

Original Article

# Evaluation of Sea Surface Temperature based $p\text{CO}_2$ Algorithm in the Southwest Bay of Bengal

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**Abstract** - The partial pressure of carbon dioxide ( $p\text{CO}_2$ ) is one of the most effective measurements of carbon dioxide in seawater, and the increases in  $p\text{CO}_2$  profoundly affect the marine carbonate system. The role of SST on  $p\text{CO}_2$  is analyzed to develop a regional  $p\text{CO}_2$  algorithm using in-situ SST and calculated  $p\text{CO}_2$  by employing the polynomial regression functions such as linear, quadratic, and cubic to develop a  $p\text{CO}_2$  map and the best-fit algorithm of the cubic function developed for the postmonsoon season with an  $R^2$  of 0.537 and SEE of  $\pm 36.543$  has been validated for remote sensing applications. Evaluation of satellite-derived  $p\text{CO}_2$  with calculated  $p\text{CO}_2$  showed  $R^2$  of 0.498 and the root mean square error (RMSE) of  $\pm 30.922 \mu\text{atm}$  with 75% of overestimation of calculated  $p\text{CO}_2$  by the satellite-derived  $p\text{CO}_2$ . The satellite-derived  $p\text{CO}_2$  map error is mainly because of the inbound errors in MODIS-derived SST products. Hence, improvement in sensor technology and retrieval algorithm would improve the retrieval of input parameters (SST), which is useful in estimating  $p\text{CO}_2$  precisely. This would enable us to understand the biogeochemical processes behind the variability of  $\text{CO}_2$  in the surface waters of the southwest Bay of Bengal.

**Keywords** - Chlorophyll,  $p\text{CO}_2$ , Regression, SST, Bay of Bengal, MODIS.

## I. INTRODUCTION

The global carbon cycle is essential for energy and mass exchange in the Earth System, as it connects the system's components (land, ocean, and atmosphere) (Garbe et al., 2014). Increases in atmospheric carbon dioxide ( $\text{CO}_2$ )

concentrations, primarily caused by the combustion of fossil fuels, cement production, and increased urbanization, are directly accountable for 60% of the average global air temperature increase (IPCC, 2013). The direct exchange of  $\text{CO}_2$  with the atmosphere at mixed-layer waters is primarily influenced by sea surface temperature (SST), dissolved inorganic carbon (DIC) levels, and total alkalinity (TA), with SST influenced by physical processes such as the mixing of water masses and DIC and TA influenced by biological processes (photosynthesis and respiration). The partial pressure of  $\text{CO}_2$  ( $p\text{CO}_2$ ) in seawater is generally modulated by both physical (SST) and biogeochemical (DIC and TA) processes (Lu et al., 2011).

The temperature mostly determines the  $p\text{CO}_2$  concentration at the sea surface at surface (SST). When seawater is warmed by  $1^\circ\text{C}$ ,  $p\text{CO}_2$  increases by four in a parcel with a fixed chemical composition (Stephans et al., 1995; Zhu et al., 2009). On the other hand, the DIC in the surface ocean varies from an average value of  $2150 \mu\text{mol kg}^{-1}$  in Polar Regions to  $1850 \mu\text{mol kg}^{-1}$  in the tropics as a result of biological processes and reduces  $p\text{CO}_2$  by a factor of 4 (Feely et al., 2001). Therefore, the effect of biological drawdown and temperature on surface water  $p\text{CO}_2$  is similar, but the two effects are often compensating. Hence, the spatial and temporal distribution of  $p\text{CO}_2$  in surface waters and  $\text{CO}_2$  flux is largely governed by a balance between the changes in seawater temperature, net biological utilization of  $\text{CO}_2$ , and the upwelling flux of  $\text{CO}_2$ -rich waters.



According to carbon dioxide measurements in the atmosphere, the oceans and terrestrial biosphere absorb roughly half of the annual anthropogenic CO<sub>2</sub> emissions (Siegenthaler and Sarmiento, 1993). Knowledge of the large-scale spatiotemporal variability in partial pressure of carbon dioxide (*p*CO<sub>2</sub>) distribution is a prerequisite to estimating oceanic CO<sub>2</sub> absorption, which is difficult to obtain from observations only (Wallace, 1995). Several researchers have utilized various methods to interpolate and/or extrapolate shipboard *p*CO<sub>2</sub> data on spatial and temporal scales using relationships with remotely sensed data, such as sea surface temperature (SST) and chlorophyll-*a* concentration. For instance, Tans et al. (1990) and Keeling and Shertz (1992) used the relationship between *p*CO<sub>2</sub> and SST to infer surface ocean CO<sub>2</sub> fields. Stephens et al. (1995) with root-mean-square (RMSE) error of ( $\leq 40 \mu\text{atm}$ ). Ono et al. (2004) included chlorophyll *a* as an additional regression parameter and reduced the RMS error to  $\leq 17\mu\text{atm}$ . Sarma et al. (2006) further developed a remote-sensing algorithm for *p*CO<sub>2</sub> by including SST, chlorophyll-*a*, and climatological salinity. Lohrenz and Cai (2006) added chromophoric dissolved organic matter (CDOM) to derive sea surface salinity as a parameter in their remote-sensing algorithm for *p*CO<sub>2</sub>. Zhu et al. (2009) studied the air-sea exchange of CO<sub>2</sub> using remotely sensed *p*CO<sub>2</sub> developed using satellite-derived SST, chlorophyll *a*, and wind speed with an RMS error of 4.6  $\mu\text{atm}$ . Recently, a regression equation for *p*CO<sub>2</sub> with SST and chlorophyll *a* was proposed by Zui et al. (2012) and Qin et al. (2014) with an RMSE of  $\pm 13.45 \mu\text{atm}$  and  $\pm 21.46 \mu\text{atm}$  with the satellite-derived *p*CO<sub>2</sub> respectively.

