

Estimation of partial pressure of CO₂ around Mount Krakatau waters, Sunda Straits, Indonesia

Susanna Nurdjaman¹, Imat Rohimat¹, Muhammad Fadli², Dayu W Purnaningtyas¹, Aditya R Kartadikaria¹, and Mutiara R. Putri¹

¹Department of Oceanography, Faculty of Earth Sciences and Technology, Bandung Institute of Technology, Indonesia

²Research Center for Deep-Sea, Indonesian Institute of Science, Indonesia

*Corresponding author: susanna@fitb.itb.ac.id

Abstract

The study aimed to develop the formula and validate the value of oceanic carbon dioxide partial pressure (pCO_{2,sea}) around Krakatau Waters in the Sunda Strait using parameters such as sea surface temperature (SST), sea surface salinity (SSS), and chlorophyll-a (Chl) based on data collected from different seasons (September 2017 and April 2018). The formulation of empirical equation followed a multivariate polynomial regression method. The empirical equation for estimating the pCO_{2,sea} was: $pCO_2 = -472.069 + 1044.043 \log(SST) - 435.897 \log(SSS) - 5.03 \log(Chl)$. This formula can be applied for both the transitional season I and transitional season II. The results showed a strong relationship between the SST parameter and pCO₂ with a correlation of 0.91 then followed by salinity with a correlation of -0.8 (R² = 0.91). The chlorophyll-a maintained a weak correlation of 0.32. Increase in SST accelerated the solubility of CO₂ from atmosphere to the sea, thereby increasing CO_{2,sea} concentration and increasing pCO_{2,sea}. There was no significant correlation between salinity and chlorophyll-a

Keywords: Partial pressure, Carbon dioxide, Temperature, Salinity, Chlorophyll-a, Polynomial regression.

Introduction

Sunda Strait has a water area of approximately 8,138 km² and a depth of about 80 m. Towards North of Java Island depth increases to about 1,575 m towards the Indian Ocean (Birowo, 1983). This can be seen by the expansion of a hotter mass of water to the south (Wirtky, 1962). Due to these characteristics, this area is interesting to observe its carbon dioxide in relation to physical and biological parameters.

The ability of sea to convert CO₂ gas into carbonate and bicarbonate ions allows the ocean to store carbon 50 times more than the atmosphere, where 90% of the amount of carbon stored in the ocean is affected by physical pumps and 10% by biological pumps (Zhu et al., 2009 in Adziima, 2016). According to Chen et al. (2016), the Partial Pressure of Carbon dioxide (pCO₂) in water is strongly influenced by oceanographic physical parameters, such as Sea Surface Temperature (SST), salinity, Mixed Layer Depth (MLD), and chlorophyll-a. The dynamics of seawater mass and the influence of monsoon and seasonal wind variations in the Sunda Strait can have an impact on SST and pCO₂. SST has a significant effect on pCO₂. When there is an increase in SST of 10°C, surface pCO₂ will increase by 4% (Takahashi, 1999 in Zhu et al., 2009).

SST can describe the level of salt and chemical conditions in sea water. Chlorophyll-a as a biological parameter can indicate the level of water fertility. In this research, the estimated pCO₂ from the relationship of SST, salinity and chlorophyll-a parameters around Mount Krakatau waters was obtained to generate an empirical model of pCO₂.

Materials and Methods

The study was conducted in the waters of Mount Anak Krakatau (Figure 1). The data collected in this study was part of research on a project on Impact of Volcanic Eruptions on Sea Fertility and Plankton Abundance on 11-12 September 2017 and 17-18 April 2018. Satellite data was used to estimate pCO₂ in Sunda Strait. CO₂, SST, salinity, and chlorophyll-a were measured using CTD, miniproceanus, refractometer, and water quality meter. Twenty-four samples were collected on 11-12 September 2017 and an equal number on 17-18 April 2018. All the data were combined for regression analysis. The regression equation was verified and tested by F-significance, p-value, student-t test, and analyzed with classic assumption test.

