model) covers the water around Iceland, but although the assembled water sample analyses used for the study included some 13 000 stations visited by multinational survey vessels between 1986 and 1999, just 203 stations were in Icelandic waters. We located additional chlorophyll data at the Marine Research Institute (MRI) in Iceland that had not previously been collated for spatial and temporal syntheses. The new dataset was treated as an independent test of the chlorophyll distributions predicted by the NEA model, then used to produce an alternative model (IS model) based on the penalized regression spline methodology. An analysis of the results and an interpretation of the findings are presented.

Material and methods

The study area, 62–69°N and 30–6.5°W, covers the shelf and slope waters around Iceland. Chlorophyll *a* data were collated from spectrophotometric and fluorimetric analysis of pigment extracts from MRI's water samples in this region from 1986 to 2005. In all, 1470 stations (Figure 1b) were collected (i) during annual hydrographic monitoring surveys in May/June, (ii) from the pumped seawater supply to flow through instruments aboard MRI vessels, and (iii) at fixed stations on the shelf sampled at varying intervals throughout the year. At each station, the interpolation scheme described by Clarke *et al.* (2006) was applied to estimate the average concentration of chlorophyll in the upper 5 m (CHL_{surf}) from the various discrete depth water samples.

Few stations were sampled during winter, and the SeaWiFS sensor is unable to provide data from high latitudes then because of the low angle of the sun. Therefore, the analysis was restricted to a 9 month period from mid February to mid November. The final number of CHL_{surf} observations used for the analysis was 1614, of which 179 were common with the dataset of Clarke *et al.* (2006).

In common with Clarke *et al.* (2006), we used the calibrated output from the 2002 NASA OC4v4 reprocessing (O'Reilly *et al.*, 1998) of the SeaWiFS data archive, compiled into multiannual (1997–2002) averages over 5' latitude \times 5' longitude pixels, composites for successive 8 d intervals throughout the year (CHL_{sat}). Full details of the procedures for filling missing pixels and processing of these data are provided by Clarke *et al.* (2006).

Aiming for an optimal distribution of the data for fitting a new model, the whole data assemblage was allocated to intervals of 8 d throughout the year, then one observation was selected per interval, at random, from each 1/4° latitude \times 1/2° longitude cell in the model region. This created a subset of 910 observations (stations) which were, as far as possible, evenly distributed in space and time. The remaining data were used as a secondary dataset for subsequent testing. Obviously, because of the over weighting of data from the annual monitoring in late May, the dataset was biased with regard to temporal distribution, especially the secondary dataset.

Seabed depths for each cell with SeaWiFS data were determined from the ETOPO2 (2' latitude resolution) global relief dataset (National Geophysical Data Centre; <http://www.ngdc.noaa.gov/mgg/global/global.html>).

The dominant circulation regime around Iceland is a clockwise flow along the shelf and shelf edge. Major rivers discharge glacier meltwater at various points, and ocean water masses are entrained into the circulation over the shelf (Figure 1a), causing changes in temperature, salinity, and nutrient concentrations. To caricature the possible effect of river discharge and entrainment on the patterns of chlorophyll distribution, the angular bearing of each sampling station from a central position in Iceland (65°N 19°W) was used as an additional covariate in the IS model.

Models were fitted to this new Icelandic dataset using the same approach as Clarke *et al.* (2006) with thin plate splines and tensor product splines (Wood, 2006). The models were fitted using the package mgcv, version 1.3.1, in R 2.1.1 (R Development Core