Considering the above facts, it is attempted to develop a regional *p*CO<sub>2</sub> algorithm using *in-situ* SST and calculated *p*CO<sub>2</sub>. The best-fit algorithm has been validated with the calculated *p*CO<sub>2</sub> measurements for remote sensing applications.

## II. MATERIALS AND METHODS

The present study was conducted along the Tamilnadu coast, falling along the southwest Bay of Bengal region. From January 2017 to June 2019, regular monthly samplings were performed at 1, 5, 7, 9, and 12 km from the coast at four sampling stations concealing the longitude and latitude of Chennai (80°23.9 E - 13°07.9 N), Cuddalore (79°48.5 E – 11°42.4 N), Parangipettai (79°51.7 E – 11°30.6 N) and Karaikal (79°55.5 E – 10°54.8 N) (Fig. 1). Based on the region's northeast monsoon, the study period was split into four seasons: postmonsoon (January to March), summer (April to June), premonsoon (southwest monsoon - July to September), and monsoon from October to December (monsoon).

### A. In-situ data

A digital multi-stem thermometer with a  $\pm 0.1^\circ \text{C}$  precision was employed to monitor in situ SST. Water

samples were taken directly from the Niskin water sampler into a 250 ml polyethylene container.

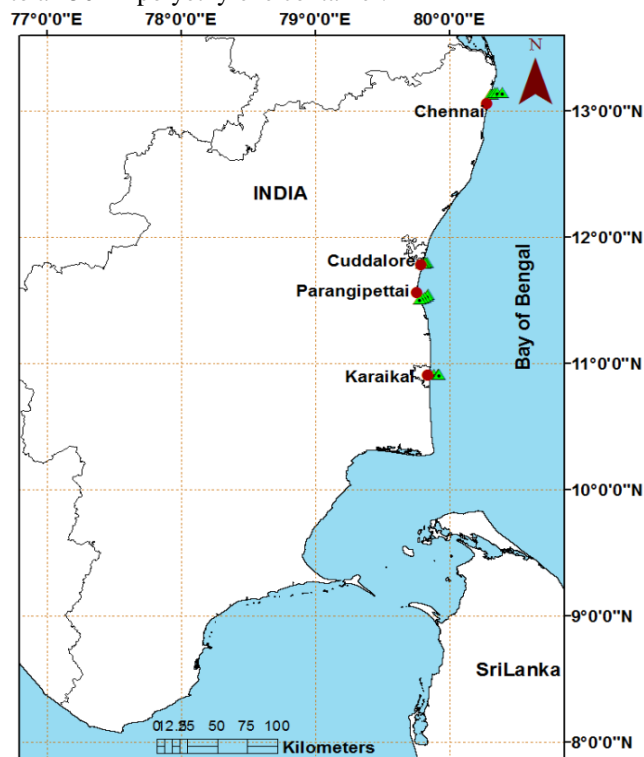


Fig. 1 Map showing the sampling stations and transects in the southwest Bay of Bengal water

clean drawing tubes with no bubbles and low turbulence with sufficient flushing to avoid contamination from the atmosphere. A hand-held refractometer was used to determine salinity (Atago hand refractometer, Japan). The samples were stored in the dark until further analysis of pH and total alkalinity (TALK) that were measured in the laboratory using a potentiometric titrator calibrated on the total scale (905 Titrando, Metrohm, Switzerland) (Frankignoulle and Borges, 2001). The *p*CO<sub>2</sub> was computed using measured temperature, salinity, TALK, and *in situ* pH (total scale). The precision for *p*CO<sub>2</sub> was 9–13  $\mu\text{atm}$  (Bhavaya et al., 2016).

### B. SST based *p*CO<sub>2</sub> Retrieval Algorithm

SST is usually the key governing element of *p*CO<sub>2</sub> in oligotrophic waters, which provides a theoretical basis for calculating *p*CO<sub>2</sub> (Zhai et al., 2005). Hence, the *in situ* SST and calculated *p*CO<sub>2</sub> datasets were subjected to two-dimensional regressions to develop the *p*CO<sub>2</sub> algorithm. Three different polynomial functions such as linear, quadratic, and cubic were applied for regression analysis

### C. Satellite Data

MODIS-Aqua derived Level-2a SST image was acquired to generate a remotely sensed *p*CO<sub>2</sub> image using satellite-derived SST. For remote sensing measurements in

the southwest Bay of Bengal, February to May is a good time to get cloud-free data; however, only occasional data sets are available attributed to the influence of both the southwest and northeast monsoons, which render the southern Bay of Bengal a more cloud-prone region in the northern Indian Ocean during the rest of the year. As a result, MODIS-Aqua derived Level-2a SST for 23<sup>rd</sup> March 2014, with a spatial resolution of 1km, was obtained from <http://modis.gsfc.nasa.gov>. ERDAS IMAGINE (9.2. ver.) and ENVI (4.7. ver.) software-generated SST and pCO<sub>2</sub> images from the data. The geometric correction was used on the SST data to remove image distortion and bring it to a standard geographic projection (Lat/Lon) with a modified Everest Datum.

**D. Evaluation Criteria**

The evaluation was carried out by comparing satellite-derived values with field measurements. SigmaPlot (Ver.12.0) statistical software was used to perform statistical fitting on these data. Mean Normalized Bias (MNB) and Root Mean Square Error (RMSE) evaluated the algorithm's performance. Mean normalized bias measures whether true values are over or understated. Root mean square error is a reliable marker of data scatter for normally distributed variables and provides vital information on satellite and in-situ data (Shanthi et al., 2013).