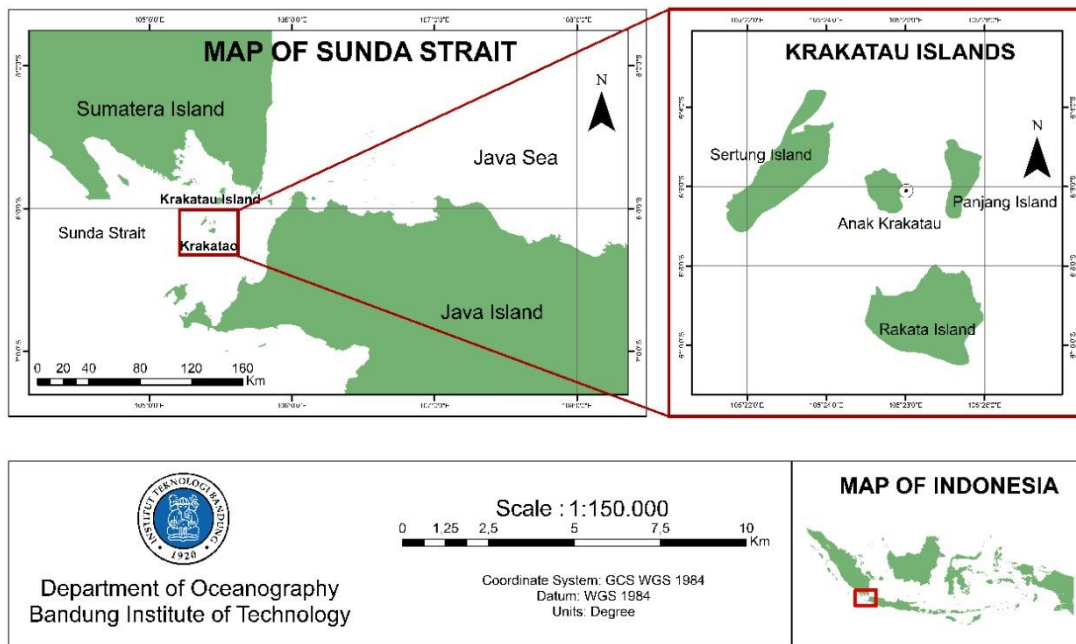


Figure 1. Mount Krakatau waters.

A model based on empirical equation was developed using the multivariate regression from the data collected in September 2017, April 2018 and a combination of the two. The pCO₂ parameter acted as the dependent variable (Y) while the SST, chlorophyll-a, and salinity as independent variables (X). The regression equation was as follows:

$$Y' = a + b_1X_1 + b_2X_2 + b_3X_3 + \dots + b_kX_k$$

Where, Y' = regression response variable, X = predictor variable, a = intercept

Results and Discussion

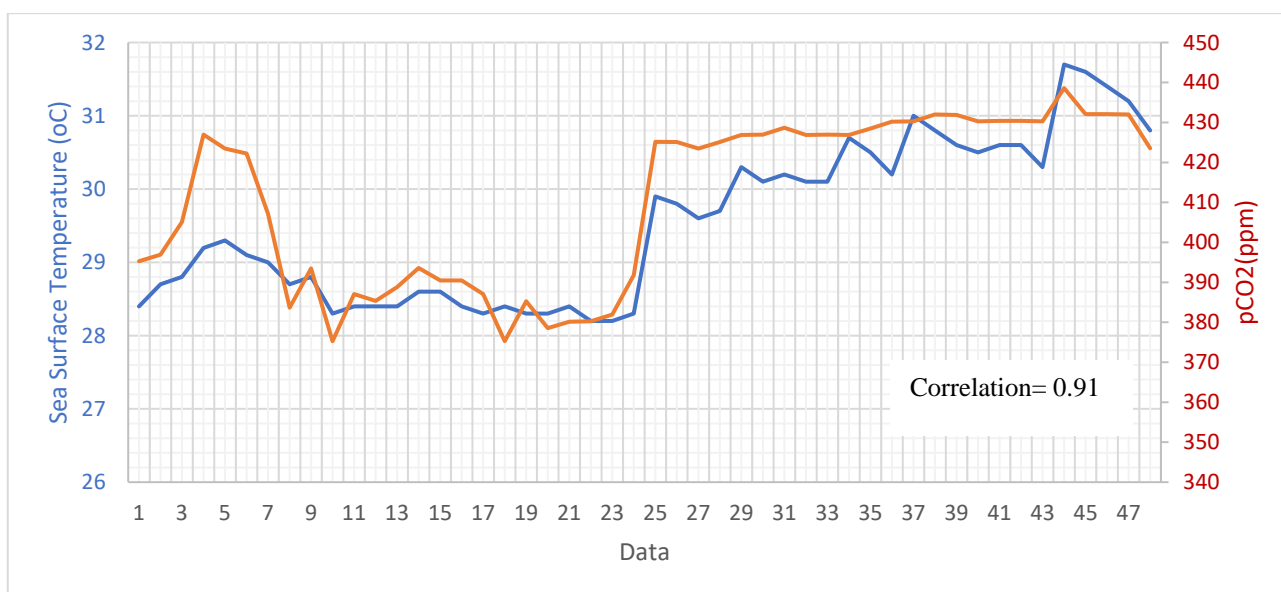


Figure 2. Relation between pCO₂ and SST based data collected on September 2017 and April 2018 (n= 48).