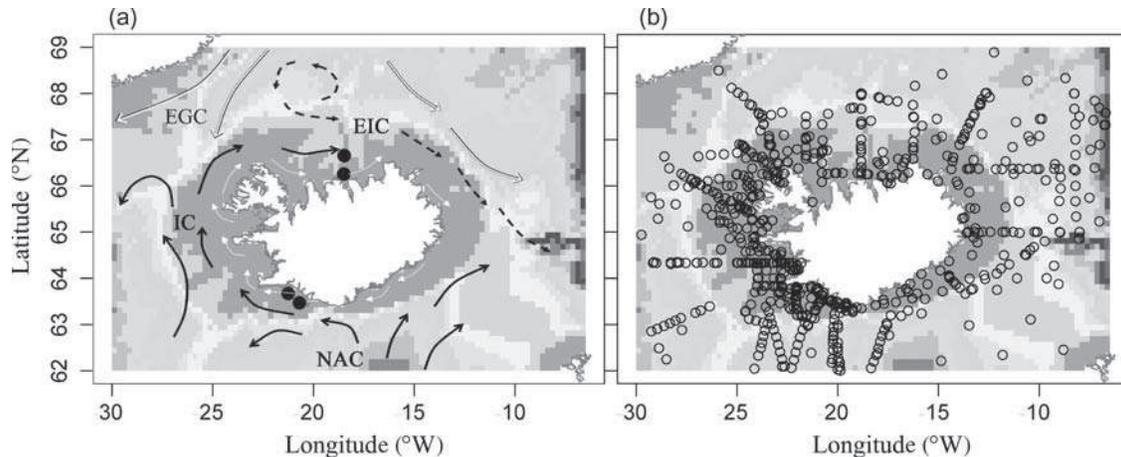


Figure 1. Maps of (a) seabed depth and the main system of currents around Iceland, the North Atlantic Current (NAC), the Irminger Current (IC), the East Icelandic Current (EIC), and the East Greenland Current (EGC), and sampling stations (dots) for time-series of chlorophyll. (b) Geographical distribution of sampling stations for the collated CHL_{surf} used in this study.

Team, 2005). Several variants of the model were tested to determine the most appropriate smoother. The degrees of freedom assigned to smoothing each explanatory variable were chosen by recursively fitting the model and systematically varying the degrees of freedom associated with each variable in turn and comparing GCV scores.

Results

Correlation between the full dataset of Icelandic sampling stations, CHL_{surf} ($n = 1614$), and the raw SeaWiFS composite values CHL_{sat} ($r^2 = 0.23$) was not markedly different from that with NEA model predictions (CHL_{NEA}) at the corresponding locations and days of the year ($r^2 = 0.27$). From this, we conclude that although the NEA model provides significant improvement in predictions of average CHL_{surf} over the whole Northeast Atlantic compared with composite SeaWiFS data, the same does not apply for Icelandic waters because of the sparseness of the available data in this region.

A GAM with one dimensional cubic spline smoothing and a normal error distribution was used for an initial exploration of the dependence of $\log(CHL_{surf})$ on each of the explanatory variables, $\log(CHL_{sat})$, square root transformed seabed depth, angular bearing around Iceland, and day of the year. The two last variables were treated as cyclic. The predictive influence and distribution of each variable over the range of values measured is shown in Figure 2.

The variance explained by the model, as covariates were added sequentially, was 31% for CHL_{sat} and increasing to 41% with the addition of day of the year. Addition of either one or both of the remaining variables (seabed depth and angular bearing) only

increased the variance explained by a further 2%. Nonetheless, the best model was a four dimensional tensor product smoother of all covariates, optimized for the degrees of freedom assigned to each explanatory variable. This IS model explained 49% of the variance in $\log(CHL_{surf})$, using the fitting dataset. Seabed depth and bearing contributed substantially to the final model, because the variance explained was 44% for a two dimensional tensor product smooth using CHL_{sat} and day of the year as predictors. The CHL_{sat} was, as expected, the primary predictive variable, but the seasonal variation was obviously important too.

The CHL_{surf} in the fitting dataset and the corresponding composite SeaWiFS CHL_{sat} values, along with the predicted values from the NEA model (CHL_{NEA}) and the new IS model (CHL_{IS}), were plotted (Figure 3) for examination of the variation in the scatter. This was then repeated for CHL_{surf} in the secondary dataset, and the corresponding squared correlation coefficients (r^2) were calculated. Although the r^2 values for the secondary dataset were low, the scores were highest for the IS model for both datasets (Table 1). To assess whether the three predictors (CHL_{sat} , CHL_{NEA} , and CHL_{IS}) were biased, we calculated the average difference between each predictor and the observed CHL_{surf} value it was being used to predict (Table 1). This value would be negative when the predictor consistently underestimated the values observed and positive when the predictor consistently overestimated those values. The IS model performed better than both the NEA model and the satellite values, apparently being almost unbiased for both the fitting and testing datasets. However, this apparent lack of bias was really the result of the model predictions being negatively biased at high observed chlorophyll values and positively biased at low values (Figure 3). This is

