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RESEARCH ARTICLE

# Advancements in Carbon Dioxide Modeling: An Algorithm Incorporating In-Situ and Satellite Data for Improved Understanding of $pCO_2$ Dynamics in the Bay of Bengal

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**ABSTRACT** Estimation of the partial pressure of carbon dioxide ($pCO_2$) in the Bay of Bengal (BoB) region plays a crucial role in better understanding the air-sea $CO_2$ fluxes. Complex physical and biogeochemical processes such as physical mixing, stratification, thermodynamic, and biological effects dominate the spatiotemporal variability of $pCO_2$ concentration over the BoB. This is difficult to estimate through in-situ platforms alone due to the time-consuming, cost-effective, and intricacies involved in water sample collection during rough oceanic weather conditions. Alternatively, remote sensing technology provides governing control parameters with high spatiotemporal resolution over large synoptic scales. Since the BoB region is influenced by the Indian monsoon system and other complex processes, existing regional and global $pCO_2$ algorithms are not adequate to estimate more accurate $pCO_2$ fields. Hence, there is a need to develop a regional $pCO_2$ algorithm over the BoB. To resolve this problem, in the present study, a Multi Parametric Regional Regression (MPRR) approach was developed over the BoB using satellite data such as sea surface temperature (SST), sea surface salinity (SSS), and chlorophyll-*a* (Chl*a*) concentration. To train and validate the MPRR approach, required in-situ measurements were obtained from the open and coastal waters of the BoB. The validation results revealed that the present MPRR approach showed better performance with significant low errors (mean relative error (MRE) = 0.012, mean normalized bias (MNB) = 0.022, and root mean square error (RMSE) = 4.75 $\mu atm$) and a high correlation coefficient ($R^2 = 0.92$). Furthermore, the study demonstrated the spatiotemporal variability of $pCO_2$and generated monthly, seasonal, and annual $pCO_2$ maps over the BoB.

**INDEX TERMS** Ocean color remote sensing, multiparametric regional regression, SST, SSS, Chl*a* and $pCO_2$.

## I. INTRODUCTION

The ocean absorbs one-third of anthropogenic $CO_2$ from the atmosphere, and mitigates the effects of global warming and climate change scenarios [1]. Since the beginning of pre-industrial era, the global oceans have absorbed approximately 165±20 PgC [2], with an annual rate of 2.5±0.6 PgC [3]. Estimation of $pCO_2$ concentration in surface oceanic waters plays a predominant role in better understanding of the global carbon cycles, air-sea $CO_2$ flux rates, source and sinks of

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$CO_2$, ocean acidification, primary productivity, absorption of $CO_2$, and biogeochemical studies related to $CO_2$ [4], [5], [6], [7]. In surface waters, $pCO_2$ concentration dynamically changes due to the interaction of various physical (physical mixing, stratification, mixed layer dynamics, ocean currents and circulations), biological (production, respiration, and biological pumps), and geochemical processes (carbonate precipitation and dissolution). These processes are in turn controlled by the corresponding physical and biogeochemical parameters, such as sea surface temperature (SST), sea surface salinity (SSS), mixed layer depth (MLD), chlorophyll-a concentration (Chl*a*), total alkalinity (TA), and dissolved inorganic carbon (DIC). Because of these complex oceanic processes and dynamic changes, estimation of spatiotemporal variability of $pCO_2$ through in-situ platforms are difficult [4]. Alternatively, the advancement of remote sensing technology and data processing/retrieval algorithms has made it possible to easily and accurately derive many of these parameters from satellite data. This approach offers distinct advantages over expensive in-situ measurements, particularly in terms of conducting spatial and temporal analysis on large scales.

In the past few decades, multiple regional and global $pCO_2$ approaches have been developed based on the in-situ and satellite observations. In pioneering work, Stephens et al. [8] investigated the distribution of $pCO_2$ over the North Pacific Ocean region using satellite derived SST data. The RMSE deviation estimated using their approach in the subtropical North Pacific Ocean region is low ($\pm 17$ $\mu atm$) due to $pCO_2$ variation in this region predominantly controlled by the SST alone. However, for extremely biologically active ocean regions, their method produced a higher RMSE deviation ($\pm$ 40 $\mu atm$) [4]. On a subsequent occasion, Ono et al. [9] incorporated Chl*a* along with SST in the development of a multiple nonlinear regression (MNR) model and demonstrated significant improvements in RMSE deviation ($\pm 14$ $\mu atm$). Furthermore, Lohrenz and Cai [10] aimed to enhance the accuracy of $pCO_2$ estimates by employing a combination of the multiple linear regression (MLR) technique and principal component analysis (PCA). They accomplished this by establishing a relationship between $pCO_2$ and biophysical parameters (Chl*a*, SST, and SSS) in the northern Gulf of Mexico's river-dominated region.