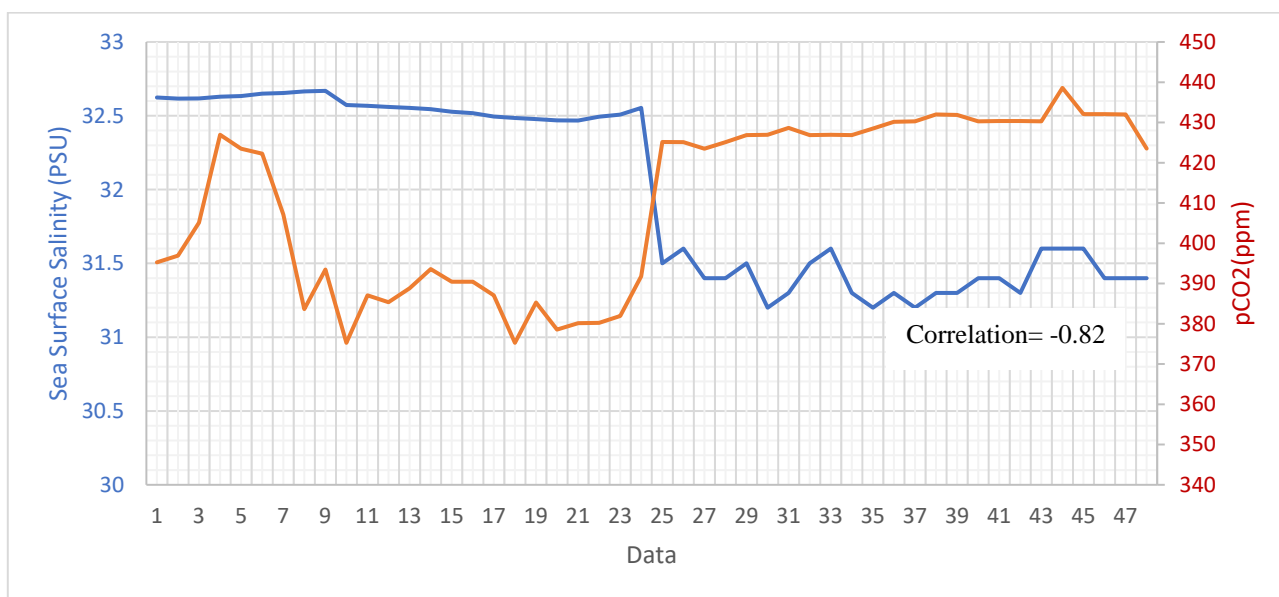


Figure 3. Relation between pCO₂ and salinity based on data collected on September 2017 and April 2018 (n= 48).

