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Development of Total Suspended Solids (TSS) Algorithm Based on Visible Spectrum Reflectance of Sentinel-2 Imagery (Case: in Suwung Estuary, Bali)

I Made Yuliara[1*], Ni Nyoman Ratini[1], Winardi Tjahyo Baskoro[1], Hendrata Wibisana[2]

[1]Faculty of Mathematics and Natural Science, University of Udayana, Badung, Indonesia.
[2]Departement of Civil Engineering, University of Pembangunan Nasional "Veteran", Surabaya, Indonesia.

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Corresponding Author:
I Made Yuliara
imdyuliara@unud.ac.id

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Abstract: This study aims to develop and build a new algorithm model that is suitable for predicting the concentration and spatial distribution of total suspended solids (TSS) in the Suwung estuary in Bali based on the visible spectrum reflectance of Sentinel-2 imagery. A total of 20 water samples were taken at selected coordinates and the time coincided with the Sentinel-2 satellite recording the research location. The TSS concentration of the samples was measured in the laboratory (in-situ) and the bottom of atmosphere reflectance correction (ρ_{BOA}) used the dark object substaction (DOS) method. The development used regression and correlation of in-situ data with imagery. Three algorithm models, namely Budhiman (2014), Guzman & Santaella (2009), and Parwati (2014) were used as an approach to developing a new TSS algorithm (AlgoNew), resulting in the Parwati model as the best model (MAPE = 3.889%, RMSE = 0.386 and R2 = 0.816). The result of AlgoNew model development is $\mathrm{TSS}(mg/L) = 4.453 - 8.777 * \rho_{\mathrm{BOA(b2)}} - 29.839 * \rho_{\mathrm{BOA(b3)}} + 227.654 * \rho_{\mathrm{BOA(b4)}}$, where the MAPE is 3.315%, RMSE = 0.332 and R2 = 0.845. The analysis results show that AlgoNew has smaller errors, is more valid, has stronger correlations, and its implications are more representative and feasible to apply compared to Parwati's algorithm (2014).

Keywords: Algorithm development; Sentinel-2; Suwung estuary; Total Suspended Solids (TSS); Visible reflectance

Introduction

The mouth of the Badung River, Bali, namely the Suwung estuary is known as a supplier of clean water for the southern part of the island of Bali, which is a densely populated residential area and tourist destination. Therefore, attention to the provision of clean water is very important. Water quality parameters such as dissolved oxygen (DO), biological oxygen demand (BOD), chemical oxygen demand (COD), electrical conductivity (EC), total dissolved solid (TDS), turbidity , temperature, heavy metals (Pb, Fe) and total suspended solids (TSS), are microplastics that are harmful to health, actively contributing to the quality and ecosystem of waters in terms of physicochemical (Hendrawan et al., 2016; Hou et al., 2017; Rinawati et al., 2016; Yuliara et al., 2023; Al Fatih et al., 2025; Yusrizal et al., 2024; Zhang et al., 2023).

Turbidity caused by contaminant particles transported by TSS can interfere with light penetration into the water, thereby affecting the habitat of aquatic life and aquatic ecosystems (Mamun et al., 2022; Elvitriana et al., 2023; Supardiono et al., 2023; Yao et al., 2022). TSS concentration plays an important role in

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relation to the flux of water contaminants, which is often also referred to as suspended sediment concentration, which mostly includes seston minerals either from terrestrial sources or resuspension of settled material and is often also used to control sedimentation dynamics in water bodies (Dey & Vijay, 2021; Sagan et al., 2020; Butler & Ford, 2018; He et al., 2019).

Routine, comprehensive and sustainable water quality monitoring activities will become very important activities for more effective clean water management in the future. The use of manual or conventional methods carried out in the field provides accurate measurement results, but for large-scale studies it takes a relatively long time, is less efficient, not comprehensive, and is expensive (Gholizadeh et al., 2016; Novoa et al., 2017). An alternative method that is comprehensive, more effective, sustainable and real-time can utilize technology, namely remote sensing satellite technology. Remote sensing involves the collection of information, carried by electromagnetic radiation, about the Earth's surface or atmosphere (Rees, 2012).

Many developed countries since the 1970s have used remote sensing satellite technology products (imagery data), to monitor water quality (Gholizadeh et al., 2016). Since satellite remote sensing is a valuable and efficient tool for monitoring water quality at high temporal and spatial resolutions, many efforts have been made to accurately estimate TSS concentration from optical remote sensing data (Novoa et al., 2017; Yu et al., 2019; Balasubramian et al., 2020).

