A multi-parameter logistic model to estimate dissolved inorganic carbon in global surface oceans from satellite data

Kande Vamsi Krishna and Palanisamy Shanmugam

Ocean Optics and Imaging Laboratory, Department of Ocean Engineering, Indian Institute of Technology Madras, Chennai-600 036, India

*Corresponding author: Email: pshanmugam@iitm.ac.in

Abstract

The estimation of dissolved inorganic carbon (DIC) in global surface ocean waters is crucial for better understanding of air-sea CO_2 flux rates, ocean acidification, and climate change. The magnitude and spatiotemporal variability of DIC fields are strongly influenced by physical and biogeochemical processes such as physical mixing, biological production, remineralisation, and circulations. In-situ sampling methods to study the spatiotemporal variations of DIC fields are less effective due to the time-consuming and expensive data collection processes. Alternatively, several space-borne sensors provide high spatial and temporal resolution data with large synoptic views. In this study, we developed a multi-parameter logistic model (MPLM) to estimate DIC fields in global surface ocean waters from satellite data. This model is more robust when compared the existing regional or global models in producing global DIC fields and capturing their full range of spatiotemporal variability across different latitudes, longitudes, and ocean basins. It overcomes the limitations of the other models that involve multiple relationships resulting in severe boundary discontinuity problems. The MPLM model utilizes chemical parameters, specifically partial pressure of carbon dioxide (pCO_2) and total alkalinity (TA) fields, along with the carbonate system calculations. The global pCO_2 fields are derived from a multiparametric non-linear regression approach (MPNR) and the TA fields from a single linear regression approach (SLR) using sea surface temperature (SST), sea surface salinity (SSS) and chlorophyll-a (Chl*a*) data. The MPLM is a robust and reliable tool for understanding carbon cycle dynamics from space and monitoring of ocean acidification and climate change.

Keywords: Dissolved inorganic carbon, carbonate system calculations, Ocean acidification, Marine Environment.

1. Introduction

Dissolved Inorganic Carbon (DIC, measured in μmol kg^{-1}) in the ocean refers to the carbon dioxide (CO_2) and other inorganic forms of carbon that are dissolved in ocean waters. Over the past few decades, anthropogenic activities such as the burning of fossil fuels, deforestation, population growth and alterations in land use land changes have led to a significant increase in atmospheric CO_2 levels (Krishna et al., 2020). Consequently, which resulted in higher levels of DIC concentration throughout the global oceans. The increased DIC concentration is a critical factor driving ocean acidification, which poses a major threat to marine ecosystems and the overall global carbon cycle (Takahashi et al., 2014). Accurate estimation of the magnitude and spatiotemporal variability of surface ocean DIC fields is crucial for a better understanding of air-sea CO_2 exchange rates and shifts in ocean biogeochemistry (Sasse et al., 2013). The concentration of DIC is primarily influenced by a complex interplay of physical processes (oceanic mixing, stratification, eddies, ocean currents and circulations), biological activities (photosynthesis and respiration), and chemical reactions (precipitation and dissolution) (Gregor and Gruber, 2021). These processes are governed by key parameters such as sea surface temperature (SST), sea surface salinity (SSS), chlorophyll-a concentration (Chl*a*), dissolved oxygen (DO), apparent oxygen utilization (AOU), nutrients availability (silicate, Si; phosphate, P; and nitrate, Ni), geographical location (latitude and longitude) and water depth (Broullón et

al., 2020; Carroll et al., 2022; Gregor and Gruber, 2021; Sasse et al., 2013; Takahashi et al., 2014). Understanding the significance of these processes and the governing parameters is essential for predicting future changes in DIC concentrations and its impact on the global climate change. In-situ measurements (though research vessels/buoys/moorings) offer one way to monitor DIC variations in the global oceans. However, in-situ methods face challenges like time-consuming, expansive, and difficult to execute in remote or adverse conditions. Alternatively, remote sensing technology is a powerful tool for estimating DIC fields in the ocean by offering global coverage, continuous monitoring, and high accuracy through the integration of multiple parameters and advanced algorithms.