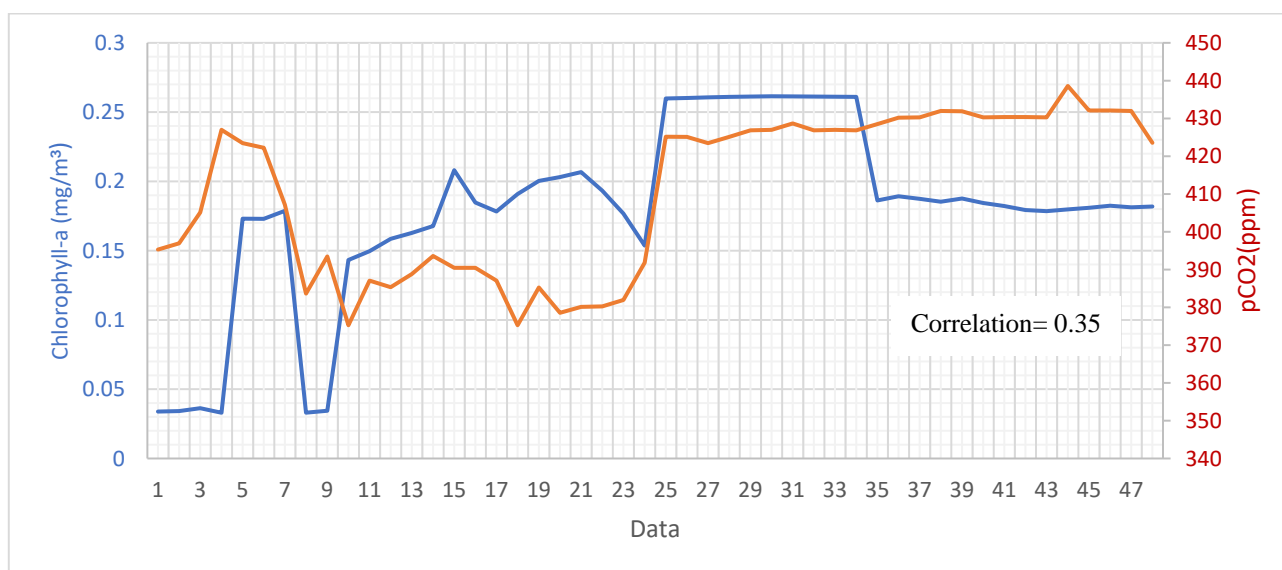


Figure 4. Relation between pCO₂ and Chlorophyll-a based on data collected on September 2017 and April 2018 (n= 48).

Correlation between SST and pCO₂ was high ($R^2 = 0.91$ (n = 48) as can be seen from Figure 2. This positive correlation indicates that pCO₂ seawaters have a comparable and strong relationship with SST. Increase in SST provides enough energy to accelerate the rate of reaction of the dissolution of H₂CO₃ in seawater and increase the concentration of CO₂, leading rise in pCO₂ in the sea (Zhu et al., 2009, in Adziima, 2016).

Figure 3. shows the relationship between pCO₂ and salinity ($R^2 = -0.82$) where, n = 48. Decrease in salinity

triggers an increase in pCO₂ and vice versa. This is in accordance with the study of Zhu et al (2009) and Adziima (2017) demonstrating a negative relationship of salinity with pCO₂. On the other hand, the relationship of pCO₂ with chlorophyll-a shows a positive correlation of $R^2 = 0.35$ (n = 48,) as shown in Figure 4. The chlorophyll-a pattern is weak. This is in accordance with William's statement (2011) which states that the influence of the biological pump only affects about 10% of the carbon cycle in the ocean.

Final Empirical Equation of pCO₂

This required assessing the best fit value of the regression - linear regression, polynomial order 2 and order 3, logarithmic and exponential models. The formula of pCO₂ was determined from value of root mean square error (RMSE) and correlation coefficient (r). The logarithmic equation so produced was assigned the name "Rohimat Model":

$$pCO_2 = -472.069 + 1044.043 \times \log(T) - 435.897 \times \log(S) - 5.03 \times \log(\log(Chl))$$

Where,

- pCO₂ = the partial pressure of CO₂ in the seawaters calculated (µatm)
- T = SST (°C)
- S = SSS (PSU)

Chl = Chlorophyll-a (mg/m³)

n = total number samples

P = p-value obtained from regression

Sig = the significance F value from the regression

Verification

The model was verified using combined data as shown in Figure 5 below. Verification results showed a correlation of 0.917 with an RMSE weighting of 8.34. This suggested the similarity with the situation in the field. This was supported by the relatively small RMSE value (<10). The model shows that the pCO₂ value in April 2018 was higher than in September 2017 due to the differences in SST in both the seasons. There was a transition season I (April 2018), where the SST was higher than in transition season II (September 2017). At that time the sun axis with earth shifted south to north and gave significant warming to the equatorial region.