Many studies have used remote sensing satellite imagery data (SPOT, Landsat 8, Sentinel-2A, MODIS, Wordview 3) to monitor and provide assessments of water quality through water quality parameters in various regions in Indonesia (Hendrawan et al., 2016; Hodgkins et al., 2016; Bioresita et al., 2018; Wang et al., 2017; Liu et al., 2017; Sukmono, 2018; Hafeez et al., 2022; Indeswari et al., 2018; Kurniadin & Maria, 2020; Baktiar & Basith, 2020).

Several studies have used satellite imagery and applied various algorithm models to monitor and measure one of the water quality parameters such as TSS. The Purwati algorithm released in 2014 is the best algorithm of the 3 types of algorithms tested to analyze TSS concentration with Worldview 3 satellite imagery in Karimunjawa waters. The accuracy and error results stated by the Root Mean Square Error (RMSE) are 1.01 mg/L and the coefficient of determination is 5.95% (Baktiar & Basith, 2020). The Laili algorithm released in 2015 was applied to estimate TSS concentration based on Sentinel-2 imagery in the Porong River, Sidoarjo, and the estimation results were better when the reflectance variable value inputted into the algorithm was the Bottom of Atmosphere (BOA) reflectance value (Bioresita et al., 2018). For Sentinel-2, the BOA reflectance correction can be obtained by applying the Sen2Cor module that has been prepared by several image processing software (Bui et al., 2022). Indeswari et al. (2018) tested 5 types of TSS algorithms, namely the Syarif Budhiman algorithm released in 2004, Parwati released in 2006, Nurahida Laili in 2015, Guzman & Santaella in 2009, and the Jaelani algorithm in 2016 to map the distribution of TSS in the waters of the Porong River estuary, Sidoarjo using multitemporal Landsat-8 satellite imagery data in 2017 and in-situ data. From the results of this study, it was found that the Budhiman algorithm had the smallest Normalized Mean Absolute Error (NMAE) value, which was 19.53%, which proves and shows that the Budhiman algorithm is most appropriate in explaining the TSS concentration conditions in the Porong river estuary.

Maulana et al. (2015) applied the Van Hengel and Spitzer (VHS) algorithm to analyze the effect of TSS in determining the shallow sea depth of the Marina coast of Semarang city, and the results of the study obtained TSS concentrations ranging from 1 to 181 mg/L, a coefficient of determination (R^2) of 0.8669 and RMSE of 14.1668. Based on the description of several studies above, it can be said that not every TSS algorithm is suitable or appropriate if applied to a different research location. The accuracy of the measurement results on the processed imagery shown by the RMSE value is influenced by the type of remote sensing satellite imagery data used. Generally, methods for estimating TSS can be directly from remote-sensing reflectance or water-leaving reflectance (Hou et al., 2017; Novoa et al., 2017; Yu et al., 2019; Wang et al., 2017; Jiyah et al., 2017; Neves et al., 2021). Concentrations of TSS of surface waters are related to remotely-sensed reflectance via empirical calibration between in-situ-sampled TSS and reflectance in a MODIS band 1-equivalent wavelength window (Hodgkins et al., 2016).

This study aims to develop the existing TSS algorithm to build a new algorithm that is suitable, appropriate for estimating TSS concentrations in the Suwung estuary. The image data used is Sentinel-2 satellite imagery data and the development of the algorithm is carried out using the regression method which involves laboratory (in-situ) TSS concentration data and reflectance values in the visible spectrum corrected at BOA.

Method

The research location is in the Suwung estuary, Denpasar city, precisely in the South Denpasar sub-district which is located at coordinates 8° 43' 26" - 8° 44' 04" South Latitude and 115° 11' 16" -115° 11' 22" East

