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Modelling Kara Sea phytoplankton primary production: Development and skill assessment of regional algorithms

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ABSTRACT

Empirical region-specific (RSM), depth-integrated (DIM) and depth-resolved (DRM) primary production models are developed based on data from the Kara Sea during the autumn (September–October 1993, 2007, 2011). The model is validated by using field and satellite (MODIS-Aqua) observations. Our findings suggest that RSM algorithms perform better than non-region-specific algorithms (NRSM) in terms of regression analysis, root-mean-square difference (RMSD) and model efficiency. In general, the RSM and NRSM underestimate or overestimate the *in situ* water column integrated primary production (IPP) by a factor of 2 and 2.8, respectively. Additionally, our results suggest that the model skill of the RSM increases when the chlorophyll specific carbon fixation rate, efficiency of photosynthesis and photosynthetically available radiation (PAR) are used as input variables. The parameterization of chlorophyll (chl *a*) vertical profiles is performed in Kara Sea waters with different trophic statuses. Model validation with field data suggests that the DIM and DRM algorithms perform equally (RMSD of 0.29 and 0.31, respectively). No changes in the performance of the DIM and DRM algorithms are observed (RMSD of 0.30 and 0.31, respectively) when satellite-derived chl *a*, PAR and the diffuse attenuation coefficient (K_d) are applied as input variables.

1. Introduction

Estimating the annual water column integrated primary production (IPP) (symbols and abbreviations are presented in Table 1) and studying its spatiotemporal variability on regional and global scales are among the main tasks of ocean biogeochemistry. Field studies provide *in situ* measurements but cannot quantify basin and global IPP dynamics without significant extrapolation (Berger, 1989; Bidigare et al., 1992; Koblentz-Mishke et al., 1970). This problem can be resolved by using bio-optical high resolution satellite-derived data (*e.g.*, surface chl *a* (Chl_0)), sea surface temperature (T_0) and incident photosynthetically available radiation (PAR) (Carder et al., 2004; McClain et al., 1998, 2004; O'Reilly et al., 1998) as input variables in the IPP models. Therefore, modelling IPP is the key approach in the investigation of primary productivity (*e.g.*, Behrenfeld and Falkowski, 1997b; Carr et al., 2006; Platt and Sathyendranath, 1993).

Numerous IPP algorithm designs and assessments of their predictive capacity on global and regional scales have been developed during the “ocean colour satellite era” (from 1978 to the present) (Campbell et al., 2002; Carr et al., 2006; Friedrichs et al., 2009; Saba et al., 2010, 2011). The results of four Primary Productivity Algorithm Round Robins (PPARR) allowed these authors to come to the following main conclusions: (i) the model's performance was independent of the algorithm's complexity, namely, the number of input variables, depth and wavelength resolution; (ii) all the models over- or underestimated the IPP by approximately a factor of 2; and (iii) the average model skill was significantly lower in shallow regions than in pelagic waters.

The same conclusions could be applied to the Arctic Ocean (AO) (Bélanger et al., 2013; Hill et al., 2013; Hill and Zimmerman, 2010; Matrai et al., 2013; Zhai et al., 2012). Hill and Zimmerman (2010) revealed that AO models over- or underestimated the observed IPP by a factor of 2 and that simple algorithms that were based on chl *a* performed better than more complex algorithms. Recently, descriptions of AO IPP models have been presented in terms of their efficiency (Babin et al., 2015; Y. Lee et al., 2015; Petrenko et al., 2013). These authors concluded that all the AO IPP models currently have significant limitations and should be used with caution.

One important factor causing problems in the development of robust IPP models for the Arctic Ocean is undersampling and a lack of suitable data on primary production and abiotic characteristics.

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Thus, comparatively few AO region-specific algorithms have been developed with Arctic Ocean datasets (Hill et al., 2013; Hill and Zimmerman, 2010; Matrai et al., 2013; Zhai et al., 2012) and applied to the assessment of AO IPP (Hill et al., 2013).