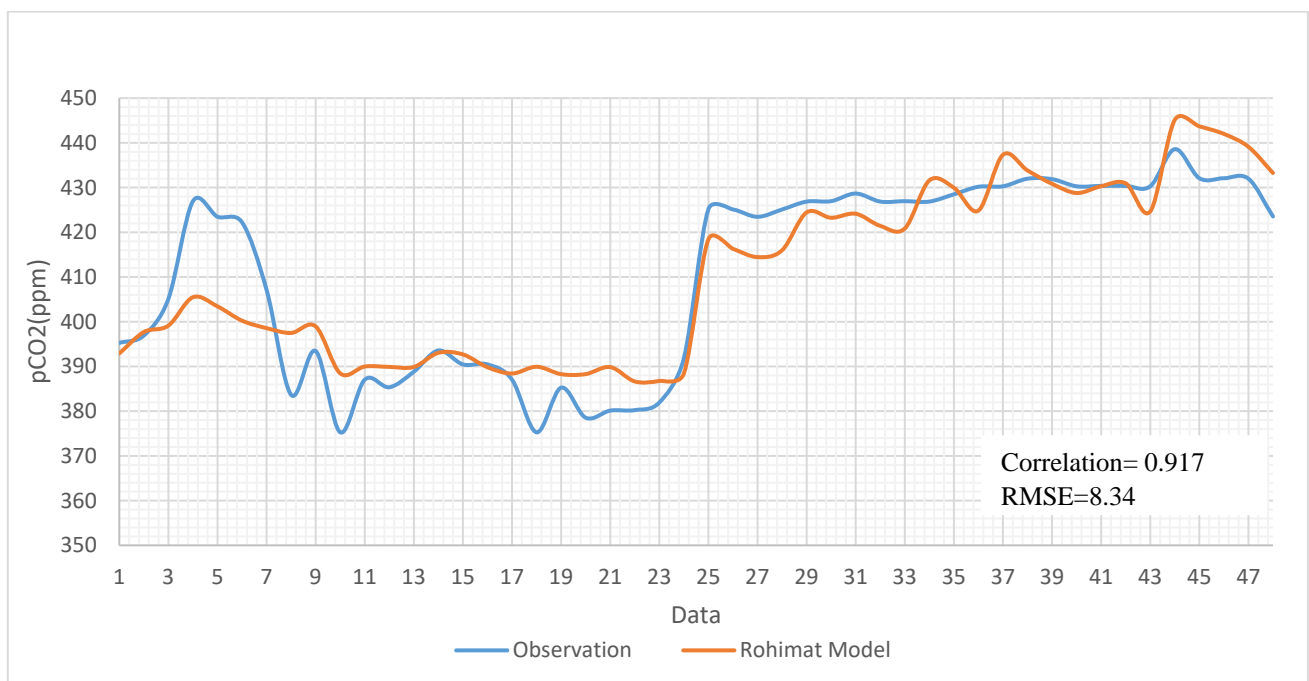


Figure 5. Comparison between observed data and Rohimat Model around the Anak Krakatau.