Recently, Chen et al. [11] employed a diverse set of machine learning approaches to estimate surface ocean $pCO_2$ in the Gulf of Mexico (GOM) region. These approaches encompassed a range of models, including multi-linear regression (MLR), multi-nonlinear regression (MNR), principal component regression (PCR), decision tree, support vector machines (SVMs), multilayer perceptron neural network (MPNN), and random forest-based regression ensemble (RFRE) method. They have incorporated essential environmental variables such as SST, SSS, Chl*a*, and diffuse attenuation of downwelling irradiance (Kd) as inputs for these models. The findings provide valuable insights into the intricate relationships between these oceanographic parameters and $pCO_2$ levels in the Gulf of Mexico, with potential implications for marine ecosystems and the global carbon cycle.

To better understand the global carbon cycle, it is crucial to monitor the surface ocean $pCO_2$ variations over the different spatiotemporal scales. Multiple $pCO_2$ models have been proposed over various ocean regions [6], [7], [12], [13], [14], [15], [16], [17], [18], [19], [20]; however, accurate estimation of surface $pCO_2$ in the Indian Ocean (IO) is yet to be defined [21]. The North Indian Ocean (NIO) has distinctive physical and biogeochemical features due to semi-annual reversing atmospheric and oceanic circulations driven by the monsoonal forcing factors [22]. The Arabian and BOB regions are widely recognizing in the NIO for its high biological production, physical mixing (upwelling and down welling), water mass transport, and stratification. In the Arabian Sea, Sarma [23] estimated surface $pCO_2$ from the carbonate chemistry parameters (DIC and TA) by considering these as a function of SST, SSS and Chl*a* using MLR approach. Mohanty et al. [24] recently employed a similar method to estimate the spatial and temporal variability of surface ocean $pCO_2$ fields in the NIO region. However, this method produced large uncertainties due to propagation of errors linked with the calculation of DIC and TA as a parametric function of SST, SSS and Chl*a*. To minimize these uncertainties, Krishna et al. [4] formulated multiparametric nonlinear regression (MPNR) approach by considering the direct $pCO_2$ relationships with SST, SSS, and Chl*a* and significantly improved the $pCO_2$ estimations in the global oceans.

Despite the fact that the BoB plays a major role in the global carbon budget, there have been very few attempts [25], [26], [27], [28] were made to investigate the $pCO_2$ variability over this region. In a recent study, Joshi et al. [29] developed and tested three machine learning methods (which includes multiple linear regression (MLR), artificial neural network (ANN), and extreme gradient boosting (XGB)) over the central BoB region using SST, SSS and $pCO_2$. While machine learning techniques offer numerous advantages, such as their capacity to learn from extensive datasets and provide accurate predictions, the lack of available large datasets for training a more precise $pCO_2$ model and validating its results presents a limitation in this study. In recent times, several researchers have investigated the seasonal and inter-annual variability of the surface ocean carbon cycle in the BoB region [24], [28], [29]. However, these studies produced higher RMSE deviations (10-30 $\mu$atm) over the region due to the consideration of limited parameters and samples in the model formulation and validation.

To address these issues, the present study used a multiparametric regional regression (MPRR) approach. This method uses a combination of in-situ ($pCO_2$, SST, and SSS) and satellite (Chl*a*) observations to develop and validate a more accurate model for estimating $pCO_2$ variability in the BoB region. By incorporating multiple parameters, the MPRR approach aims to provide a more comprehensive

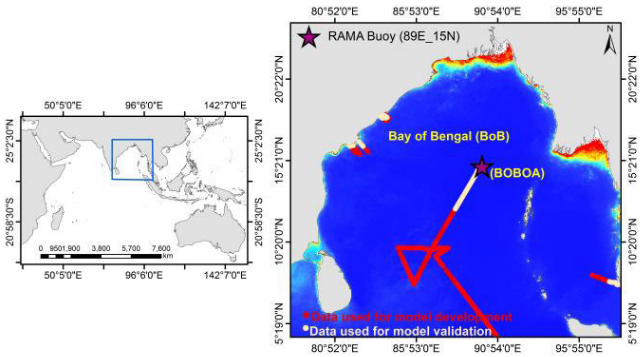


**FIGURE 1. Location of the study region and spatial distribution of in-situ sample locations used for developing (solid red) and validating (solid white) the MPRR algorithm.**

understanding of the complex interactions between these variables, resulting in improved accuracy and reliability in estimating $pCO_2$ fields. To develop and validate the MPRR approach, a significant amount of high-quality in-situ measurements were collected from both the open and coastal waters of the BoB region. The developed MPRR approach is validated using independent in-situ measurement data, the validation results revealed that the present MPRR approach showed better performance with significant low errors and a high correlation coefficient. Finally, to demonstrate the spatiotemporal variability of surface $pCO_2$ fields over the BoB, the developed MPRR approach was implemented on the satellite data products (SST, SSS and Chl*a*) and generated $pCO_2$ maps (monthly/seasonal/annual).