Longitude. There are 20 water samples taken at selected coordinate points and the time coincides with the passage of the Sentinel-2 satellite to record, take data at the research location. Measurement of TSS concentration of water samples in the laboratory (in-situ) using the Gravimetric method. The image data used is Sentinel-2 image data and the acquisition time is June 5, 2024. The stages of Sentinel-2 satellite image processing are carried out starting from converting raw images to reflectance values at the Bottom of Atmosphere (ρ_{BOA}); performing geometric, radiometric, atmospheric corrections using the DOS (Dark Object Subtraction) method; performing visible and near infrared spectrum image copping of the research area; continuing with image masking to separate land and water; applying 3 TSS algorithm models as shown in Table 1 which are used as an approach; and developing the algorithm. Statistical and descriptive analysis was conducted through validity and correlation tests using TSS regression tests from laboratory measurements (in-situ) against the results of the 3rd model of the approach algorithm and TSS from the development algorithm. The accuracy test was evaluated using the root mean square error (RMSE) and the average absolute error was analyzed using the mean absolute percentage error (MAPE) whose formula is presented in Equations (1) and (2), namely:

$$\mathrm{RMSE} = \sqrt{\frac{\left(X_{\mathrm{insitu}} - X_{\mathrm{prediction}}\right)^2}{n}} \quad (1)$$

$$\mathrm{MAPE} = \frac{1}{n}\sum_{1}^{n}\left|\frac{X_{\mathrm{prediction}} - X_{\mathrm{insitu}}}{X_{\mathrm{insitu}}}\right| \times 100 \quad (2)$$

Where: $X_{prediction}$ = TSS data from imagery
X_{insitu} = laboratory TSS data
n = number of data

The complete research stages are shown in Figure 1.

Table 1. Summary of 3 TSS concentration algorithm models

Name of algorithm	TSS algorithm model
Syarif Budhiman (2004), case study in the waters of Mahakam Delta, East Kalimantan.	TSS (mg/L) = 8.1429*exp(23.704*ρ_{B4})
Guzman & Santaella (2009) in Restele et al. (2022), case study in the waters of Mayaguez Bay, Puerto Rico.	TSS (mg/L) = 602.63*(0.0007*exp(47.755*ρ_{B4}))+3.1481
Parwati (2014) in Baktiar & Basith (2020)	TSS (mg/L) = 0.6211*(7.9038*exp(23.942*ρ_{B4}))*0.9645

Description: ρ_{B4} is the reflectance of band 4 (red).

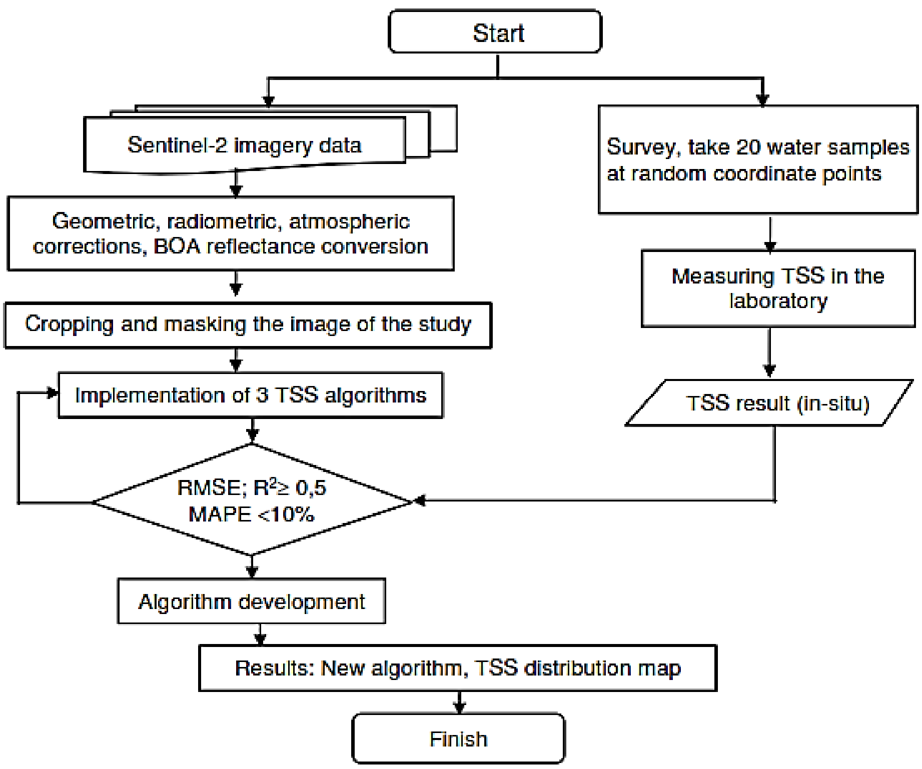
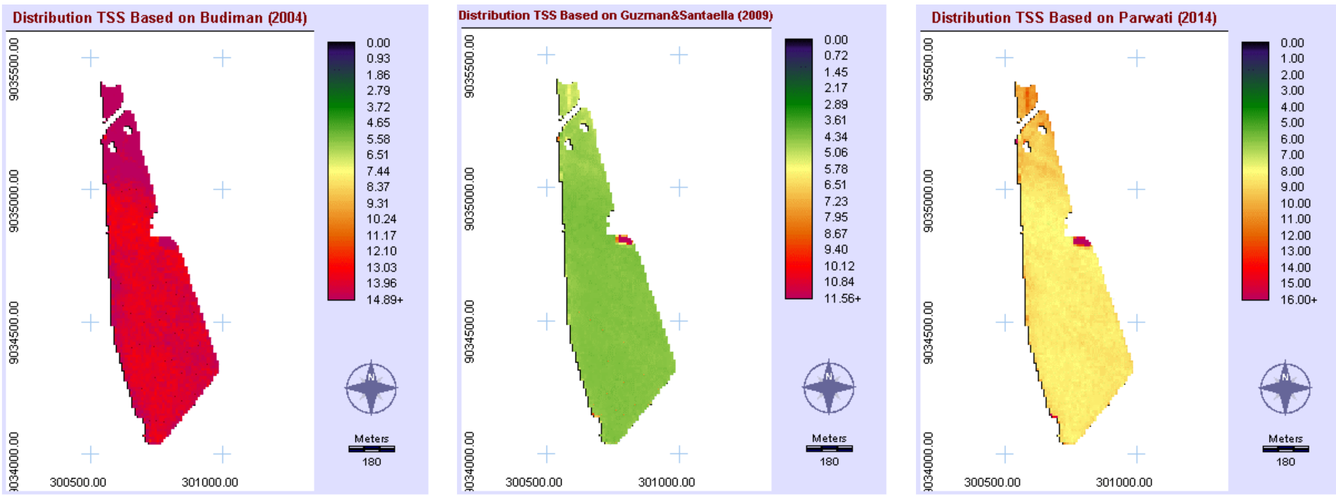