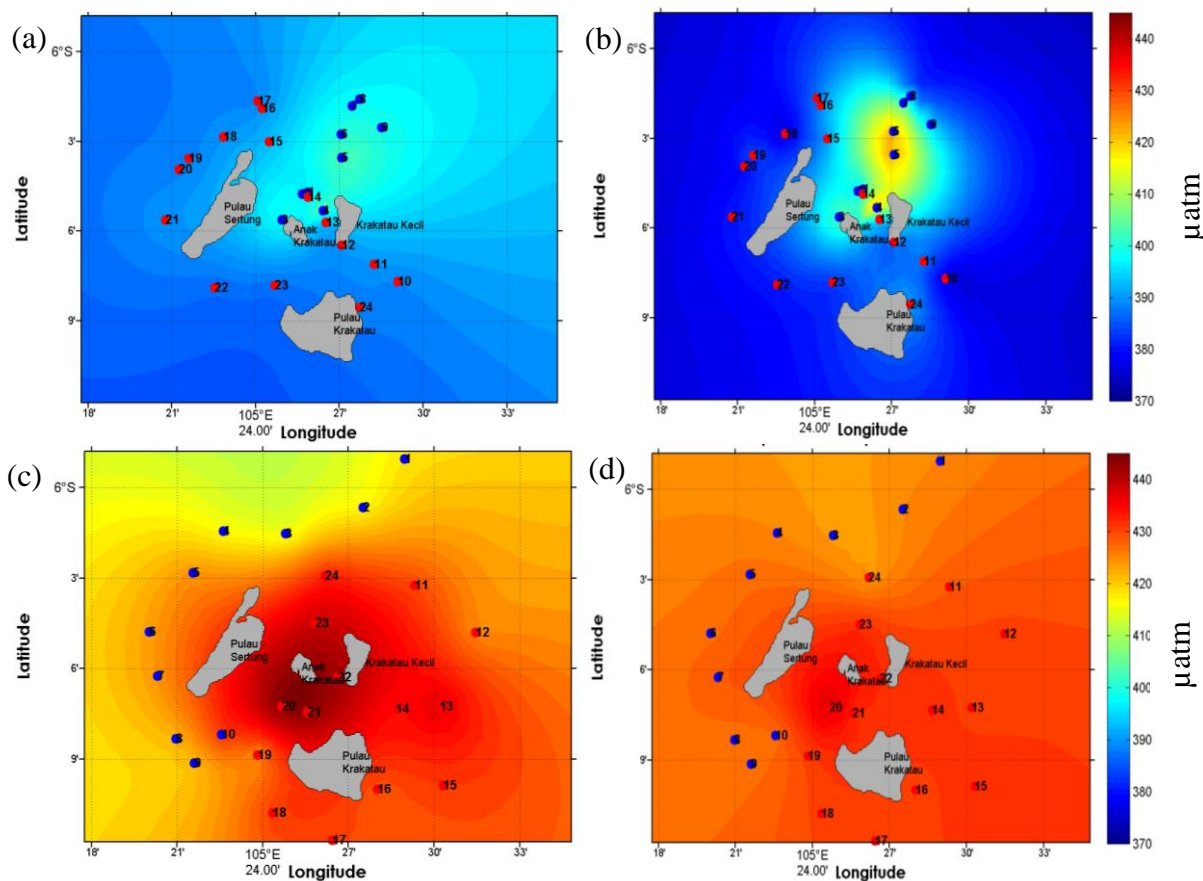


Figure 6. Comparison of pCO₂ distribution pattern between Rohimat Model (right) (a) 11-12 September 2017; (c) 17-18 April 2018 and observed data (right) (b) 11-12 September 2017; (d) 17-18 April 2018.

Figure 6 shows the comparison of pCO₂ from model with pCO₂ from field measurements. Data collected in September shows that the highest pCO₂ was 401 µatm in the northern part of Krakatau and the lowest 388 µatm in the southern part of Krakatau. There are also similarities in the actual pCO₂ data in the field and in September the highest pCO₂ was north of Krakatau. The range of pCO₂ values from the estimation model in September also has a range that is almost the same as the field pCO₂ at 388-401 µatm (field pCO₂ 375-426 µatm).

Estimation model results in April showed highest pCO₂ in the middle of Anak Krakatau Island, with value of pCO₂ about 444 µatm. These results also demonstrated similarities with the actual pCO₂ in the field. In April the highest pCO₂ value was in the middle of Krakatau, precisely south of Anak Krakatau Island. The range of values in the model pCO₂ with field pCO₂ were close to around 423-438 µatm for the field pCO₂ and 417-444 µatm for the pCO₂ model.

Comparison with previous models

Table 1. Model verification results with observation data.

No	Model	Correlation	RMSE
1	Model Rohimat (2018)	0.917	8.345
2	Zhu et al., (2009)	0.462	18.863
3	Zhai et al., (2005)	0.904	42.531
4	Dai et al., (2009)	-0.853	51.250
5	Hermawan (2016)	0.247	143.863

Table 2. Empirical equations of pCO₂ estimates from previous studies.

Research studies	Models
Rohimat Model (2018)	$pCO_2 = -472.069 + 1044.043 \log(T) - 435.897 \log(S) + 5.03(-\log(Chl))$
Zhu et al., (2009)	$pCO_2 = 6.31(T^2) + 61.9(K^2) - 365.85T - 94.41(Chl) + 5715.94$
Zhai et al., (2005)	$pCO_2 = 350 + 20e^{(0.0423(T-26))}$
Dai et al., (2009)	$pCO_2 = 27.607(S) - 2.632(T) - 428.586$
Hermawan (2016)	$pCO_2 = -3012.54 + 56.52(T) - 87.31(Chl) + 166.94(S) - 0.89(T^2) + 13.31(Chl^2) - 2.59(S^2)$