## II. DATA AND METHODS

### A. IN-SITU DATA

In order to develop and validate the MPRR approach, the in-situ measurements (SST, SSS and $pCO_2$) were obtained from the National Centers for Environmental Information (NCEI) - National Oceanic and Atmospheric Administration (NOAA) (https://www.ncei.noaa.gov/access/ocean-carbon-acidification-data-system-portal/). Note that, the NCEI data repository is not available over the coastal region of BoB; hence, 300 in-situ observational data collected during a field visit conducted by the National Remote Sensing Centre (NRSC) were also included. In addition to this, the Bay of Bengal Ocean Acidification (BOBOA) mooring measurements were employed to account for the seasonal fluctuations of surface ocean $pCO_2$.

The BOBOA moored buoy, deployed in the BoB on November 23, 2013, provides crucial data on $pCO_2$ variability and air-sea $CO_2$ flux. As the first buoy of its kind in the Northern Indian Ocean, it plays a vital role in understanding seasonal and inter-annual $CO_2$ fluctuations and associated biogeochemical processes. The spatial distribution of in-situ data over the study region is shown in Fig.1, whereas corresponding metadata (parameter, number of samples, location, and date) are presented in Table 1. Although, the in-situ measurements are spatially biased, which represent significant oceanic features and processes, such as major gyre systems, varying temperature and density profiles (warming and stratification conditions), mixing and dilution processes, and biological activity regions. The in-situ data comprises fugacity of $CO_2$ ($fCO_2$) measurements, which were converted to $pCO_2$ using the following equation [14].

$$pCO_2(\mu\text{atm}) = fCO_2(\mu\text{atm}) \times [1.00436 - 4.669 \times 10^{-5} \times \text{SST}(^{o}\text{C})] \quad (1)$$

### B. SATELLITE DATA

In order to illustrate and demonstrate the spatiotemporal variability of surface $pCO_2$ fields over the BoB, Moderate Resolution Imaging Spectroradiometer ( MODIS) - Aqua sensor Level-3 products of SST and Chl*a* (spatial resolution: 4 km) were obtained from the NASA ocean color website (https://oceancolor.gsfc.nasa.gov/). In addition to this, Multi-Mission Optimally Interpolated - Sea Surface Salinity (MMOI-SSS) data (spatial resolution: 25 km) were obtained from the Jet Propulsion Laboratory (https://podaac.jpl.nasa.gov/dataset). For the purpose of satellite data analysis, SeaWiFS Data Analysis System (SeaDAS) software developed by NASA Ocean Biology Processing Group (OBPG) was used. To conduct satellite validation analysis, the in-situ measurements corresponding to the satellite pixels at 25 km spatial resolution were averaged to establish matchups. Using monthly, seasonal, and annual satellite data (SST, SSS, and Chl*a*) for the reference year 2017, the spatiotemporal variability of surface ocean $pCO_2$ was described.

### C. MODEL PARAMETRIZATION

The BoB region is strongly influenced by the Indian monsoon cycle (south-west monsoon, SWM and north-east monsoon, NEM), enormous amount of freshwater inflow from the in the spatiotemporal variability of surface $pCO_2$ fields [4]. For this variability, a MPRR approach was adopted by relating surface pCO2 with SST, SSS, and Chl*a*. In total, 20284 quality-controlled in-situ measurement data (9784 from the NCEI data repository, 10200 from the BOBOA buoy, and 300 from the NRSC field campaign) were considered to formulate and validate the present MPRR approach. Based on the spatiotemporal coverage, these measurements were randomly divided into model development (12000 points) and validation (8284 points) datasets. In this study, MODIS-Aqua Level-3 daily binned Chl*a* data (spatial resolution: 4 km) corresponding to in-situ locations were used due to the unavailability of concurrent in-situ Chl*a* observations with NCEI datasets. In-situ measurements are instantaneous and continuous, but corresponding satellite derived Chl*a* have 4 km spatial resolution. Hence, there is a spatiotemporal mismatch between in-situ (SST, SSS and $pCO_2$) and satellite data (Chl*a*). For the purpose of spatiotemporal matchup analysis between in-situ and satellite data, all the in-situ measurements were converted into 4 km spatial resolution provided by the satellite

**TABLE 1. In-situ data used for the development and validation of MPRR approach.**

| Region | Date | N | Latitude & Longitude | Vessel name | Observer |
|---|---|---|---|---|---|
| Bay of Bengal | 1-27$^{th}$ April 2016 | 9784 | 5.70-17.88°N 84.75-98.36°E | Roger Revelle | Wanninkhof RikPierrot Denis |
| Bay of Bengal (near coast) | 15-26$^{th}$ October 2016 | 300 | 17.20-17.92°N 94.39-84.17°E 16.33-16.17°N 81.76-81.82°E 15.16-16.21°N 82.69-82.64°E | Local survey boat | NRSC |
| Bay of Bengal (open ocean waters) | Nov. 2013-Dec. 2014; Dec. 2014-Jun. 2015 Mar. 2016-Jan.2017; Jan. 2017-Nov. 2018 | 10200 | 15N, 90E | BOBOA buoy | Adrienne Sutton Rudolf Hermes Chris O' Brien |

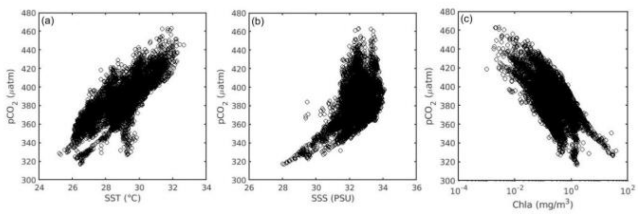


**FIGURE 2. Scatter plots of the relationships of $pCO_2$ with (a) SST, (b) SSS, and (c) Chla at 4km resolution.**

sensor (MODIS-Aqua), which reduces the number of sample points to 6864. Furthermore, these available sample points were used to establish parametric relationships between in-situ $pCO_2$ and regulating control parameters (SST, SSS, and Chl*a*) (Fig.2).