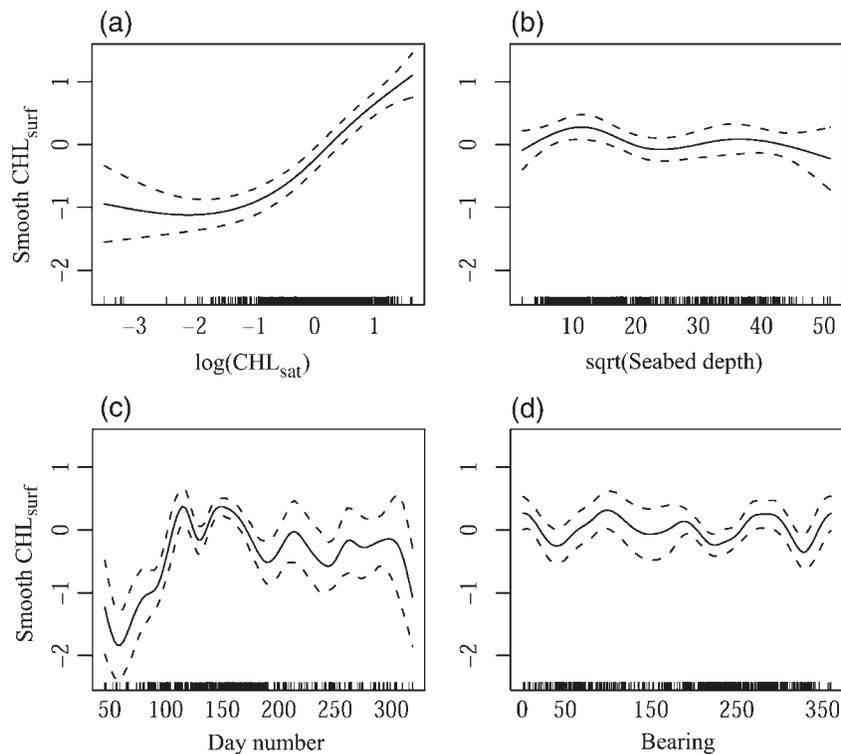


Figure 2. Mean and standard error of the four explanatory variables: (a) 8-d composite of satellite chlorophyll a 1997–2002, (b) day of the year, (c) seabed depth, and (d) the bearing to the sampling location from a central point on Iceland, fitted and smoothed (d.f. = 3, 3, 6, and 12, respectively). The distribution of data pairs is shown by marks along the x -axis.