**III. RESULTS AND DISCUSSION**

The oceanic partial pressure of CO<sub>2</sub> (pCO<sub>2</sub>) is highly variable, and it is difficult to assess spatial and temporal variability because of the scarcity of measurements. In general, pCO<sub>2</sub> and SST have a strong relationship, mainly in oceanic regions where significant physical and biological factors are. The thermodynamic effect of temperature on pCO<sub>2</sub> (at constant salinity, alkalinity, and dissolved inorganic carbon) is about 4°C (Copin-Montegut, 1989). At the same time, the equilibrium of the carbonate system in seawater is altered by the influence of SST in the absence of external exchanges (Qin et al., 2014). Hence, the two-dimensional approach of SST and pCO<sub>2</sub> regression fits are attempted to understand the role of SST on pCO<sub>2</sub> in the southwest Bay of Bengal coastal waters; the polynomial regression analysis for different functions like linear, quadratic, and cubic have been carried out to generate pCO<sub>2</sub> maps.

**A. 2D-Regression Analysis and Pco2 Algorithm Development**

In-situ SST and calculated pCO<sub>2</sub> concentrations (Eq. 2) were obtained by monthly coastal samplings at four sampling stations from January 2017 to June 2019 in the southwest Bay of Bengal region. The data points (20) matching the date

of satellite-derived SST data were treated separately for validation purposes. Finally, 334 points were taken for regression analysis accounting for 94% of the total data.

Where N= Number of points. On the whole cubic, the function was a better fit than other functions. It produced a significant relationship during the postmonsoon season (R<sup>2</sup>=0.537) with a minimum standard error of estimation (± 36.543 µatm), and the derived pCO<sub>2</sub> algorithm was used to generate the pCO<sub>2</sub> images. The pCO<sub>2</sub> algorithm implies the following equation:

$$pCO_2 = 263581.4877 - 27820.7825*SST + 980.9763*SST^2 - 11.5396*SST^3$$

**Postmonsoon**

pCO<sub>2</sub>=1590.7218-43.4352\*SST → (1) Linear

pCO<sub>2</sub>=-2922.0693+272.4418\*SST-5.5244\*SST<sup>2</sup> → (2) Quadratic

pCO<sub>2</sub>=263581.4877-27820.7825\*SST+980.9763\*SST<sup>2</sup>-11.5396\*SST<sup>3</sup> → (3) Cubic

**Summer**

pCO<sub>2</sub> = 2594.7694-76.0582\*SST → (4) Linear

pCO<sub>2</sub>=9892.4125-555.7563\*SST +7.8763\*SST<sup>2</sup>→(5) Quadratic

pCO<sub>2</sub>=-4167.8615+832.0346\*SST-37.7442\*SST<sup>2</sup>-0.4995\*SST<sup>3</sup> → (6) Cubic

**Premonsoon**

pCO<sub>2</sub> =2983.6552-88.1427\*SST → (7) Linear

pCO<sub>2</sub>=29285.3892-1881.4403\*SST +30.5341\*SST<sup>2</sup> (8) Quadratic

pCO<sub>2</sub>=-151226.738+16636.935\*SST-602.1762\*SST<sup>2</sup>-7.1998\*SST<sup>3</sup>→(9) Cubic

**Monsoon**

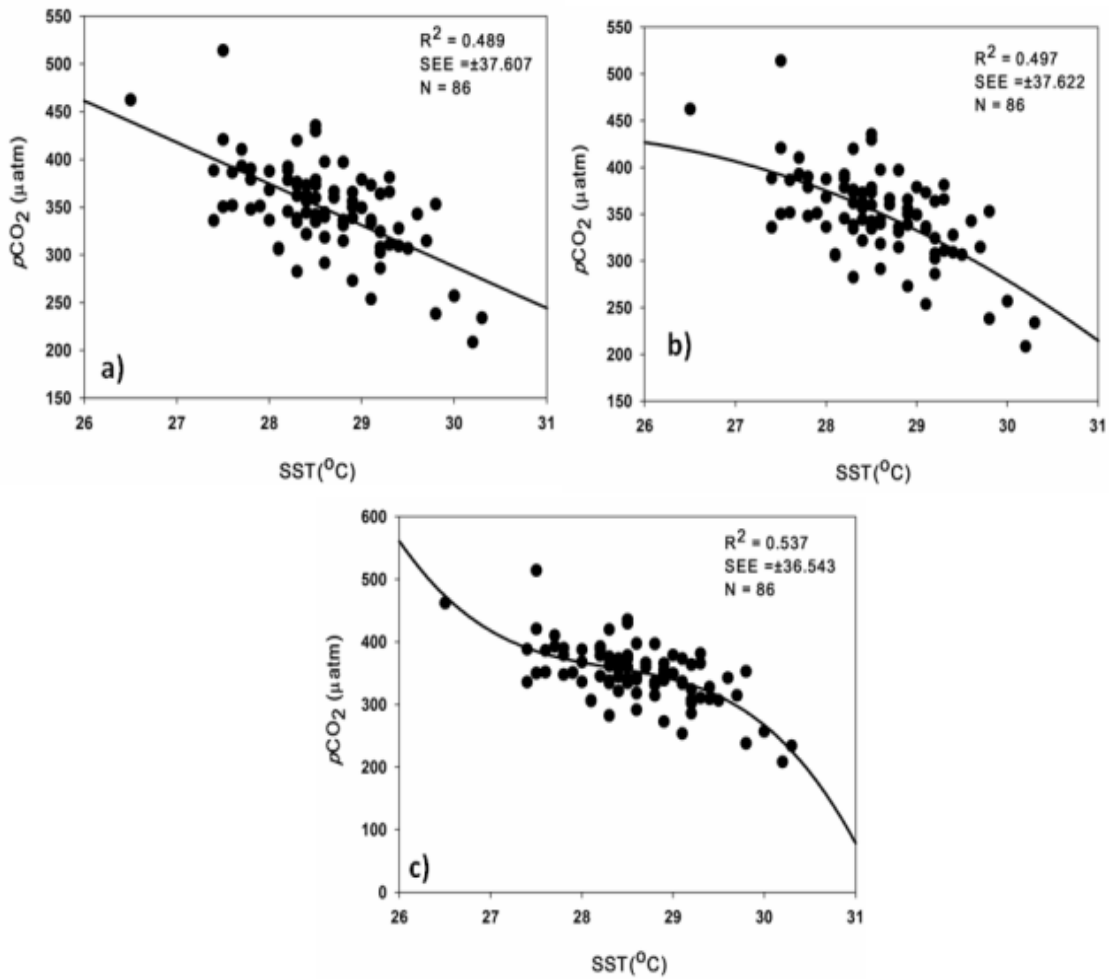
pCO<sub>2</sub> = 2755.7601-77.9496\*SST → (10) Linear