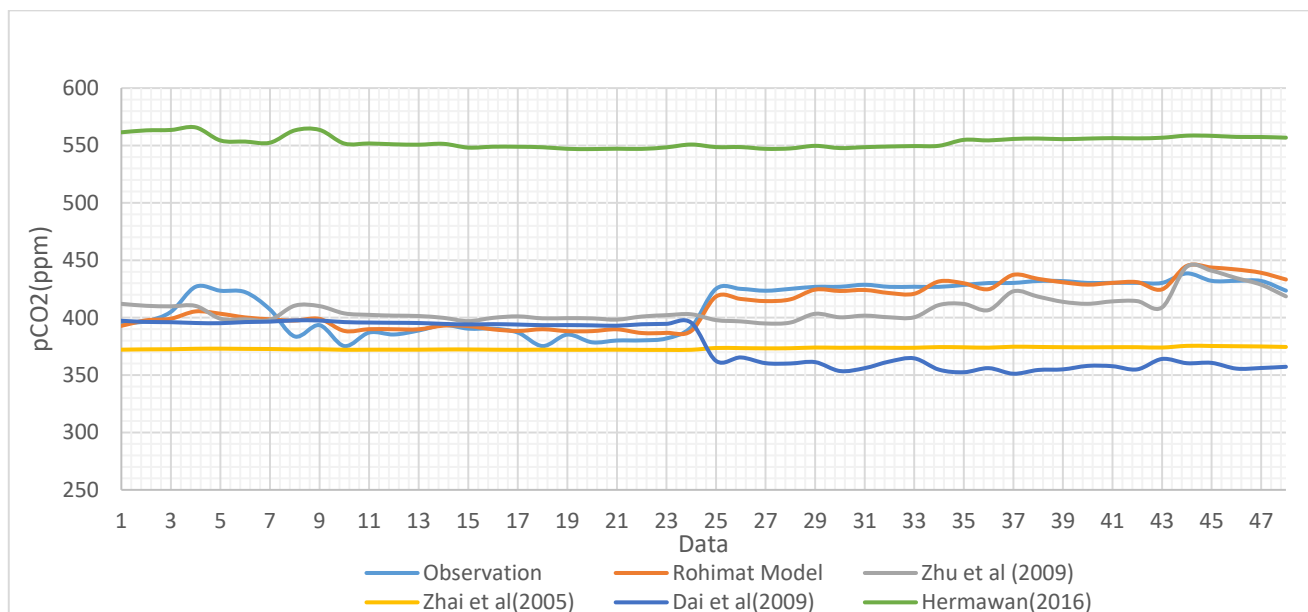


Figure 7. Comparison with previous models.

The model was compared with previous equation models suggested by Zhu et al. (2009), Zhai et al. (2005), Dai et al (2009) and Hermawan (2016) as shown in Table 2. The pCO₂ were estimated using SST, salinity and chlorophyll-a data from field measurements on 11-12 September 2017 and 17-18 April 2018 in Mount Krakatau waters, Sunda Strait. Comparison revealed that models produce a range of pCO₂ values between 350-350 μatm except using the Hermawan model (2016) which indicated that the value of pCO₂ was too high (Overestimate) - 550 μatm vulnerable (Figure 7).

Rohimat model has the highest correlation of 0.917 and the lowest error value of 8.345 (Table 1) following the calculation based on model of Zhu et al. (2009) with a correlation of 0.462 with RMSE 18.863. Calculations from the empirical model Zhai et al. (2005) showed a correlation of 0.904 but high RMSE value of 42.531. The model of Dai et al. (2009) presented a negative correlation value of -0.853 with RMSE 51.250 while the Hermawan model (2016) produces the lowest correlation of the six models (0.247) with a very high RMSE value of 143.86. It is apparent that using the combined verification of 48 sets of data in September and April, the calculation of the Rohimat model has a better correlation and a smaller RMSE value than the models from previous studies.

Conclusion

Models developed using the quantitative parameters described above provide fairly accurate results for field data with a correlation of 0.91 and RMSE 8.34. Models developed based on data collected in September produced a significant correlation of 0.86 but for April field data the value was 0.77.

Logarithmic equations for estimating the pCO₂ value related to SST, salinity and chlorophyll-a parameters yielded the following empirical equation:

$$pCO_2 = -472.069 + 1044.043x \log(T) - 435.897x \log(S) - 5.03x \log(\log(-Chl))$$

The results showed a strong relationship between the SST and pCO₂ with a correlation of 0.91, followed by salinity with a correlation of -0.82. Chlorophyll-a did not show any significant correlation as evident from the value of 0.32. Increase in SST accelerated the rate of reaction of CO₂ formation due to the dissolution of H₂CO₃ in seawater, thereby increasing the concentration of CO₂ and increasing pCO₂. Increasing salinity has a weak effect. Rise in salinity reduces the concentration of dissolved CO₂, thereby reducing pCO₂.

Acknowledgement

This research is part of the National Strategic Research, RistekDikti 2017-2018.

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