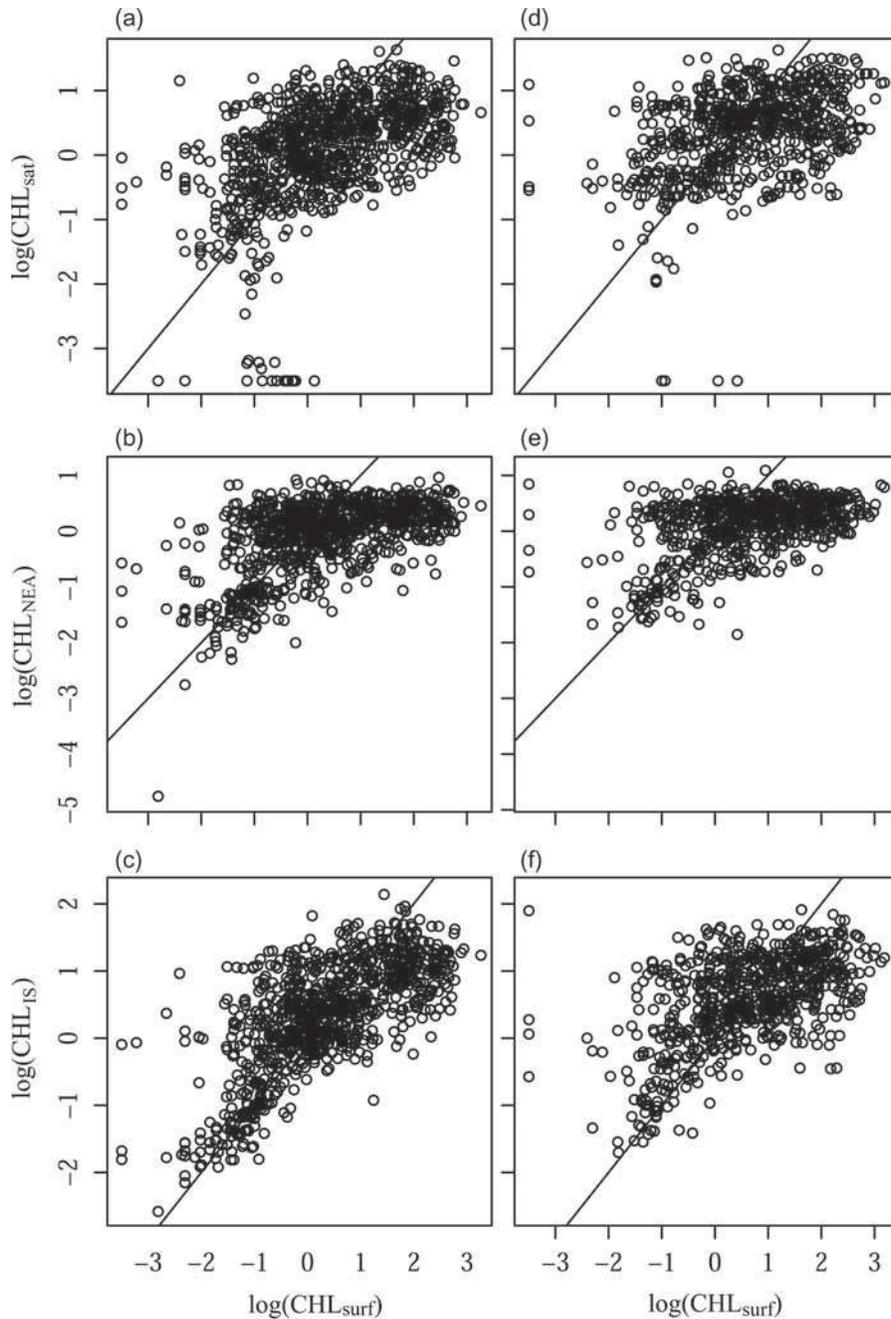


Figure 3. The scatter of log-transformed chlorophyll *a* concentrations at the surface, measured from water samples from above 5 m deep (CHL_{surf}) vs. (a and d) 8-d composites of SeaWiFS records, averaged for the years 1997–2002 (CHL_{sat}), (b and e) predicted by the NEA-model, and (c and f) predicted by the IS-model, respectively, for fitting and testing data.

a well known problem with satellite data, which the model has partially overcome for these data. The NEA model performs the worst, being the most (negatively) biased, again a well known phenomenon in that using predictions from inappropriate models is likely to cause bias. The fact that the results are similar for both the fitting and the test datasets supports our contention that the high r^2 in the test dataset is attributable to high variability in the data rather than poor predictions.

Extreme values of CHL_{surf} were poorly predicted by all predictors (Figure 3). Broken down by month (Figure 4), the correlations for the IS model during the months May–July were clearly weaker

than for the rest of the year. For closer examination, we performed separate model analyses, on the one hand restricted to data from waters north and east of Iceland (cold Arctic waters) and on the other hand to waters to the south and west (warm Atlantic waters), to determine whether systematic differences in seasonality between these regions might account for the weaker fit in May/June. However, the analyses did not result in any substantial change in the overall explained variance or suggest any obvious and plausible hypotheses.

For visual examination of the changes in horizontal distribution during the growth season, the fitted model was used to

predict average surface chlorophyll (CHL_{IS}) on the first day of each month between March and November over a 5' latitude \times 5' longitude grid of seabed (Figure 5). Further, at four locations where detailed annual time series were available in the dataset (Figure 1a), the relationships between *in situ* measurements (CHL_{surf}), SeaWiFS CHL_{sat} , and predicted CHL_{surf} according to the models were examined (Table 2). The IS model predictions provided the closest correlation with the observed variable CHL_{surf} at three of the locations and similar or lower bias than the composite SeaWiFS data and the NEA model predictions.