pCO<sub>2</sub>=-2378.7502+283.9733\*SST-6.3704\*SST<sup>2</sup> (11) Quadratic

pCO<sub>2</sub>=-596822.233-63293.5995\*SST-2240.349\*SST<sup>2</sup>-26.443\*SST<sup>3</sup>→(12) Cubic

**B. Development of  $pCO_2$  algorithm based on in-situ SST**

The regression analysis of the full dataset for three polynomial functions reveals an insignificant association with an  $R^2 \leq 0.330$  and  $SEE \geq \pm 92 \mu atm$  between SST and  $pCO_2$ . The thermal capacity of the ocean is very large, and it varies from season to season, and space coinciding with this  $pCO_2$  also shows fluctuations. Hence it is not appropriate to treat the entire dataset in one cluster. Therefore, the seasonal regression analysis between SST and  $pCO_2$  was made to develop an SST-based  $pCO_2$  algorithm for three polynomial linear, quadratic, and cubic functions. The regression plots were illustrated in figures 2-5, and the polynomial regression equations were given as follows. SST plays a major role in influencing the seasonal variability of  $pCO_2$  because temperature determines the solubility of  $CO_2$  to a large extent (Sabine et al., 2000). Higher SST makes the air lighter, shifts the air to the upper atmosphere, and reduces the air-sea interaction, thereby  $CO_2$  dissolution on the water's surface. In the regression analysis, SST portrays the constant negative relationship with  $pCO_2$  in all the seasons, and it is clear from the regression equations that  $pCO_2$  decreases with increasing temperature (Lefevre and Taylor, 2002). SST in the Bay of Bengal varies more seasonally, with high temperatures during the summer months and low temperatures during the monsoon and postmonsoon seasons, which coincide with river inputs and winter cooling. Hence it is attempted to treat them on a seasonal scale.



**Fig. 2 Regression analysis of postmonsoon dataset between in-situ SST and calculated  $pCO_2$  for linear (a), quadratic (b), and cubic (c) polynomial functions**

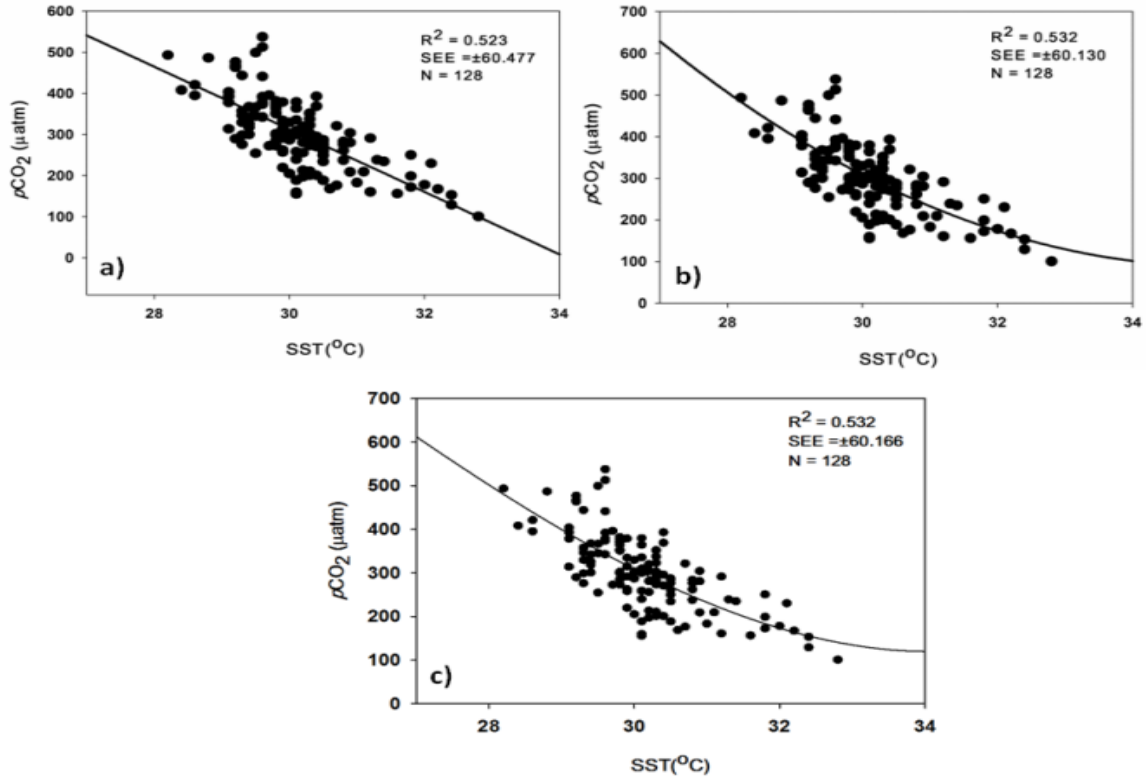


Fig. 3 Regression analysis of summer dataset between *in-situ* SST and calculated pCO<sub>2</sub> for linear (a), quadratic (b), and cubic (c) polynomial functions