Parametric analysis indicates that surface $pCO_2$ have strong correlations with SST, SSS, and Chl*a*. Based on the formulations of Krishna et al. [4] and strong parametric relationships over the BoB, more accurate and precise regional regression coefficients were obtained from the MPRR approach. The present MPRR approach improved the regression coefficients of MPNR approach by considering the vast number of quality-controlled in-situ measurements covering over the coastal and open oceans regions of BoB. Although the in-situ measurements are biased spatially, this represents warming and stratification conditions, mixing and dilution, and biological productive regions of BoB.

$$\begin{aligned} pCO_2 = {} & 11.855\,SST + 4.753\,SSS \\ & - 21.777\log_{10}Chla - 125.557 \end{aligned} \tag{2}$$

The robustness and effectiveness of present MPRR approach and accuracy assessment was carried out using independent in-situ $pCO_2$ datasets to generate $pCO_2$ maps.

### D. MODEL ACCURACY ASSESSMENT

The MPRR model accuracy assessment was carried out using standard statistical parameters such as mean relative error (MRE), mean normalized bias (MNB), root mean square error (RMSE), correlation coefficient ($R^2$), slope, and intercept.

$$MRE = \frac{1}{N}\sum_{i=0}^{N}\frac{\left|(pCO_2^{estimated} - pCO_2^{in-situ})\right|}{pCO_2^{in-situ}} \tag{3}$$

$$MNB = \frac{\sum_{i=0}^{N}(pCO_2^{estimated} - pCO_2^{in-situ})}{N} \tag{4}$$

$$RMSE = \sqrt{\frac{\sum_{i=0}^{N}(pCO_2^{estimated} - pCO_2^{in-situ})^2}{N}} \tag{5}$$

The MRE and RMSE provide the systematic and random errors, whereas other statistical parameters The MRE and RMSE provide the systematic and random errors, whereas other statistical parameters such as MNB, intercept, slope, and $R^2$ values are used to investigate the deviations of the estimated $pCO_2$ from the measured in-situ $pCO_2$ values.

## III. RESULTS AND DISCUSSION

This section presents the validation and inter-comparison results of the present MPRR approach with existing studies using in-situ and satellite observations. Furthermore, the spatial distribution and temporal variability of surface $pCO_2$ fields are demonstrated using satellite oceanographic data.

### A. VALIDATION AND INTER-COMPARISION RESULTS

The daily MODIS-Aqua Level-3 SST and Chl*a* data (spatial resolution: 4 km) and the associated 7-day MMOI-SSS composite data (spatial resolution: 25 km) were used to validate the satellite-derived $pCO_2$ data with the in-situ observations over the BoB. The Level-3 MODIS-Aqua SST/Chl*a* and MMOI-SSS products had different spatiotemporal resolutions. To reduce the spatiotemporal mismatches in the validation datasets, the MODIS-Aqua (4 km) products were resampled according to the SSS products (25 km) using the nearest neighborhood technique. Finally, 1300 sample points available after elimination of points with no satellite data and binning to 25 km spatial resolution, these points are used for validation of in-situ and satellite data. Validation

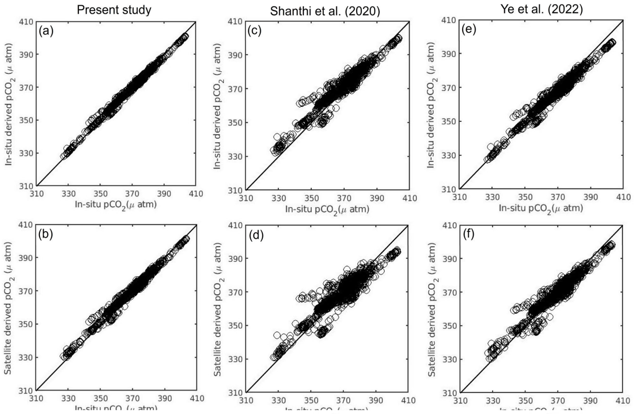


**FIGURE 3.** **Validation and comparative scatter plots (a, b) of present study, with (c, d) Shanthi et al. [26] and (e, f) Ye et al. [30].**

