Computational Marine Ecological Modelling

Analysing water column phytoplankton distribution and assessing Chlorophyll-a concentration from Sentinel-3 satellite images using NUM model

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1 Introduction

1.1 Background

Understanding the links between the structure of primary producer communities and physical components of the ocean is an important research frontier bridging community and physical oceanography. Primary producers like phytoplankton are essential to marine biogeochemical cycles and ecosystems since they contribute to about half of the global primary production. Physical properties like temperature also play a crucial role in phytoplankton physiology and metabolic processes. Additionally, based on previous studies, phytoplankton growth rates increases with the increase of temperature, almost doubling with each 10°C increase in temperature (Q10 temperature coefficient) [6] and water temperature is identified as the primary driver of blooms of particular species. However, other factors like light-saturated conditions and non-limiting nutrient conditions also increase the specific phytoplankton productivity and phytoplankton nutrient uptake, respectively, with an increase in temperature [2].

Various studies indicate that phytoplankton productivity, and thus phytoplankton levels, have fallen in the North Atlantic in the last century, which coincides with the start of the industrial era and the large-scale release of greenhouse gases.

Chlorophyll concentration, which is normally used as the proxy for phytoplankton concentration, can be measured using various methods such as spectrophotometry, high-performance liquid chromatography etc. but these methods require an high expertise to generate consistently efficient results [5]. Moreover, for various reasons such as the need for collecting samples at regular time intervals, there is an inability to continuously monitor Chl-a [3]. Therefore, scientific community have started to rely on satellite imagery data for the research as it can provide spatio-temporal data over large water areas which contrasts with field methods where a lot of measurements would be needed. In 2016, the Ocean and Land Colour Instrument (OLCI) was launched on board of Sentinel-3A, which was based on ENVISAT's Medium Resolution Imaging Spectrometer (MERIS) [1] and currently, this intstrument is the main source of global color reading.

1.2 Objective

The main purpose of this research is to analyze phytoplankton pigment distribution on different levels of water column for multiple time steps and assess the efficiency of OC4Me algorithm used by Sentinel-3 for the calculation of Chl-a in the Atlantic ocean. The analysis will be concluded using the Nutrient-Unicellular-Multicellular (NUM) model [7], which considers various physical and biological factors like water column temperature, light intensity at the surface, nutrient uptake, diffusivity etc. In order to assess the local impact of input factors' variation on model response, local sensitivity is done using the change in temperature gradient across different water columns. Furthermore, The model output will be used to calculate the uncertainty in phytoplankton concentration calculated usign OC4Me algorithm in Sentinel-3 satellite.

2 Methods and materials

The study area is defined as the latitudinal strip in the Atlantic ocean at the longitudinal value of 20°W where one day timestamp (2022-05-10) has been selected for the analysis because of temporary unavailability of longer timestamps.

Ocean and Land Colour Instrument (OLCI) used in sentinel-3 satellite has the field of view of the five cameras arranged in a fan-shaped configuration in the vertical plane and radiance passes via a calibration assembly to one of five cameras. Since, its not possible to differentiate whether the radiance is calculated from surface or certain depth of the area, camera captures data as 2D image of the covered region. In the process, it captures 21 OLCI spectral bands with different wavelength which are normally used for different functions. In order to calculate chl-a concentration, 4 bands (Oa03, Oa04, Oa05, Oa06) are used with ranging wavelength between 442nm and 560nm [5].

2.1 Satellite data

For analysis, Level-1 reduced resolution data from sentinel-3A is used where spatially re-gridded top Of Atmosphere (TOA) radiances for the 21 OLCI spectral bands data are available. Data is further processed to extracted 4 required bandwidths along with geo coordinates for each data point. Afterwards, data is extracted for study area and further analysed using OC4Me algorithm.