Based on the significant benefits of remote sensing technology, various regional DIC algorithms have been developed for the Atlantic Ocean (Boteler et al., 2023), Pacific Ocean (Sarma et al., 2006; Yasunaka et al., 2021), Indian Ocean (Bates et al., 2006), Southern Ocean (McNeil et al., 2007), and Arctic Ocean (Arrigo et al., 2010). While regional DIC models provide valuable insights into DIC variability within specific regions, they may not be suitable for generating global DIC fields due to the lack of more in-situ data and model parameters covering the full range of spatiotemporal variability of DIC fields. Although estimation of global-scale DIC fields is possible by combining various regional models, which poses a significant challenge due to the complexity of the multiple relationships involved at different spatiotemporal scales results in severe boundary discontinuity problems (Krishna et al., 2020; Krishna and Shanmugam, 2023). Hence, a more comprehensive approach which integrates multiple sources of data and incorporates complex biogeochemical processes may be necessary to accurately estimate global surface ocean DIC fields. To address this problem, Sasse et al., (2013) developed the self-organizing multiple linear output (SOMLO) method to estimate DIC fields in the global oceans by considering the essential parameters such as SST,SSS, DO and nutrients. In another study, Takahashi et al., (2014) improved DIC mapping precision through the use of extensive long-term in-situ climatological data with exclusion of high intra/inter-annual variability regions of the equatorial Pacific Ocean and global coastal regions. Furthermore, Broullón et al., (2020) constructed a feed-forward neural network (FFNN) approach to estimate global monthly DIC fields using the data from the Global Ocean Data Analysis Project (GLODAP) and the Lamont-Doherty Earth Observatory (LDEO).

Recently, Gregor and Gruber, (2021) employed the geospatial random cluster ensemble regression (GRaCER) method to generate global surface ocean DIC maps. They derived observational data from two key sources: the surface ocean CO2 Atlas (SOCAT) for partial pressure of carbon dioxide (pCO_2) measurements and the GLODAP for total alkalinity (TA) data. The in-situ climatological data-based models face limitations in terms of spatial coverage, temporal sparsity, data bias, and potential inaccuracies due to variable quality and resolution. They often lack the ability to provide future projections and may struggle to capture fine-scale climate processes or extreme events. To address the limitations and challenges mentioned earlier, this study introduced a multi-parameter logistic model (MPLM) for estimating DIC fields in the global surface oceans using satellite oceanographic data. This innovative approach relied on chemical parameters, specifically pCO_2 and TA fields along with the carbonate system calculations. The global pCO_2 fields are derived using the Multiparametric non-linear regression approach (MPNR), while the TA fields are obtained through the single linear regression approach (SLR) by establishing parametric relationships with SST, SSS and Chl*a* concentration. Furthermore, the proposed study demonstrated global DIC fields through satellite oceanographic data. This study showcases the advancements in DIC estimation through carbonate system calculations, providing a robust and reliable approach for understanding carbon cycling dynamics and enabling better monitoring of ocean acidification and global climate change scenarios.

2. Data and Methods

2.1 In-situ data

To validate the MPLM model, in-situ measurements were obtained from the National Centers for Environmental Information – National Oceanic and Atmospheric Administration (NCEI-NOAA) (https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system-portal/) and the GLODAP (https://www.glodap.info/index.php/data-access/). These two data repositories provide high-quality oceanographic data contributed by various research institutes through oceanographic cruises across the Atlantic, Pacific, Southern, Indian, and Arctic oceans, conducted at different times to capture seasonal variations. Fig. 1 illustrates the spatial distribution of these measurements that encompass various physical and biogeochemical regions including areas with mixing and regions rich in biological production.

2.2 Satellite data

In order to demonstrate the MPLM model effectiveness in capturing the dynamic spatiotemporal patterns of global surface ocean DIC fields, we obtained satellite data from various sources. This included Moderate Resolution Imaging Spectroradiometer (MODIS) - Aqua sensor Level-3 data for SST and Chl*a* concentration sourced from the Goddard Space Flight Centre - National Aeronautics and Space Administration (GSFC-NASA) (https://oceancolor.gsfc.nasa.gov). Additionally, global mapped Level-4 SSS data obtained from the Jet Propulsion Laboratory (JPL) (https://podaac.jpl.nasa.gov).