Discussion

The highly variable correlations between CHL_{surf} and CHL_{sat} found for case 2 waters are attracting increased attention (Hu

et al., 2000; Cota *et al.*, 2003; Gregg and Casey, 2004; Magnuson *et al.*, 2004; Maritorena and Siegel, 2005; Brown *et al.*, 2008; Komick *et al.*, 2009). The variations are for the most part considered to be caused by material of variable colour dissolved or suspended in the seawater (Morel and Bélanger, 2006) that is misinterpreted as chlorophyll when using standard algorithms for calculating CHL_{surf} from satellite records. Some suggestions for resolving the problems have been proposed (Hu *et al.*, 2000; Magnuson *et al.*, 2004; Siegel *et al.*, 2005a; Wynne *et al.*, 2006), but await further tests and evaluation. Given the shortage of available CHL_{surf} data that meet the criteria set for validating algorithms (Werdell and Bailey, 2005) for our study area, an alternative is to analyse climatological satellite data and multiannual observations.

The analysis described here produced a fitted statistical model (IS model), based on averaged 8 d composites of SeaWiFS chlorophyll data, day of the year, seabed depth, and the angular bearing to the location of water sampling around Iceland. The model, adjusted to the data available inside the study area, may be used to predict the surface chlorophyll for any day and location inside the region modelled. The predictions were tested against measurements of chlorophyll *a* in water samples, and the calculated values of r^2 were compared with that of predictions according to a model for the whole Northeast Atlantic (NEA model) and the average SeaWiFS composite values, testing the relative performance (Figure 3, Table 1). Further, the correlations between water sample measurements of surface chlorophyll *a* and either the values inverted from satellite ocean colour records or those predicted by the IS model at four locations used for seasonal studies (Table 2) support the

Table 1. Correlation coefficients (r^2) and bias estimate calculated for the primary fitting dataset and the secondary testing dataset of measured *in situ* chlorophyll *a* concentrations (CHL_{surf}) vs. the corresponding 8-d composite SeaWiFS (OC4v4) averages for the years 1997–2002, and the predicted values according to the NEA- and IS-models.

Source	Fitting data ($n = 910$)		Testing data ($n = 704$)	
	r^2	Bias	r^2	Bias
SeaWiFS	0.26	0.26	0.17	0.25
NEA model	0.31	0.42	0.21	0.50
IS model	0.49	0.00	0.30	0.04

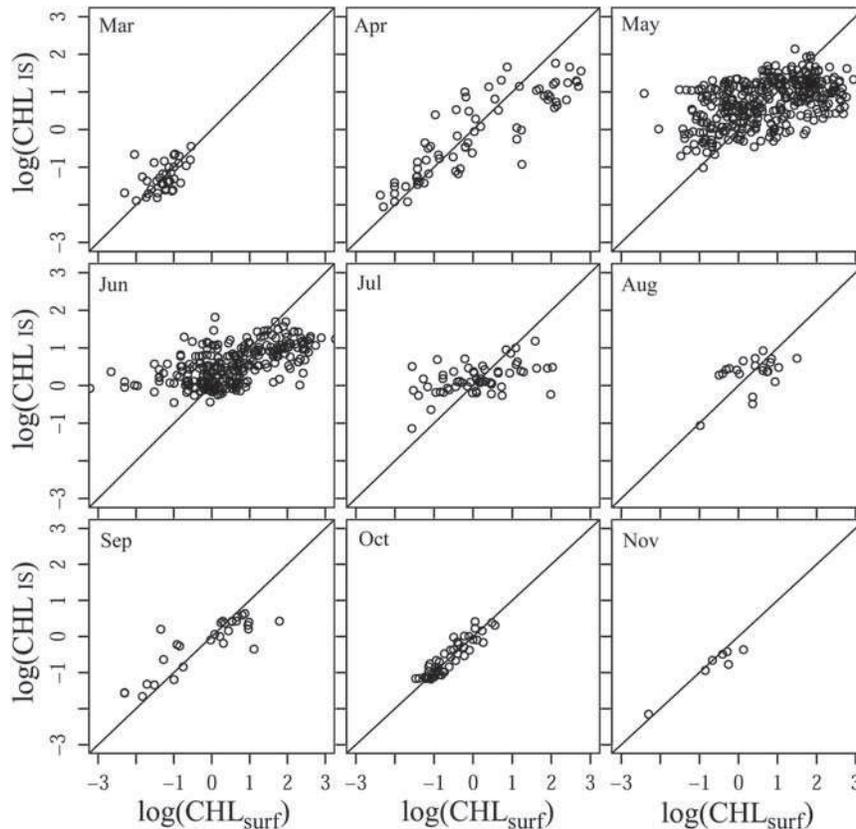


Figure 4. The scatter of chlorophyll *a*, measured from water samples vs. that predicted according to the IS-model for the months March–November.