Figure 1. Research flow diagram

Result and Discussion

The resulting image of the application of 3 TSS equation models or algorithms as listed in Table 1 which is used as an approach to build a new algorithm on Sentinel-2 satellite imagery is presented in Figure 2. In this study, the measurement of TSS concentration in the processed image was carried out on pixels whose coordinate positions have been selected as observation points (OP). The number of water samples was 20 samples taken at the same time as the Sentinel-2 satellite passed over the research location area, namely June 5, 2024. The results of measuring water quality parameters representing TSS at 20 OPs on image pixels resulting from the application of 3 algorithm models as shown in Table 1 and also the results of laboratory tests (in-situ) are presented in Table 2.



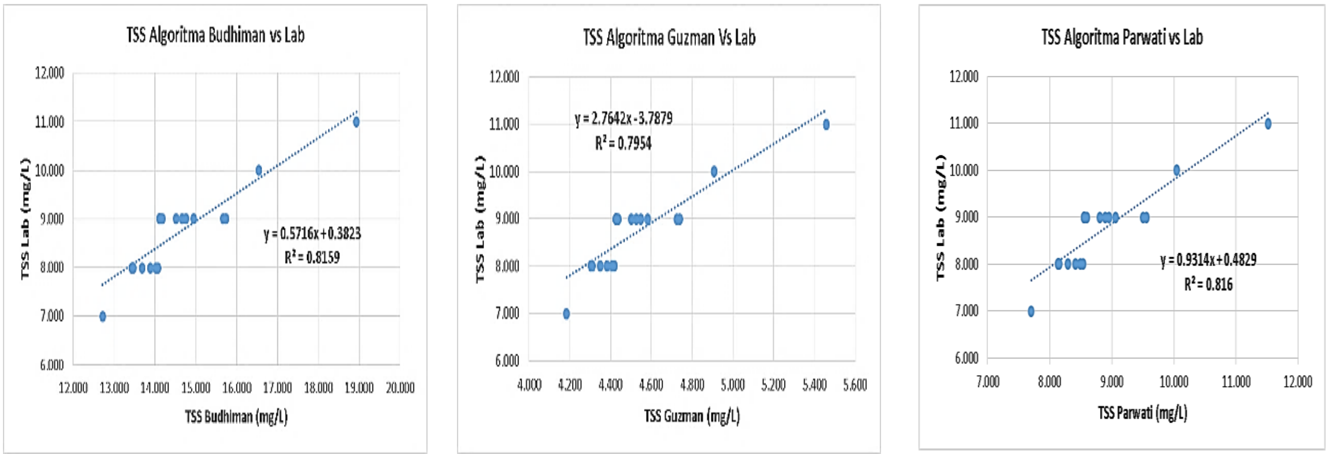
. (a) Budhiman (2004) (b) Guzman & Santaella (2009) (c) Parwati (2014)