The accuracy of IPP models that were developed based on the World Ocean dataset decreases at the regional scale, and significant regional differences exist in the performance of algorithms (Campbell et al., 2002; Ishizaka et al., 2007; Z. Lee et al., 2015; Saba et al., 2010; Siegel et al., 2001). Therefore, we can assume that region-specific algorithms perform better than non-regional algorithms. The development of region-specific IPP algorithms for the Kara Sea seems obvious. The Kara Sea is characterized by specific environmental conditions that lead to particular processes of organic matter synthesis because of intense river runoff and a wide shelf zone (Dittmar and Kattner, 2003; Hanzlick and Aagaard, 1980; Holmes et al., 2012; Le Fouest et al., 2013; Stein, 2000). Fresh water discharge into the Kara Sea shelf leads to sharp stratification (Kubryakov et al., 2016; Zatsepin et al., 2010) and high particulate (POM) and coloured dissolved (CDOM) organic matter and terrigenous mineral suspension concentrations (Amon, 2004; Dittmar and Kattner, 2003; Rachold et al., 2004; Vetrov and Romankevich, 2004). Consequently, the Kara Sea waters are characterized by high turbidity, low transparency (average Secchi disk depth (Z_s) of 8 m) and a small photosynthetic layer (Z_{ph}) (22 m on average) (Burenkov et al., 2010; Demidov et al., 2014; Mosharov, 2010; Mosharov et al., 2016; Vedernikov et al., 1994). Therefore, the development of region-specific models could be one method to improve IPP estimation in the Kara Sea's optically complex waters.

Choosing appropriate model coefficients and input variables is very important to increase the algorithm's efficiency. As recently shown, the IPP in the Kara Sea during autumn weakly depends on the chl *a* concentration. On the other hand, the chlorophyll specific carbon fixation rate (P^b_{opt}) and PAR greatly affect the Kara Sea's primary production (Demidov et al., 2014). At the end of the vegetative season, the PAR level should be considered the main factor that defines the primary production in the Kara Sea. Ignoring the chl *a* vertical distribution, specifically, the subsurface chlorophyll maximum (SCM), may be another reason for decreasing of model's efficiency (Ardyna et al., 2013; Arrigo et al., 2011; Hill et al., 2013).

Thus, the main purposes of this study are as follows: (1) the development of a region-specific Kara Sea IPP depth-integrated (DIM) and depth-resolved (DRM) models; (2) the skill assessment of developed models with *in situ* and satellite datasets; (3) a comparison of the predictive skill of region-specific and non-region specific algorithms; (4) the assessment of the effect of photophysiological parameters and PAR on model performance; and (5) the parameterization of vertical chlorophyll profiles in waters with variable productivity and an investigation of the influence of the vertical chl *a* distribution on the model accuracy.

2. Data and methods

2.1. Data sources, sampling and Kara Sea trophic sub-regions

The field data that were used in the model's development were collected during three Kara Sea expeditions: the 49th cruise of the R/V "Dmitry Mendeleev" (from 30 August to 19 September 1993) and the 54th and 59th cruises of the R/V "Akademik Mstislav Keldysh" (from 9 September to 30 September 2007 and from 15 September to 4 October 2011, respectively) (Fig. 1a). Only two stations were established on 30 and 31 August and were included in the autumn database. The chl *a* concentration was measured at 113 stations and the primary production at 85 stations. The PP, chl *a* and PAR data that were used for model validation (Supplementary material S1) were collected at 31 sites during the 125th cruise of the R/V "Professor Shtokman" (from 3 September to 20 September 2013) (Fig. 1b). The PP and chl *a* data and the incident and subsurface PAR (see below) were used to calculate the model coefficients and to obtain the average chl *a* vertical profiles.