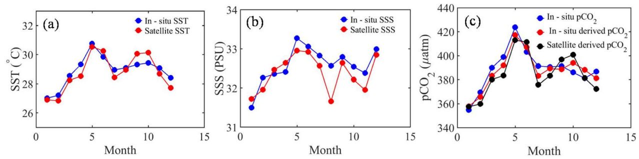


**FIGURE 4.** **Monthly variations of satellite derived (a) SST, (b) SSS and (c) $pCO_2$ with the in-situ observations over the BoB region (2017).**

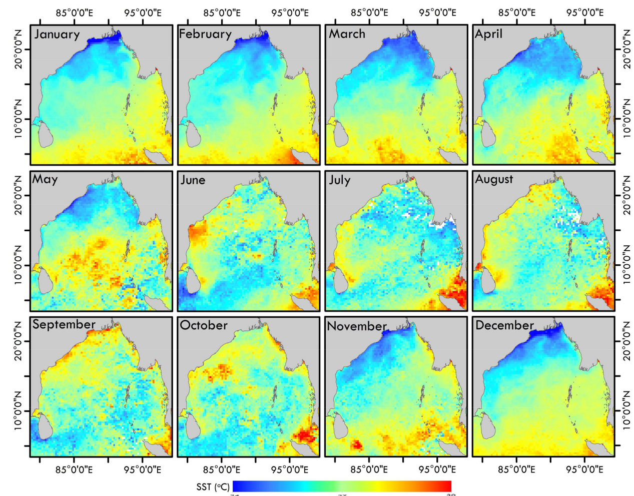


**FIGURE 5.** **Spatial distribution of monthly satellite derived SST at 25-km resolution over the BoB region (2017).**

results indicate that, direct in-situ $pCO_2$ values are consistent and closely correlated with in-situ derived (MRE=0.012, MNB=0.022, RMSE= 4.75 $\mu$atm, and $R^2 = 0.92$) and satellite derived (MRE=0.020, MNB=0.032, RMSE=4.94 $\mu$atm, and $R^2 = 0.91$) $pCO_2$ values.

### B. COMPARITIVE ANALYSIS

Furthermore, we conducted a comparative analysis and performance assessment of MPRR approach with existing regional algorithms [26], [30]. The validation scatter plots are shown in Fig. 3, whereas corresponding statistical parameters are shown in Table 2.

In contrast, our evaluation of existing regional algorithms, specifically those designed for BoB region reveals higher errors and deviations in $pCO_2$ estimations. The inter-comparison of the existing regional BoB algorithms produced the errors and deviations as: MRE 0.064–0.146, RMSE 7.64–14.26, $R^2$ 0.71–0.85 and slope 0.70–0.82 (Table 2). The effectiveness of the MPRR approach can be attributed to its comprehensive consideration of dominant parameters and by incorporating a diverse dataset of spatiotemporal in-situ data for model development. The MPRR approach provides a promising alternative, effectively mitigating the limitations and uncertainties associated with existing algorithms.

### C. SPATIOTEMPORAL VARIABILITY OF $pCO_2$ FIELDS

The air-sea $CO_2$ fluxes and its effects on global climate change largely depend on the spatiotemporal variability of $pCO_2$ fields. These fluxes are primarily controlled by the thermodynamic effects, which depend on SST variations.

Stephen et al. [8] reported that $pCO_2$ increases by 4.23 % for every 1°C rise in SST. Similarly, the $pCO_2$ field alters due to the seasonal changes in biological production (strongly controlled by the Chl*a*). Hence, the surface variations of $pCO_2$ fields are mainly driven by the thermodynamic (SST), stratification (SSS) and biological (Chl*a*) production. Generally, high biological productions with low stratification and thermodynamic affected regions have lower $pCO_2$ values, whereas low biological production with high stratification and thermodynamic influenced regions have higher $pCO_2$ values [4]. The comparison between monthly variation of satellite derived SST, SSS, and $pCO_2$ values and corresponding in-situ measurements are shown in Fig. 4.

The BoB region exhibits significant variations in SST due to the factors such as atmospheric circulation patterns, monsoon systems, ocean currents, and local climatic conditions [31]. The variations in SST significantly influence the $pCO_2$ levels in seawater. Warmer SST leading to higher $pCO_2$ levels, while cooler SST resulting in lower $pCO_2$ levels [4], [8]. During the pre-monsoon season (March to May), the BoB experiences relatively warm temperatures as the region transitions from the cooler winter months to the upcoming monsoon season. The monsoon season (June to September) in the BoB is characterized by heavy rainfall and increased freshwater discharge from river runoff and precipitation. These monsoonal influences can lead to decreased solar radiation penetration due to cloud coverage, resulting in relatively cooler SST values compared to the pre-monsoon season [32]. The monsoon season, which occurs from June to September, brings significant rainfall and cloud cover to the BoB region, leading to cooling of the ocean surface. However, after the monsoon period, the influence of the monsoon weakens, resulting in reduced cloud cover and precipitation. As a consequence, the reduction in cloud cover allows more solar radiation to reach the ocean surface, leading to increased