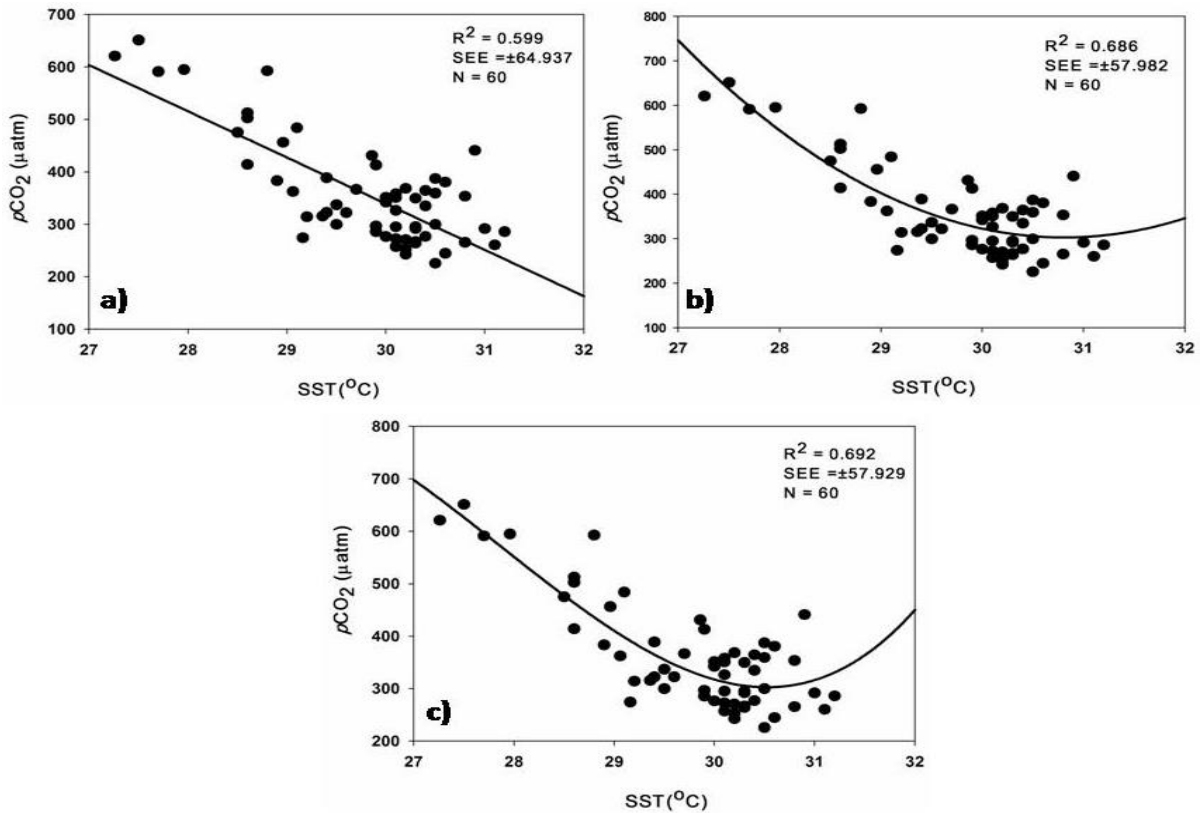


Fig. 4 Regression analysis of premonsoon dataset between *in-situ* SST and calculated pCO<sub>2</sub> for linear (a), quadratic (b), and cubic (c) polynomial functions