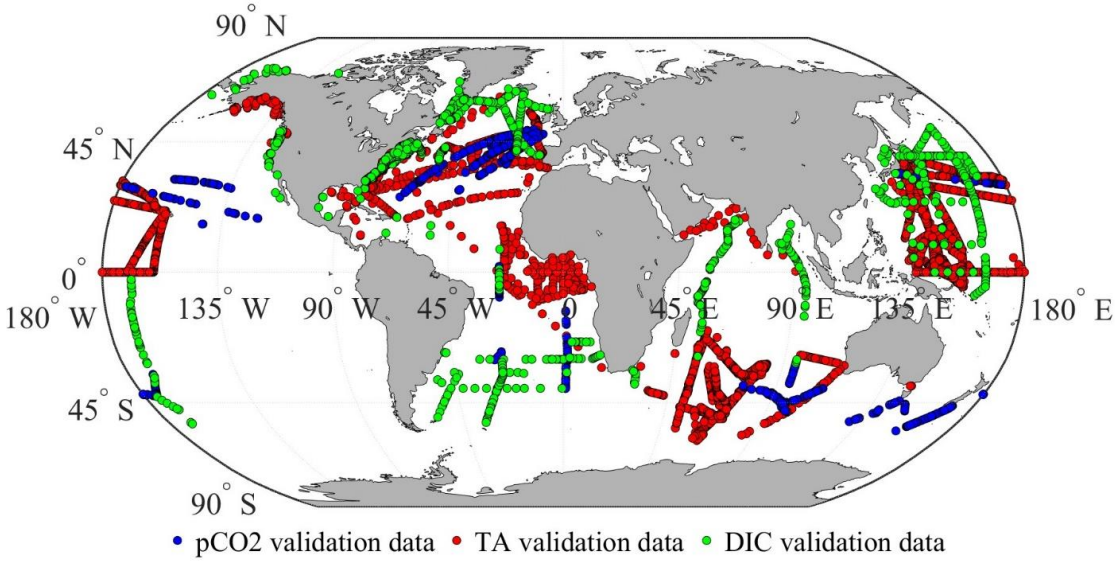

Figure 1. Depicts a map of the in-situ sampling locations for validation of pCO_2, TA and DIC fields

2.3 Methodology

The magnitude and spatiotemporal variability of global surface ocean DIC fields are driven by a complex physical as well as biogeochemical processes and governing control parameters. The estimation of global ocean DIC fields though regression approaches present substantial challenges owing to the sparse in-situ measurements and the intricate DIC trends across diverse spatiotemporal scales leading to pronounced boundary discontinuity issues (Broullón et al., 2020; Gregor and Gruber, 2021; Takahashi et al., 2014). To address these limitations and challenges, this research introduced an innovative multi-parameter logistic model (MPLM) designed to estimate DIC fields using satellite oceanographic data. The MPLM approach

integrates crucial chemical parameters including pCO_2 and TA in conjunction with carbonate system calculations. The CO2SYS (carbon dioxide system) calculations used in the present study are consisted with the previous studies (Gregor and Gruber, 2021; Takahashi et al., 2014). The MPLM model derives global pCO_2 fields using the MPNR approach developed by Krishna et al. (2020) and TA fields through a SLR approach proposed by Krishna and Shanmugam (2023). In the following, the visual representation of the MPLM approach flowchart was presented in Fig. 2.