**TABLE 2. Comparitive statistics of present study and other regional studies.**

| Validation | MRE | MNB | RMSE | $R^2$ | SLOPE | Reference |
|---|---|---|---|---|---|---|
| In-situ | 0.012 | 0.022 | 4.75 | 0.92 | 0.91 | Present study |
| Satellite | 0.020 | 0.032 | 4.94 | 0.91 | 0.89 | |
| In-situ | 0.124 | 0.246 | 12.24 | 0.75 | 0.71 | Shanthi et al. [26] |
| Satellite | 0.146 | 0.282 | 14.26 | 0.71 | 0.70 | |
| In-situ | 0.064 | 0.072 | 7.64 | 0.85 | 0.82 | Ye et al. [30] |
| Satellite | 0.086 | 0.094 | 8.24 | 0.83 | 0.79 | |

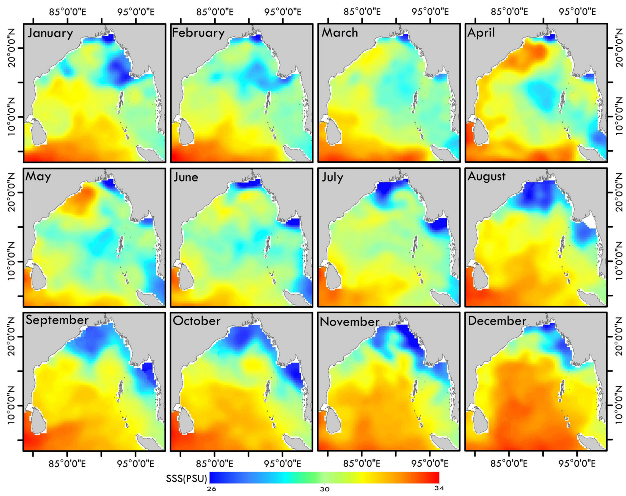


**FIGURE 6. Spatial distribution of monthly satellite derived SSS at 25- km resolution over the BoB region (2017).**

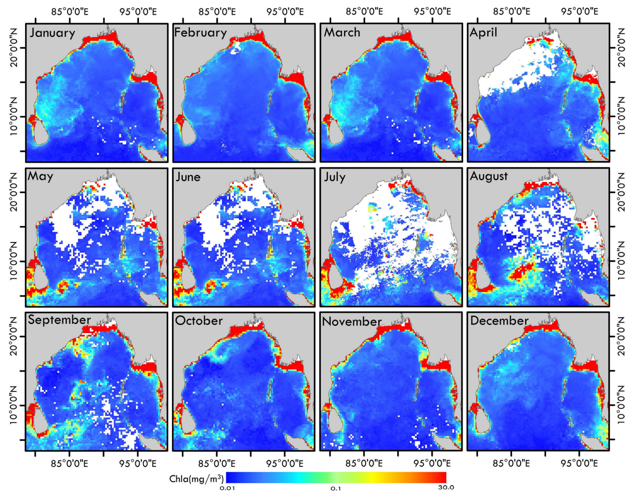


**FIGURE 7. Spatial distribution of monthly satellite derived Chla at 25-km resolution over the BoB region (2017).**

heating of the upper layer of seawater. The decrease in cloud cover and weakening of the monsoon's cooling effect cause SST to rise during the post-monsoon period (October to November).In winter season (December to February), the BoB region experiences relatively cooler SST values due to prevailing northeasterly winds and cold air advection from the Asian landmass [33]. It is important to note that SST is just one of the factors influencing $pCO_2$ variations in seawater. Other factors, such as biological activity, air-sea $CO_2$ exchange, and vertical mixing, also play significant roles in determining $pCO_2$ levels. The seasonal variability of SSS in the BoB can have significant influences on $pCO_2$ levels during different periods of the year [24]. During the pre-monsoon season, the BoB experiences warmer temperatures and reduced rainfall. These conditions lead to increased evaporation, which contributes to higher SSS in the surface waters. The higher SSS can cause seawater to become more saline, reducing its ability to dissolve $CO_2$. As a result, $pCO_2$ levels tend to be higher during the pre-monsoon period due to reduced $CO_2$ solubility.

The monsoon season in the BoB is characterized by heavy rainfall and increased freshwater discharge from river runoff and precipitation. This influx of freshwater leads to a decrease in SSS in the surface waters. The lower SSS during the monsoon season enhances the ocean's capacity to dissolve and hold $CO_2$. Consequently, $pCO_2$ levels tend to be lower during the monsoon period due to higher $CO_2$ solubility. The post-monsoon season have reduced rainfall and a gradual decrease in freshwater input, leading to a slight increase in SSS compared to the monsoon period. The higher SSS during the post-monsoon season may cause a reduction in $CO_2$ solubility, contributing to higher $pCO_2$ levels in the surface waters. The winter season in the BoB is characterized by cooler temperatures, but there is limited seasonal variation in SSS during this period.SSS remains relatively stable during the winter, so its impact on $pCO_2$ levels is less pronounced compared to other seasons [34].