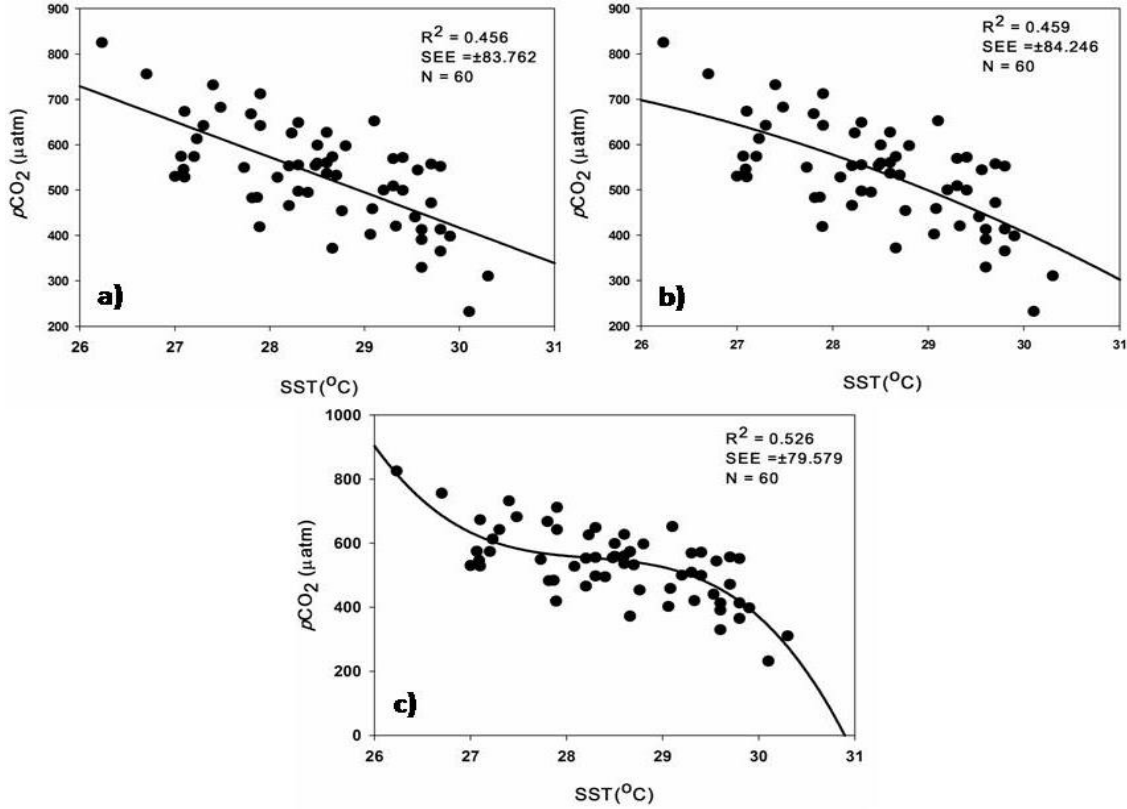


Fig. 5 Regression analysis of monsoon dataset between *in-situ* SST and calculated *pCO<sub>2</sub>* for linear (a), quadratic (b), and cubic (c) polynomial functions

The  $R^2$  values and standard error of estimate (SEE) obtained for different seasons using the polynomial regression analysis are summarized in table 1. Among the three polynomial functions used, the cubic function provided better agreement for all the seasons than other functions. Still, the standard error of the estimate remained high ( $> 50\mu\text{atm}$ ) for summer, premonsoon, and monsoon seasons. The polynomial regression analysis of different seasons showed the significant  $R^2$  values during premonsoon season ( $R^2 = 0.599$ ,  $\text{SEE} = \pm 64.937$ ;  $R^2 = 0.686$ ,  $\text{SEE} = \pm 57.982$  and  $R^2 = 0.692$ ,  $\text{SEE} = \pm 57.929$ ) for linear, quadratic, and cubic functions respectively than other seasons. So after that summer explained the better relationship between SST and  $p\text{CO}_2$  and poor correlation co-efficient is observed during monsoon and postmonsoon seasons with the  $R^2$  values for different functions.

Table 1. Results of regression analysis between *in-situ*  $p\text{CO}_2$  and SST

Season	N	Linear		Quadratic		Cubic	
		$R^2$	SEE( $\pm$ )	$R^2$	SEE( $\pm$ )	$R^2$	SEE( $\pm$ )
POM	86	0.49	37.61	0.50	37.62	<b>0.54</b>	<b>36.54</b>
SUM	128	0.52	60.48	0.53	60.13	0.53	60.17
PRM	60	0.60	64.94	0.69	57.98	0.69	57.93
MON	60	0.46	83.76	0.46	84.25	0.53	79.58

The cubic function provided a better predictive capability for all seasons with a marginal improvement in the correlation coefficient than the other two functions. Conversely, Olsen et al. (2008) investigated the different regression diagnostics from single parameter relationships of  $f\text{CO}_2$  with SST, chlorophyll *a*, and mixed layer depth. They found a poor correlation of SST with  $f\text{CO}_2$  in seawater during winter ( $R^2 \leq 0.001$ ) and a strong correlation with chlorophyll *a* and mixed layer depth in summer. In the present study, the cubic function offers an improved correlation coefficient ( $R^2 = 0.537$ ) during the postmonsoon season, with a minimum standard error of estimate ( $\pm 36.543$ ). Thus, a cubic function-derived algorithm has been applied to develop satellite-derived  $p\text{CO}_2$ .

**C. Evaluation of SST based pCO<sub>2</sub> algorithm**

To generate a satellite-derived pCO<sub>2</sub> field, MODIS-Aqua retrieved SST data was used for the postmonsoon season (23<sup>rd</sup> March 2014) (Fig. 6). Satellite-derived SST (MODIS-Aqua) and modeled pCO<sub>2</sub> images are validated with the *in-situ* SST and calculated pCO<sub>2</sub> data of the same date at different locations of the southwest Bay of Bengal. Evaluation of MODIS-SST with *in-situ* SST shows a negative bias (MNB = -0.009) with RMSE of ±0.491°C (Fig.7a), which is greater than the error (±0.38°C) observed by Gentemann (2014) and could be attributed to possible errors in cloud removal, contaminated aerosol retrievals, or sampling. Moreover, SST measured using infrared radiometers will estimate with high resolution only under cloud-free conditions, and it has been evident from the regression results (R<sup>2</sup>=0.700 and SEE ±0.244°C). The data points fall outside the 95% confidence band, suggesting that the satellite-derived values were higher or lower than they should be in natural waters. However, a comparison plot of *in-situ* SST with MODIS-derived SST revealed that the MODIS-SST, scattered about the 1:1 line, underestimated 70% of the *in-situ* data and inflated 30% of the *in-situ* data (Fig.7b).