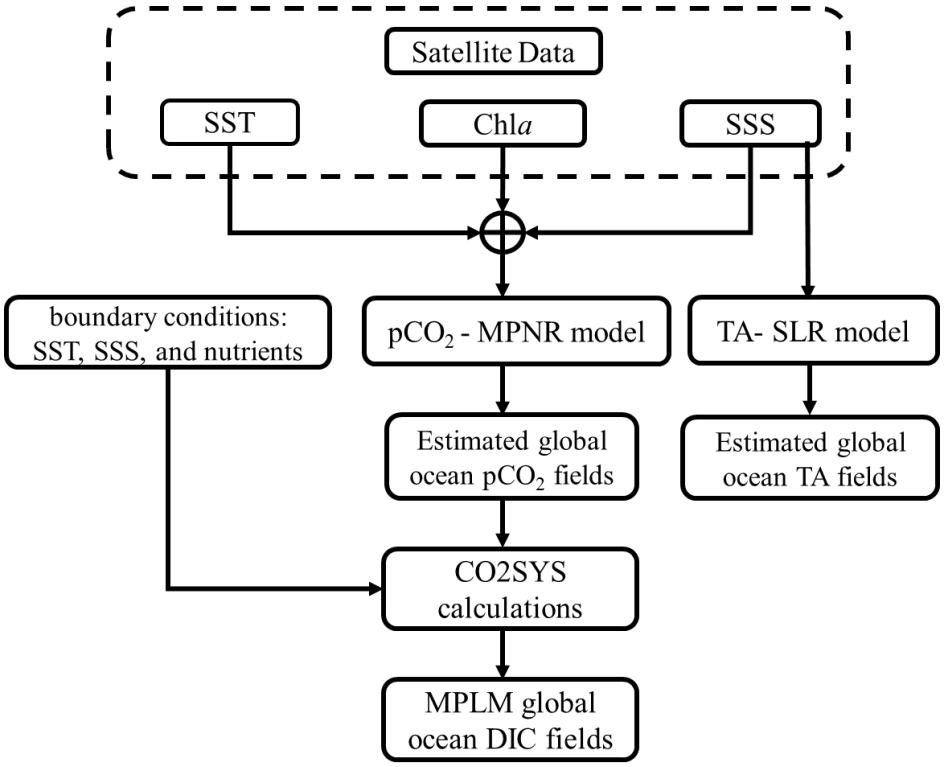

Figure 2. Flowchart showing the architectural framework of MPLM approach.

4. Accuracy assessment

The MPLM model accuracy assessment employed various standard statistical parameters. These parameters included mean relative error (MRE), mean normalized bias (MNB), root mean square error (RMSE), correlation coefficient (R^2), slope, and intercept. The MRE and RMSE were used to quantify systematic and random errors, whereas MNB used to identify and address any consistent biases present in the estimates. The correlation coefficient (R^2) quantifies the degree of linearity between predicted and measured DIC values. Additionally, the slope and intercept parameters allowed for potential calibration adjustments to improve the model accuracy. This comprehensive evaluation ensured a robust understanding of the MPLM model accuracy by considering various aspects of its performance and enabling a more informed assessment of its predictive capabilities in relation to in-situ DIC measurements.

$$\mathrm{MRE}=\frac{1}{N}\sum_{i=0}^{N}\frac{|(\mathrm{DIC_{modeled}}-\mathrm{DIC_{in-situ}})|}{\mathrm{DIC_{in-situ}}} \quad (1)$$

$$\mathrm{MNB}=\frac{\sum_{i=0}^{N}(\mathrm{DIC_{,modeled}}-\mathrm{DIC_{in-situ}})}{N} \quad (2)$$

$$\mathrm{RMSE}=\sqrt{\frac{\sum_{i=0}^{N}(\mathrm{DIC_{modeled}}-\mathrm{DIC_{in-situ}})^2}{N}} \quad (3)$$

5. Results and discussion

This section presents validation results using in-situ data and the global DIC fields derived from satellite oceanographic data. The MPNR approach relies on the data from pCO_2 and TA fields for its calculations. To ensure the accuracy and reliability of this approach, a thorough validation analysis was carried out using a significant number of TA, pCO_2 and DIC measurements. The validation results indicate that these parameters exhibit strong correlation and low uncertainties (Table 1) between the in-situ and modeled derived values. However, it is worth noting that when compared to other parameters, the DIC fields showed slightly higher uncertainties. This can be attributed to error propagation originating from the pCO_2 and TA fields as well as the complex calculations associated with the CO_2 system calculations. Despite this, these errors remained within a specified acceptable range and did not compromise the ability of the approach to generate global DIC fields accurately.