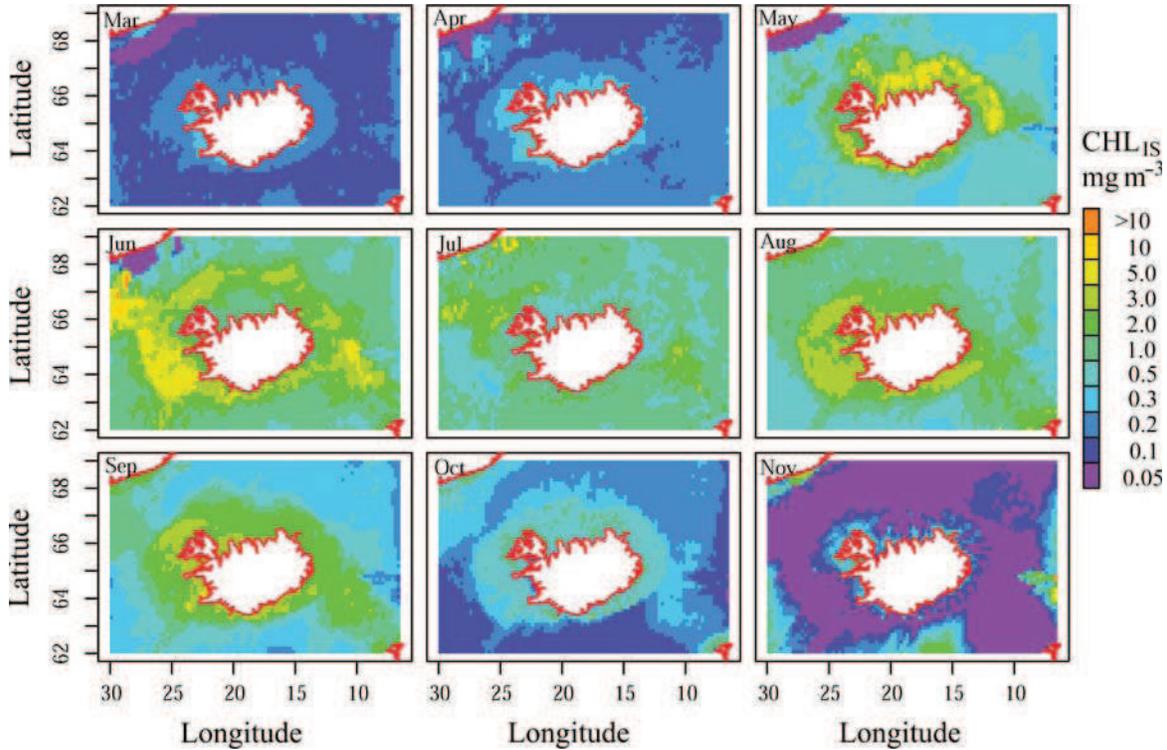


Figure 5. The IS-model predictions of horizontal distribution of chlorophyll *a* in the surface layer, for the 1st of each month, March – November.

Table 2. Correlation coefficients (r^2) and bias estimate calculated for *in situ* measurements of chlorophyll *a*, the corresponding values from the 8-d composite SeaWiFS (OC4v4) averages for the years 1997–2002, and predictions from the NEA- and IS-models calculated for available time-series at GR (Grímsey 66°15'N 18°34'W), EY (Eyjafjörður 66°28'N 18°04'W), SW1 (63°46'N 21°04'W), and SW2 (63°29'N 20°20'W).

Source	GR (<i>n</i> = 79)		EY (<i>n</i> = 12)		SW1 (<i>n</i> = 117)		SW2 (<i>n</i> = 115)	
	r^2	Bias	r^2	Bias	r^2	Bias	r^2	Bias
SeaWiFS	0.12	0.36	0.38	0.40	0.16	0.34	0.40	1.03
NEA model	0.15	0.78	0.60	1.01	0.19	1.20	0.26	1.68
IS model	0.22	0.23	0.49	0.29	0.24	0.61	0.46	1.20

notion that the IS model is an improvement on the perception of climatological spatial and temporal patterns of surface chlorophyll around Iceland. The predicted CHL_{IS} explains more of the variance in the available *in situ* measurements of surface chlorophyll measured from water sampled around Iceland than the raw SeaWiFS composite data and the NEA model predictions.