Figure 2. TSS distribution image resulting from the application of 3 algorithm models

Table 2. Values of TSS concentration from 3 algorithm models and in-situ

OP	Concentration of TSS (mg/L)			
	Budhiman (2004)	Guzman & Santaella (2009)	Parwati (2014)	In-situ
1	13.427	4.304	8.136	8.000
2	14.113	4.425	8.555	9.000
3	14.939	4.581	9.061	9.000
4	14.113	4.425	8.555	9.000
5	13.685	4.349	8.293	8.000
6	13.881	4.383	8.413	8.000
7	14.013	4.407	8.494	8.000
8	15.664	4.724	9.506	9.000
9	13.459	4.309	8.155	8.000
10	14.519	4.501	8.805	9.000
11	14.079	4.419	8.535	8.000
12	16.542	4.907	10.044	10.000
13	18.935	5.457	11.512	11.000
14	13.472	4.304	8.136	8.000
15	12.715	4.183	7.699	7.000
16	14.113	4.425	8.555	9.000
17	15.739	4.739	9.551	9.000
18	14.763	4.547	8.953	9.000
19	13.427	4.304	8.136	8.000
20	14.113	4.425	8.555	9.000

The lowest TSS concentration from the in-situ results as seen in Table 2 is 7 mg/L and the highest is 11 mg/L. Then, the lowest TSS concentration results of the Budhiman algorithm are 12.715 mg/L and the highest are 18.935 mg/L, the lowest TSS concentration from the Guzman algorithm is 4.183 mg/L and the highest is 5.457 and from the Parwati algorithm the lowest is 7.699 mg/L and the highest is 11.512 mg/L. In general, the larger the in-situ TSS values, the larger the values generated by the algorithm. There is a relatively linear correlation across the TSS data. Linear calibration facilitates a wider range of TSS values than areal extent, especially pixel-by-pixel TSS values (Hodgkins et al., 2016). The increasing TSS values in this study convincingly reflect the overall increase in turbidity. The difference in TSS values that arise between the results of applying the 3 algorithm models used as an approach with the in-situ results is evaluated using MAPE and R^2. The best algorithm model (1 of 3 algorithm models) that produces the smallest difference value is selected to develop and build a new algorithm, which in this study uses the MAPE value requirement < 10% and $R^2 \geq 0.5$. The correlation graph of TSS in-situ measurements and 3 algorithm models is presented in Figure 3, while the results of MAPE calculations, and R^2 and correlation coefficient (R) are presented in Table 3.



(a) (b) (c)

Figure 3. Correlation graph of the results of TSS measurements using the algorithm and in-situ; a) Budhiman with Lab, (b) Guzman&Santaella with Lab and (c) Parwati with Lab

Table 3. Results of MAPE, R2 and R calculations for the three algorithm models

Model algorithm	MAPE (%)	R^2	R
Budhiman (1004)	67.50	0.8259 (81.59%)	0.9033
Guzman & Santaella (2009)	47.80	0.7954 (79.54%)	0.8919
Parwati (2014)	3.90	0.8160 (81.60%)	0.9033

From Table 3, when viewed from the correlation coefficient value, namely R, the three algorithm models analyzed correlate very strongly with the in-situ TSS results and from the R^2 value it expresses that the pixel values of the TSS image results from the three algorithm models can explain the in-situ TSS measurements well. The smallest MAPE value is produced by the Parwati (2014) algorithm compared to the other 2 algorithms, which is 3.9% where this value is < 10% as required in this study. The TSS Parwati (2014) algorithm is a development result that shows very good, accurate performance applied to single-band Landsat 8 images, namely the red band (band 4, wavelength 636 - 673 nm), and when applied to Worldview 3 (band 5, wavelength 630-690 nm) also shows good performance results, but if the number of water samples analyzed is very small, the correlation with image data is very weak (R^2 is small) (Baktiar & Basith, 2020). It can be emphasized again that, of the 3 algorithm models tested and used as an approach, the results of the Parwati (2014) algorithm show better results and meet the requirements, so the Parwati (2014) algorithm is chosen as an approach in developing a new TSS algorithm ($Algo_{New}$).