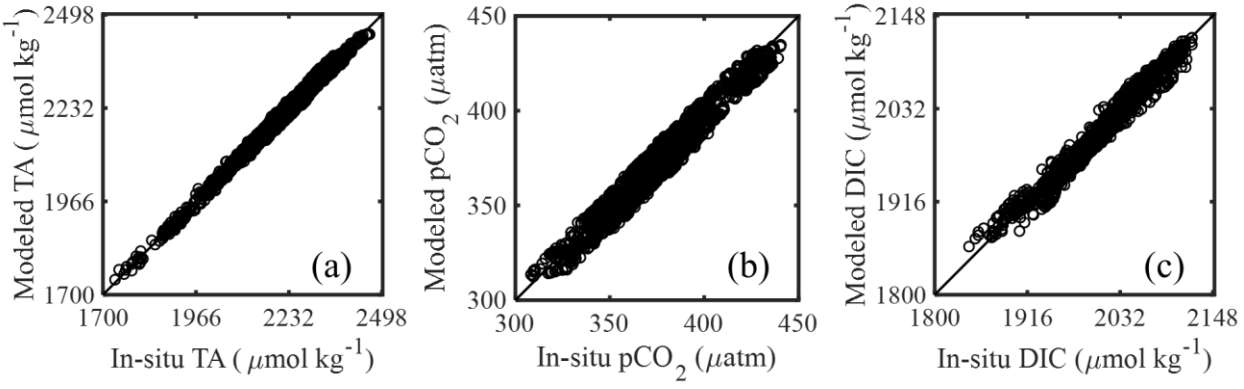

Figure 3. Depicts a visual representation of the validation scatter plots between in-situ and model derived values for (a) TA, (b) pCO_2, and (c) DIC fields.

Understanding the magnitude and spatiotemporal variability of DIC fields is crucial for accurately modeling the carbon cycle of the ocean and predicting its response to changing environmental conditions, such as ocean acidification and global warming. Fig. 4 presents the global surface ocean DIC fields derived from the MPLM approach. The Pacific Ocean with its vast size and dynamic circulation patterns exhibits significant variations in DIC fields. The subtropical regions of the Pacific Ocean generally have higher DIC concentrations, while the equatorial and subpolar regions tend to have lower DIC concentrations. On the other hand, the tropical and subtropical regions of the Atlantic Ocean have higher levels of DIC fields ranging from 2100 to 2300 μmol/kg.

Table 1. Statistics of in-situ and modeled derived TA, pCO_2 and DIC fields

Parameters	MRE	MNB	RMSE	R^2	Slope	Intercept	Data points
TA	0.003	-1.202	9.48	0.98	1	-18.74	19750
pCO_2	0.007	-0.514	3.21	0.97	0.98	4.66	9102
DIC	0.003	-3.239	9.52	0.97	1	-7.93	1581