2.1.1 Analysis using OC4Me algorithm

Chlorophyll concentration, Chl, is defined by the "OC4Me" Maximum Band Ratio (MBR) semi-analytical algorithm, developed by Morel et al [4]. OC4Me is a polynomial based on the use of a semi-analytical model typically uses 4 bands (Oa03, Oa04, Oa05, Oa06) with ranging wavelength between 442nm and 560nm. The equation is given as:

$$C = 10^{A_0 + A_1 R + A_2 R^2 + A_3 R^3 + A_4 R^4} \tag{1}$$

where C is the derived concentration of chl-a in mg/m3, coefficients $A_0, A_1, A_2, A_3 and A_4$ are 0.450, 3.259, 3.522, 3.359, and 0.949 respectively and R is defined as:

$$R = log_{10}(max((R_{443}, R_{490}, R_{510})/R_{555})) \tag{2}$$

where $R_{443}, R_{490}, R_{510}, R_{555}$ are the irradiance reflectance at the wavelength of 443, 490, 510, and 555nm, respectively [5].

2.2 NUM model

Nutrients–Unicellular–Multicellular (NUM) paradigm is an alternative to the NPZ modelling paradigm defined to investigate the patterns of body sizes and traits that emerge within the planktonic communities. In paper [7], it is used to estimate the carbon export originating from copepod fecal pellets. Current research is using this paradigm to model the phytoplankton chlorophyll concentration and understand the effect the change in temperature gradient in the water column.

2.2.1 Analysis

As model output, chlorophyll (chl-a) concentration is extracted and used to compare with satellite data. Extracted Chl-a is the output for a water column upto certain depth at given timestamp and same process is followed for multiple positions in the study area. In order to compare model generated chl-a concentration with one calculated from the satellite data, column chl-a is aggregated using formula:

$$C_M = \frac{\int_0^{z_d} C(z) exp(-2k_d z) dz}{\int_0^{z_d} exp(-2k_d z) dz} \tag{3}$$

where C_M is the cumulative in-situ concentration of water column chl-a, k_d is the attenuation coefficient, $C(z)$ is the model chl-a concentration expressed in mg/m3, and z_d is the depth of water column.

3 Result Assessment

Using algorithms mentioned in section 2, results have been generated based on both satellite data and NUM model.

In order to analyse the water column distribution of phytoplankton on different latitudinal positions, NUM model is used to capture chl-a concentration upto 100m depth (figure 1). Results have shown that chl-a concentration in the temperate regions is significantly higher than the tropical region both at shallower and deeper depths, however upto 30°N, there is not much difference in chl-a concentration. It can also be visualized that chl-a concentration is increasing abruptly below 50m depth which is probably due to the high nutrient flux in the bottom layer of water column. However, below 80m concentration is decreasing again which is due to the fact that sunlight is unable to reach this deep and restrict the phytoplankton growth.