The development of the algorithm to build a new algorithm is carried out using the multiple regression method. As an independent variable is the visible spectrum reflectance of the Sentinel-2 image where this reflectance is in band 2, band 3 and band 4, while the dependent variable is the TSS value from in-situ measurements. From the regression analysis, the resulting multiple regression equation or model that expresses the TSS prediction on Sentinel-2 imagery is $Y = 4.453 - 8.777*B2 - 29.839*B3 + 227.6541*B4$ where the Y variable represents the new TSS value ($Algo_{New}$). Variable B2 is the BOA band 2 reflectance ($\rho_{BOA(b2)}$), variable B3 is the BOA band 3 reflectance ($\rho_{BOA(b3)}$) and

B4 is the BOA band 4 reflectance ($\rho_{BOA(b4)}$). The TSS Algo$_{New}$ algorithm is the result of TSS development involving all visible wave BOA reflectance of Sentinel-2 imagery, so that the form of the algorithm model can be written:

$$\mathrm{TSS(mg/L)} = 4.453 - 8.777 * \rho_{BOA(b2)} - 29.839 * \rho_{BOA(b3)} + 227.654 * \rho_{BOA(b4)} \quad (3)$$

The results of multiple regression analysis using IBM SPPS statistical software version 22 showed that the TSS prediction algorithm model developed was able to explain variance or dependent variables up to 84.448% (R^2), while the significance level of the algorithm model obtained was 1.06034 x 10^{-6}. This shows that the algorithm model built using the BOA reflectance value has a confidence level of up to above 99%, meaning that the prediction error rate using the model built is less than 1.06034 x 10^{-4}%. The regression coefficients for the independent variables B2 (Blue) and B3 (Green) reflectance each have a negative effect of -8.777 and -29.839 on the Algo$_{New}$ model, while the coefficient for the B4 (Red) reflectance variable has a positive effect of 227.6541. The coefficient value of 227.6541 shows that the contribution and influence of B4 reflectance is very large in building Algo$_{New}$ to predict TSS. The TSS algorithm based on linear regression results obtained from the correlation of B4 band reflectance of Sentinel-2 images with in situ TSS measurement results is a good and fairly accurate algorithm for evaluating TSS concentration predictions (Restele et al., 2022). The results of the statistical analysis also show that the P value representing the smallest prediction error probability is owned by B4 which is 2.24 x 10^{-5}% and the largest is owned by B2 which is 81.342%. Statistically, it can be seen that the probability of prediction error caused by a single variable (B2 and B3) is quite large (> 20%).

In general and actually, the algorithm model built using the BOA reflectance value is quite acceptable considering that, in addition to the influence of other factors that cannot be controlled when the satellite is recording or acquiring data in the research area (such as weather for example), there is also a multi-collinearity condition between the variables of the three bands that commonly occur in multispectral images. To overcome this, it can be done with a principal component analysis (PCA) transformation on all bands used in building a new algorithm (Rees, 2012).

The results of the TSS value calculation using the Algo$_{New}$ algorithm and the Parwati algorithm and in-situ measurement data are presented in Table 4. The evaluation of the Algo$_{New}$ model and its level of accuracy are determined by calculating the RMSE and validation of the Algo$_{New}$ TSS algorithm measurements against in-situ data. The results are presented in Table 5.

Table 4. Values of TSS from AlgoNew, Parwati (2004) and in-situ

OP	TSS (mg/L)		
	Algo$_{New}$	Parwati (2004)	In-situ
1	8.085	8.136	8.000
2	8.504	8.555	9.000
3	9.109	9.061	9.000
4	8.583	8.555	9.000
5	8.225	8.293	8.000
6	8.281	8.413	8.000
7	8.333	8.494	8.000
8	9.413	9.506	9.000
9	7.977	8.155	8.000
10	8.720	8.805	9.000
11	8.552	8.535	8.000
12	9.972	10.044	10.000
13	11.126	11.512	11.000
14	8.092	8.136	8.000
15	7.443	7.699	7.000
16	8.502	8.555	9.000
17	9.171	9.551	9.000
18	8.775	8.953	9.000
19	8.412	8.136	8.000
20	8.718	8.555	9.000