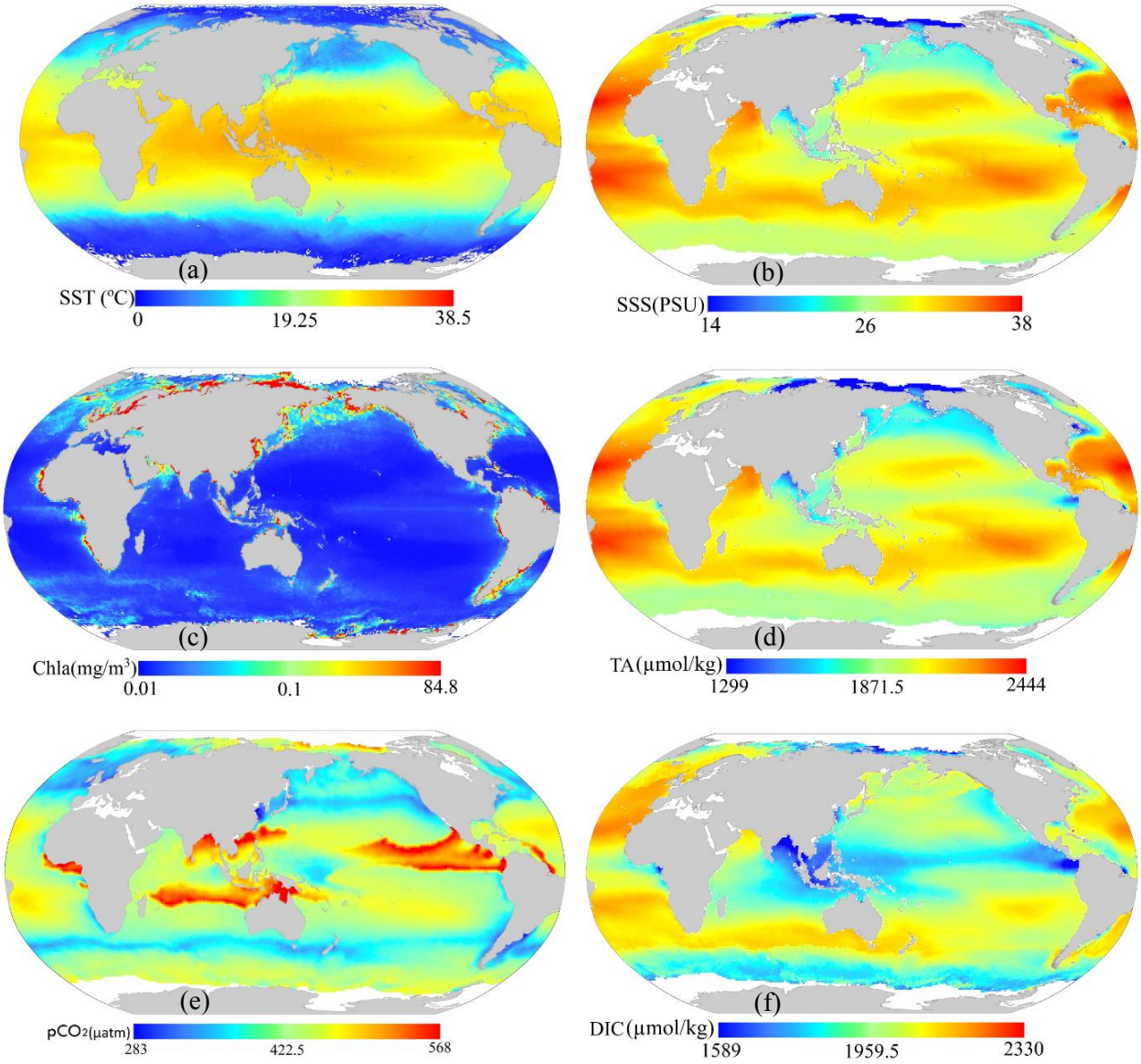

Figure 4. Demonstrate the spatial distribution of global surface ocean (a) SST, (b) SSS, (c) Chl*a*, (d) TA, (e) pCO_2 and (f) DIC fields for the reference year 2014.

In the Indian Ocean, DIC concentrations are influenced by the monsoon-driven circulation and the upwelling of carbon-rich water from the deep ocean. The DIC concentrations are relatively high in the Arabian Sea due to the upwelling of nutrient-rich water, which leads to increased biological productivity and subsequently increased DIC uptake by marine organisms. In contrast, the Bay of Bengal experiences lower DIC concentrations due to the influx of freshwater from rivers, which leads to reduced biological productivity and lower DIC uptake by marine organisms. The spatiotemporal structures of DIC fields observed in the global oceans are consistent with previous studies (Broullón et al., 2020; Carroll et al., 2022; Sasse et al., 2013; Takahashi et al., 2014). This consistency reinforces the importance of continued research and monitoring of oceanic DIC dynamics for accurate modelling and prediction of changes.

5.Conclusion

A novel multi-parameter logistic model (MPLM) was developed for estimating the spatiotemporal variability of global surface ocean DIC fields using satellite oceanographic data. Unlike previous models that relied on limited in-situ data and multiple regression equations for particular regions/seasons and few confirmed DIC trends, the MPLM approach demonstrated robustness in providing continuous coverage of DIC fields with greater accuracy. The MPLM approach was rigorously validated using in-situ data, indicating its potential as a promising tool for estimating global surface ocean DIC fields. The MPLM is capable of generating different spatiotemporal scales of DIC fields using satellite oceanographic data. This advancement could significantly enhance our current understanding of the global carbon cycle, air-sea CO_2 fluxes, ocean acidification, and changes in the biogeochemistry of the ocean with an emphasis on the current climate change scenarios.

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