The seasonal variability of Chl*a* in the BoB influences $pCO_2$ levels through its impact on biological productivity and $CO_2$ uptake by phytoplankton [29]. During the pre-monsoon season, the BoB experiences relatively warm temperatures and reduced rainfall. These conditions may lead to lower Chl*a* concentrations as nutrients become limited. The lower Chl*a* concentrations imply reduced biological activity and primary productivity, resulting in less $CO_2$ uptake by phytoplankton during photosynthesis. As a consequence, $pCO_2$ levels tend to be higher during the pre-monsoon period, as less $CO_2$ is being absorbed from the surface waters. The monsoon season in the BoB is characterized by heavy rainfall and increased freshwater discharge, which can enhance nutrient availability and stimulate biological productivity [35]. During the monsoon period, Chl*a* concentrations typically increase due to the abundance of nutrients, promoting phytoplankton growth and higher biological activity. The higher Chl*a*

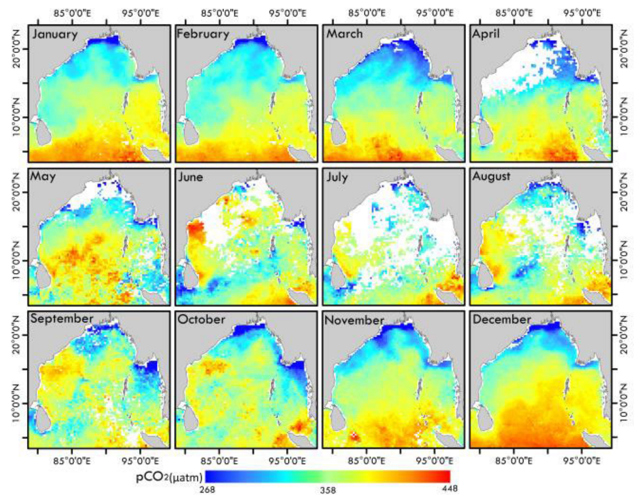


**FIGURE 8.** Spatial distribution of monthly satellite derived $pCO_2$ at 25-km resolution over the BoB region (2017).

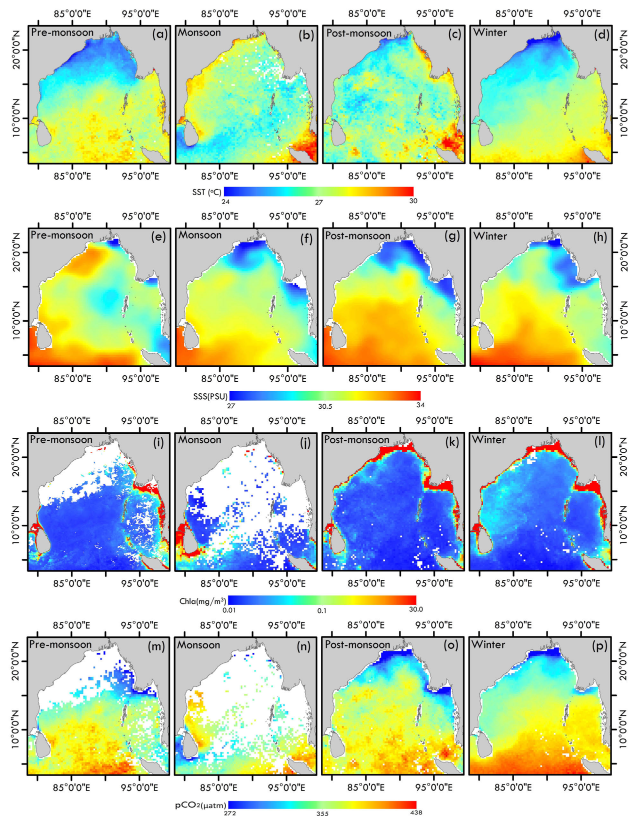


**FIGURE 9.** Seasonal maps of MODIS-Aqua SST (a-d), SSS (e-h), Chla (i-l), and $pCO_2$ (m-p) data at 25km spatial resolution for the year of 2017 [Mar-May (Pre-monsoon); Jun-Sep (Monsoon); Oct-Nov (Post-monsoon); Dec-Feb (Winter)].

concentrations imply increased $CO_2$ uptake by phytoplankton during photosynthesis, leading to lower $pCO_2$ levels in the surface waters as more $CO_2$ is being removed from the system [24]. The post-monsoon season have reduced rainfall and gradual changes in nutrient availability, which can lead to variations in Chl*a* concentrations. Depending on the nutrient