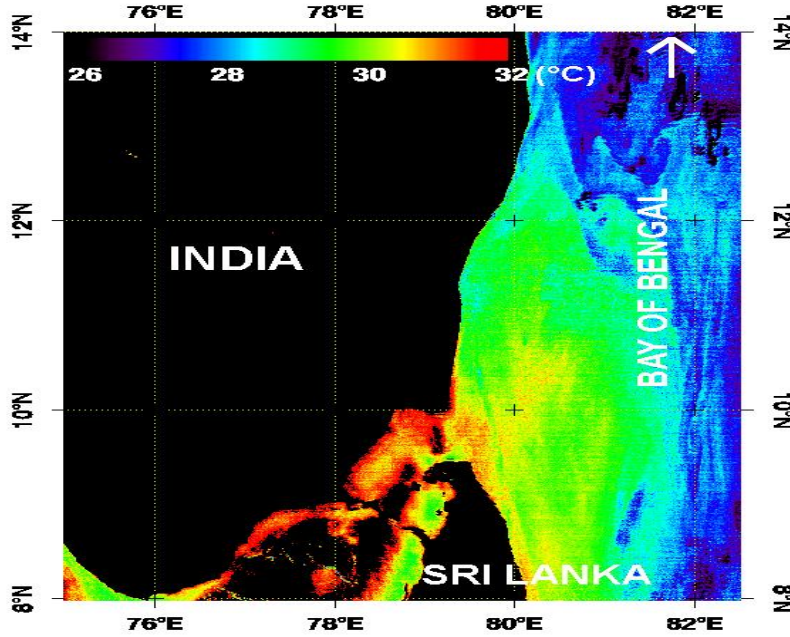


Fig. 6 MODIS-Aqua derived SST image of 23<sup>rd</sup> March 2014

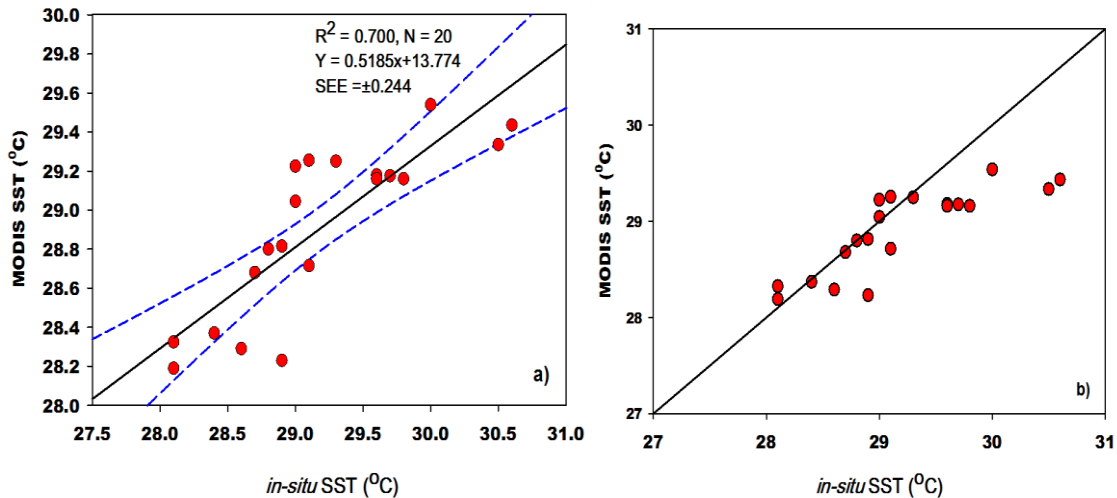


Fig. 7 Regression (a) and comparison (b) plots of *in-situ* SST Vs. MODIS-Aqua derived SST

The statistical results reported in this study are analogous to MODIS SST validation using *in-situ* observations along the western Pacific coasts (Barton and Pearce, 2006) with a bias of -0.32°C; western North Pacific (Hosoda et al., 2007) with a bias of -0.06°C and RMSE of ±0.81°C, Taiwan coast (Lee et al., 2010) with a bias of 0.42°C and RMSE of ±0.86°C, San Matías Gulf of Argentina (Williams et al., 2013) with an R<sup>2</sup> of 0.89 and Bay of Bengal (Narayanan et al., 2013) with a bias of

1.80°C and reported the overestimation of the satellite product. However, with a correlation of  $R^2 = 0.700$ , the regression fit was determined to be substantial. Hence MODIS-derived SST data was used to construct an SST-based  $pCO_2$  algorithm to generate remotely sensed  $pCO_2$ .

**D. Validation of Remotely Sensed  $pCO_2$**

The algorithm developed for the postmonsoon season is applied with MODIS-Aqua-derived SST to generate the remotely sensed  $pCO_2$  fields. The algorithm's predictive capability has been examined by comparing the calculated  $pCO_2$  with remotely remote sensed  $pCO_2$  data. Validation of remotely sensed  $pCO_2$  was carried out to assess the SST-based algorithm's performance by using calculated  $pCO_2$  data (Fig.8). The validation results found that there is no significant coefficient of determination ( $R^2 = 0.428$ ) with the SEE of  $\pm 12.510$ , MNB (0.071), and RMSE (30.922), indicating the poor agreement between remotely sensed  $pCO_2$  and calculated  $pCO_2$  (Fig.9a). A comparison plot of remotely sensed  $pCO_2$  with calculated  $pCO_2$  showed 75% overestimation and 25% underestimation of calculated  $pCO_2$  data (Fig. 9b). Similarly, Metzl et al. (1995) observed seasonal  $pCO_2$ -SST relationships to reconstruct  $pCO_2$  from climatological SST in the Indian and Antarctic Oceans. Stephans et al. (1995) also used the  $pCO_2$ -SST relationship to extrapolate  $pCO_2$  distribution by using satellite-derived SST in the North Pacific basin and obtained an RMSE of  $\pm 17 \mu atm$  and  $\pm 40 \mu atm$  for the northeast and western Pacific. The change is due to the impact of biologically produced variations in DIC.