The paramount reason for the high variability, found when analysing the relationship between spectral reflectance and chlorophyll, is connected to seasonal change (Figures 2 and 4). An obvious explanation is the variation in chlorophyll concentration observed in these waters, such as may be caused by storms (Thórdardóttir, 1986).

The angular bearing of locations around Iceland was used to represent possible differences between the Arctic waters masses overlying the shelf north and east of Iceland and the Atlantic waters overlying the southern and western shelf, as well as other variable environmental influence near land (e.g. silt in glacial

ivers and wind borne dust). Seabed depth, as a single predictive variable, contributed least to explaining the variability in CHL_{surf} . Leaving seabed depth out of the analysis, however, resulted in a greater reduction in overall variance explained than the contribution of the variable alone implied, indicating an interaction with other covariates, probably the angular bearing, because the two together act as a spatial index.

Like the NEA model, the IS model was based on the SeaWiFS chlorophyll data averaged for the years 1998–2002. The aim was to produce a climatological interpolation and synthesis of the available water sampling data. However, there are considerable inter-annual differences in date specific CHL_{surf} at given locations around Iceland, owing to both the variable entrainment of Atlantic and Arctic water north of Iceland (Thórdardóttir, 1984; Gudmundsson, 1998) and meteorological conditions south of Iceland (Thórdardóttir, 1986). The water samples and SeaWiFS data span different years, a fact that has not been taken into account in the analyses. However, examination of the variance for each year, separately for northeast and southwest of Iceland, did not reveal any recognizable or significant trend (not shown).

As most of the collated data were collected during the latter half of May, during the annual regional monitoring surveys, there is an unavoidable bias in terms of temporal distribution. Moreover, as the first selection for the fitting dataset aimed for a uniform spatial and temporal distribution, the remaining secondary dataset was obviously and inevitably biased towards the sampling in May. The monthly plots of CHL_{IS} vs. CHL_{surf} (Figure 4) illustrate the scatter in the months May–July, during the high growth season. In light of the uneven distribution towards the latter half of May at the time of the spring bloom in the region (Gudmundsson, 1998), one may expect low values of r^2 , especially when testing the correlations for the secondary dataset (Table 1). Therefore, a

reason for the poor fit during the high growth season may be that CHL_{sat} are averaged values, from several years of SeaWiFS records, whereas CHL_{surf} are highly variable *in situ* measurements. Obviously, the two subsamples of data are not entirely comparable.

Visual examination of isopleths drawn according to the results of measurements of chlorophyll in water samples during annual cruises around Iceland, and comparison with corresponding 8 d composite images of chlorophyll distribution made available by NASA, had demonstrated some correlation. However, for a detailed study on the exact correlation between CHL_{sat} and CHL_{surf} one needs simultaneous high quality datapoints, which are not yet available. Calculating the average values of satellite chlorophyll for a number of years was a mean to obtain a complete dataset on satellite chlorophyll for the whole region, needed because the persistent cloud cover results in poor coverage of satellite data in the region (Clarke *et al.*, 2006).

Our study has demonstrated the need for local corrections of CHL_{sat} , shown here for a multiannual average of 8 d composites from SeaWiFS ocean colour data. The results confirm the method of Clarke *et al.* (2006) as a valuable approach to adjust inverted chlorophyll from satellite ocean colour records to average CHL_{surf} and show that a locally adapted model is needed to produce realistic predictions of CHL_{surf} in a regional domain. The next rational step will be to initiate a sampling scheme for high quality sea truth measurements (Gregg and Casey, 2004; Yuan *et al.*, 2005), intended to construct a regionally adapted algorithm to correct regional CHL_{sat} values or to test some general algorithms that may be able to cope with both case 1 and 2 waters and seasonal and local variations. To date, the IS model predictions presented here are the best available information (interpolation) on spatial and temporal distribution of surface chlorophyll around Iceland.

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