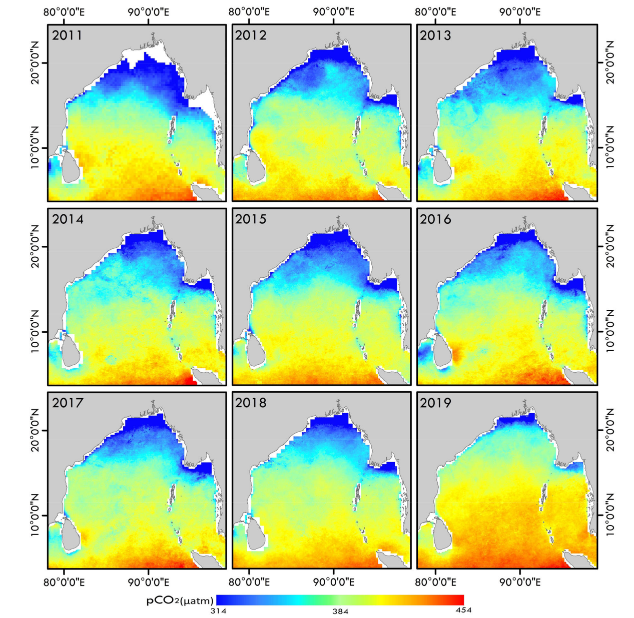


**FIGURE 10.** Spatial distribution annual satellite derived $pCO_2$ at 25-km resolution over the BoB region (2017).

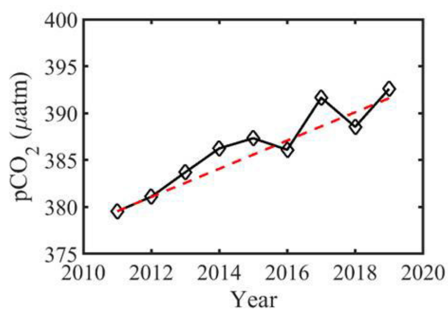


**FIGURE 11.** Inter annual variability of $pCO_2$ over the BoB region (2011-2019).

levels, Chl*a* concentrations may either decrease or remain relatively stable during this period. If Chl*a* concentrations decrease, biological activity and $CO_2$ uptake by phytoplankton may also decrease, contributing to higher $pCO_2$ levels in the surface waters. Conversely, if Chl*a* concentrations remain stable, their impact on $pCO_2$ levels may be less pronounced during the post-monsoon season. The winter season in the BoB is characterized by cooler temperatures and relatively low biological activity. The surface Chl*a* concentrations tend to be lower during the winter due to reduced light availability and nutrient limitations.

The lower Chl*a* concentrations imply reduced $CO_2$ uptake by phytoplankton during photosynthesis, potentially leading to higher $pCO_2$ levels in the surface waters. During pre-monsoon, BoB have higher biological production with moderate thermodynamic and stratification, which signifies all the three parameters play essential role in $pCO_2$ variations. In the post-monsoon season, $pCO_2$ fields are principally controlled by the thermodynamic and stratification effects as compared to the biological production, indicating that $pCO_2$ variations are mainly controlled by the SST and SSS variations rather than Chl*a*.

For the purpose of graphical demonstration of spatiotemporal variability of surface $pCO_2$ fields over the BoB region, the developed MPRR approach was implemented on the collocated satellite data of SST, SSS and Chl*a* at 25km spatial resolution (for spatial consistency of all the satellite derived products) and generated monthly (Fig. 5-8), seasonal (Fig. 9) and annual (Fig.10) maps. Monthly maps were useful for understanding short-term trends and fluctuations in $pCO_2$ levels. Seasonal maps allowed for identifying patterns in $pCO_2$ levels over different seasons, such as the influence of monsoons on carbon dioxide levels in the BoB. Finally, annual maps provided a broader perspective on how $pCO_2$ levels change over an entire year, which can be useful for assessing long-term trends and informing policy decision related to carbon management and climate change mitigation strategies in the BoB region.

The spatiotemporal variability of $pCO_2$ fields over the BoB region predominantly controlled by the Indian monsoon system such as SWM season (June-August), and NEM season (December-January). Due to SWM season, the BoB region experiences high precipitation and receives large amount of fresh water inflow from the major Indian rivers leads to strong stratification (caused by the low SSS) [15], which leads to low $pCO_2$ fields ($<350\ \mu atm$) (Fig.8).

In the coastal region of BoB, strong seasonal $pCO_2$ fluctuations are observed (Fig. 9) due to the higher variability of seasonal biological production, changes in SSS (freshwater inflow), strong vertical mixing, cyclonic eddies, organic and inorganic carbon inputs from the rivers. Sarma et al. [15] reported that BoB have higher $pCO_2$ fields in the south-western region and lower $pCO_2$ fields in the north-western region than to the atmospheric $CO_2$ level; the similar structures are observed in the present study (Fig. 10 & 11). The lower $pCO_2$ fields in north-western BoB are caused due to the strong influence of physical and biological processes over the region.

## IV. CONCLUSION

A MPRR approach was developed using simultaneous in-situ measurements of SST, SSS and Chl*a* collected during the oceanography cruises covering open and coastal waters of BoB. In-situ and satellite validations revealed that the MPRR derived $pCO_2$ values are in very good agreement with direct in-situ measurements with significantly very low RMSE deviation (4.75 $\mu atm$). Hence, the MPRR approach is more robust and accurate in assessing the $pCO_2$ fields over the BOB. Although the present study improved $pCO_2$ estimations over the BoB, inclusion of satellite derived Chl*a* data instead of in-situ measured Chl*a* in the model development dataset leads to slight deviations and uncertainties due to the spatiotemporal mismatch analysis. In future, $pCO_2$ estimations can be improved by developing in-water algorithms rather than in-situ and satellite matchup-based approaches.

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