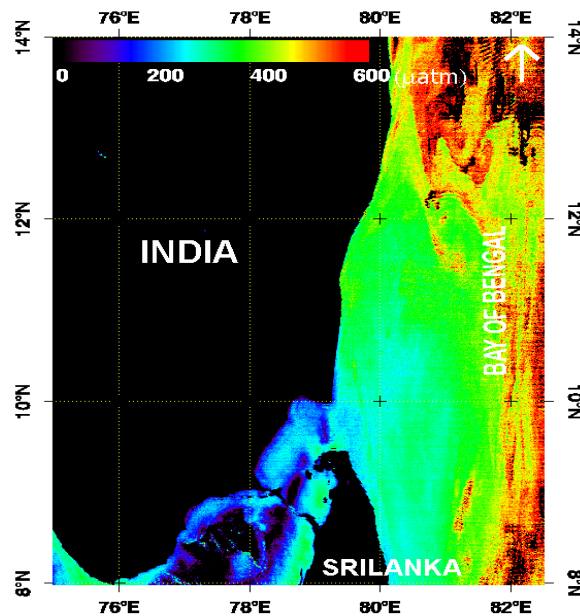


Fig. 8 SST based satellite-derived  $pCO_2$  image for 23<sup>rd</sup> March 2014

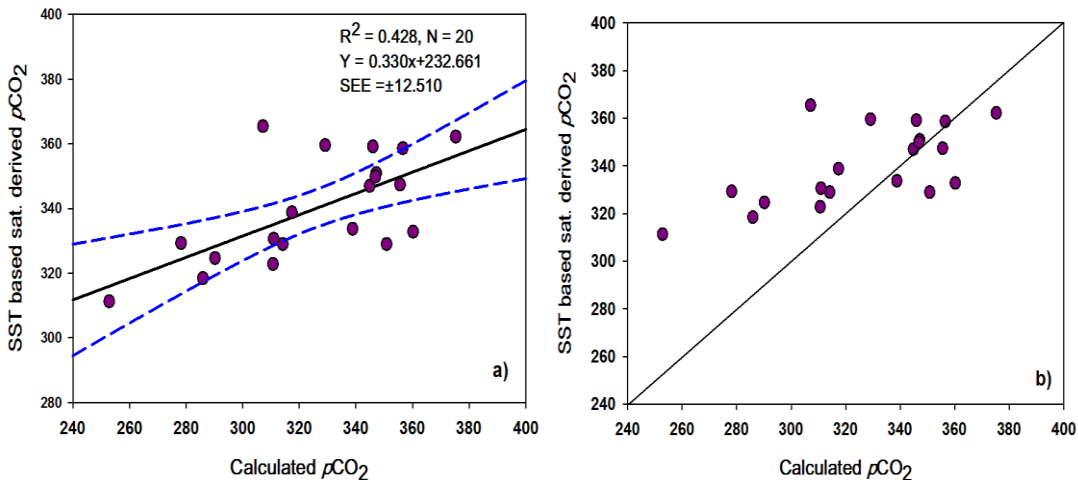


Fig. 9. Regression (a) and comparison (b) plots of calculated  $pCO_2$  vs. SST-based satellite-derived  $pCO_2$ .



Landrum et al. (1996) and Lee et al. (1998) described the relation of  $p\text{CO}_2$  with SST in subtropical and subarctic (30–43°N) waters and found an insignificant correlation ( $R^2 = 0.38$ ). These results indicated that SST alone would not serve as an accurate estimate of basin-scale  $p\text{CO}_2$ . Furthermore, our data showed little improvement in the relationship of  $p\text{CO}_2$  with SST ( $R^2 = 0.537$ ) over Landrum et al. (1996) and significantly supported Stephans et al. (1995) findings of poor predicting ability (RMSE =  $\pm 30.922$  atm). Lee et al. (1998) also extrapolated surface  $p\text{CO}_2$  in the Pacific Ocean based on the relationship of  $p\text{CO}_2$  with SST and found low interannual variability in the recent  $\text{CO}_2$  uptake of atmospheric  $p\text{CO}_2$ . Zhai et al. (2005) also reported underestimating field measurements of 0–50  $\mu\text{atm}$  by the  $p\text{CO}_2$ -SST relationship in the Northern South China Sea. From the present results and literature, it is inferred that SST plays a vital role in the  $p\text{CO}_2$  distribution and has a significant impact on the  $p\text{CO}_2$  distribution in the Bay of Bengal.

#### IV. CONCLUSION

The seasonal regression analysis showed significant seasonal variability in the relationship of  $p\text{CO}_2$  with SST. The  $p\text{CO}_2$  and SST had a strong inverse relationship in all the seasons, suggesting that increased SST reduces  $\text{CO}_2$  dissolution in seawater, lowering the  $p\text{CO}_2$  in seawater. The distribution of  $p\text{CO}_2$  fits well with the cubic curve in each season, and the best fit is found for the postmonsoon season. Further, an SST-based algorithm has been employed to generate a  $p\text{CO}_2$  map using MODIS-Aqua-derived SST data. The validation of the  $p\text{CO}_2$  map exhibited poor prediction capacity with an RMSE of  $\pm 30.922 \mu\text{atm}$ . The satellite-derived  $p\text{CO}_2$  map error is mainly because of the inbound errors in MODIS-derived SST products. As a result, advancements in sensor technology and retrieval algorithms will undoubtedly improve the retrieval of input parameters (SST), which will be valuable in accurately determining  $p\text{CO}_2$ . This would enable us to understand the biogeochemical processes behind the variability of  $\text{CO}_2$  in the surface waters of the southwest Bay of Bengal.

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