The boundaries of the Kara Sea were established in a previous work (Hill et al., 2013). The sampling depths were defined after a preliminary sounding of temperature, conductivity and chlorophyll fluorescence by a CTD probe (Seabird Electronics; SBE-19 and SBE-32). Niskin bottles were deployed at the stations to obtain water samples from discrete depths within the upper 100-m layer. Trace metal cleaning procedures (*e.g.*, Teflon coated covers and springs for the Niskin bottles) were used during all the cruises.

The Chl *a*, PP and PAR data were divided according to the trophic categories as determined by the surface chl *a* concentration (Morel and Berthon, 1989; Uitz et al., 2006) in the following ranges: 0.1–0.5 mg m^{-3} (I); 0.5–1.0 mg m^{-3} (II); 1.0–2.0 mg m^{-3} (III) and > 2 mg m^{-3} (IV). The average trophic level values of the primary productivity and abiotic parameters are presented in Table 2. The relative contributions of waters with different productivity in the Kara Sea regions and water masses (WM) (Demidov et al., 2014; Pivovarov et al., 2003) are presented in Fig. 2. Category I and II waters (Chl_0 = 0.1–1.0 mg m^{-3}) characterize the northern WM. The south-western WM was principally characterized by category I and III waters. Category II and III waters (Chl_0 = 0.5–2.0 mg m^{-3}) primarily characterized the river runoff WM. The high chl *a* concentration in the category IV waters ($Chl_0 > 2.0$ mg m^{-3}) is an inherent property of the Ob and Enisey estuaries (Fig. 2).

As recommended in previous studies of the vertical chl *a* distribution, stratified and mixed waters should be considered separately. The ratio of photosynthetic to upper mixed layers (Z_{ph}/UML) was chosen as the index of water column stability (Morel and Berthon, 1989; Uitz et al., 2006). Here, we define the photosynthetic layer as the layer up to the compensation depth, where the PP that is measured by the radiocarbon method equals 0. Waters where $Z_{ph}/\text{UML} > 1$ were considered as stratified and $Z_{ph}/\text{UML} < 1$ as mixed. A sharp pycnocline in the upper 10-m layer was observed in the Kara Sea during the autumn (UML = 7–10 m). The photosynthetic layer commonly exceeded the UML and ranged on average from 6 to 47 m in different Kara Sea regions (Demidov et al., 2014). Thus, we considered all the Kara Sea waters as stratified and classified vertical chl *a* profiles according to entirely trophic categories.

2.2. Primary production, chlorophyll and light measurements

The methods for primary production and chl *a* determination are described in detail in previous studies (Mosharov, 2010; Mosharov et al., 2016; Vedernikov et al., 1994) and are summarized in Demidov et al. (2014). Primary production was estimated on board by using a radiocarbon technique (Steemann Nielsen, 1952). The chl *a* concentration was determined by using a spectrophotometric method (Jeffrey and Humphrey, 1975; SCOR–UNESCO, 1966) or fluorometrically (JGOFS, 1994). The PP and chl *a* data that were obtained by these methods were used for model development.

The intensity of the surface irradiance was measured with a pyranometer (Vedernikov et al., 1994) or an LI-190SA (LI-COR) sensor. The daily PAR was obtained from integration in the LI-1400 module for five-minute intervals (mol quanta m^{-2}) and saved in the internal memory. The diffuse attenuation coefficient for downwelling solar radiation in the visible spectrum (K_d) was measured by an alphameter (Vedernikov et al., 1994). In the absence of underwater hydrooptical measurements, K_d was calculated by using empirical Kara Sea region-specific relationships among K_d, the Secchi depth (Z_s) and Chl_0 as shown in the Supplementary material (S2). Vertical profiles of underwater light were retrieved according to Beer's law.

2.3. Satellite ocean colour data, PAR, K_d and chlorophyll region-specific algorithms

Moderate Resolution Imaging Spectroradiometer (MODIS-Aqua)