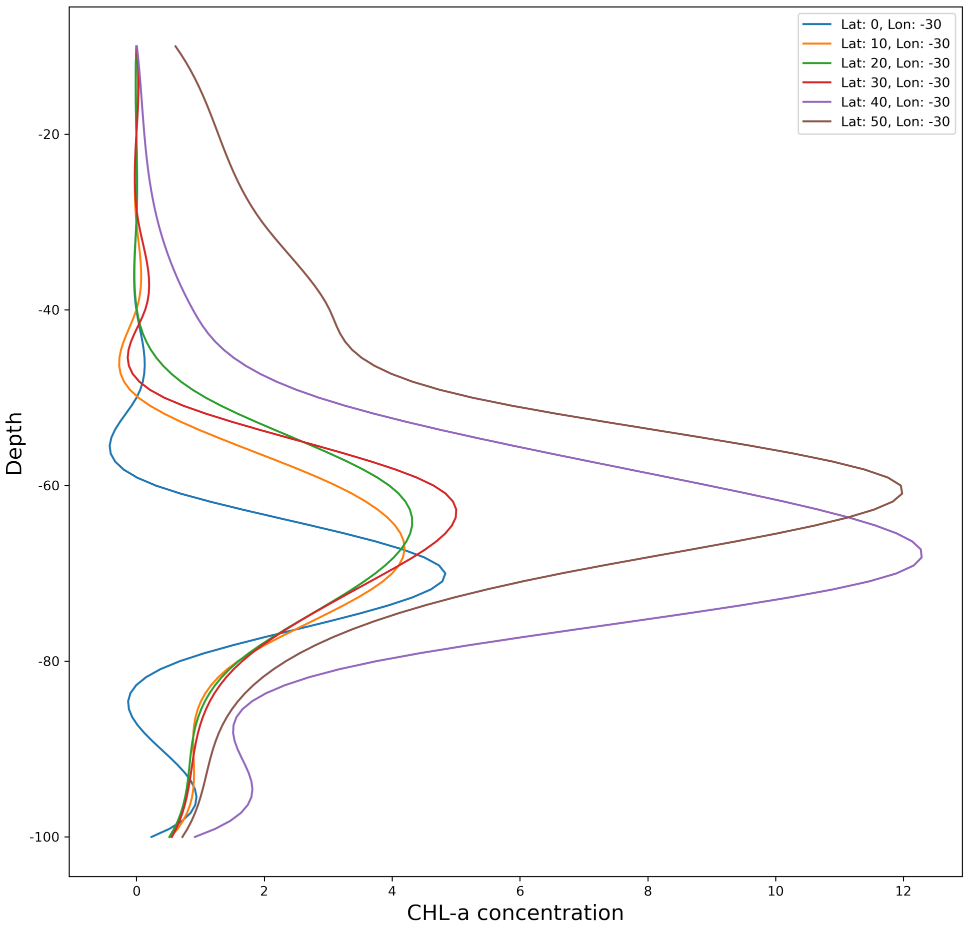

Figure 1: Phytoplankton concentration in water profile for latitudinal strip

To calculate the uncertainty of chl-a concentration measured from satellite, model outputs from NUM model are integrated using 3 under the assumption that satellite spectral beams can penetrate water upto certain depth. However, to limit the penetration of beams based on realistic scenarios, attenuation coefficient k_d is taken as 0.05 which is equivalent to the one used in NUM model in the case of light intensity.

The comparison model output and satellite data in table 1 has been made based on only one timestamp i.e. only one day has been used. Under this scenario, comparison has shown both high and low uncertainties at certain points (red and green coloured respectively). Apparently at high latitudes, satellite seems to underestimate the chl-a concentration while no such argument can be given for low latitudinal positions. The overall mean squared error is calculated to be **0.5850** mg/m3 which seems very high for given latitudinal positions. The most plausible explanation for this behavior is the limited availability of data and one model is used for calculating chl-a from satellite observation. Also, the coefficients used to calculate satellite chl-a concentration are universal which makes the model less accurate.

The accuracy can be improved by implementing multiple models with different hyperparameters to estimate chl-a concentration and by using parameters which are defined regionally. Furthermore, one timestamp is also insufficient to give any concrete analysis on chl-a concentration therefore, it would be interesting to see the trend over multiple years and compare with model output.

(Lat, Lon)	NUM model (chl-a conc.)	Satellite data (chl-a conc.)	Abs. error
$(0, -30)$	0.45258614	1.32679751	-0.87421137
$(5, -30)$	0.58966875	0.34628792	0.24338083
$(10, -30)$	0.84449868	1.33094984	-0.48645116
$(15, -30)$	0.88085586	0.38415335	0.49670251
$(20, -30)$	0.83098116	1.2512843	-0.42030314
$(25, -30)$	0.75448292	0.90134132	-0.14685841
$(30, -30)$	0.8830773	0.02741203	0.85566526
$(35, -30)$	1.25556215	0.01635022	1.23921193
$(40, -30)$	1.75931511	1.56279278	0.19652232
$(45, -30)$	2.22806407	0.46175531	1.76630877
$(50, -30)$	1.31054438	1.20304273	0.10750166
$(55, -30)$	0.92408548	1.20220296	-0.27811748

Table 1: NUM Model and Satellite data comparison

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