Table 5. RSME, MAPE and R2 values of the Parwati and AlgoNew algorithm models

Algorithm models of TSS		RSME	MAPE (%)	R^2
Parwati:	TSS (mg/L) = 3.3238*e(34.099*ρ_{B4})	0.386	3.889	0.816
Algo$_{New}$:	TSS (mg/L) = 4.453 – 8.777*$\rho_{BOA(b2)}$ – 29.839*$\rho_{BOA(b3)}$ + 227.654*$\rho_{BOA(b4)}$	0.332	3.315	0.845

Of the 2 algorithm models analyzed and validated, the results of which are shown in Table 5, statistically the newly built algorithm (Algo$_{New}$) is more representative and suitable compared to the Parwati algorithm to be applied in predicting TSS distribution in the Suwung estuary. The application of 2 different TSS algorithm models in the same study area gives different prediction results and likewise, 1 TSS algorithm model if applied in different areas will give different prediction results when validated with in-situ measurements (Kurniadin & Maria, 2020). Increasing the accuracy of the prediction of measurement results from the algorithm can be done by selecting a more appropriate atmospheric correction method. The Sen2Cor atmospheric correction method provides a higher reflectance value than the DOS method, especially in the visible spectrum and the correction at top of atmosphere (TOA) always outperforms BOA in terms of a higher determination coefficient (Ginting et al., 2024; Medina, 2020). The prediction of TSS spatial distribution based on the TSS $Algo_{New}$ algorithm is presented in Figure 4.

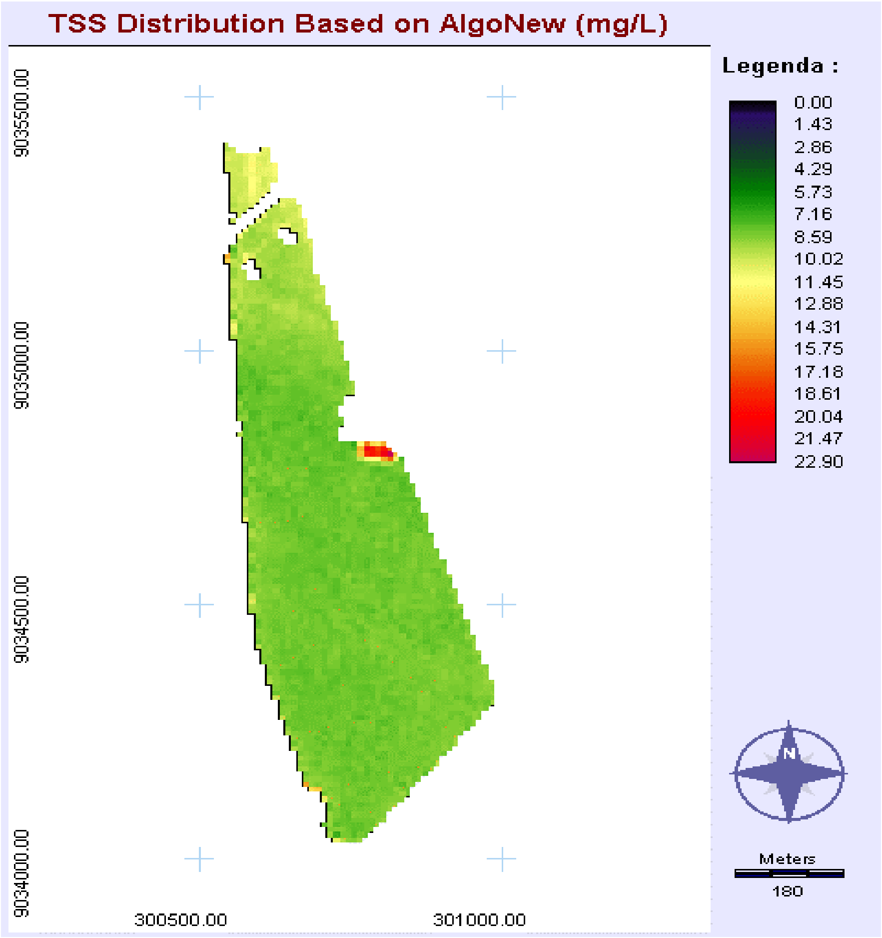


Figure 4. Predicted image of TSS distribution using the AlgoNew algorithm model

Conclusion

The new TSS algorithm ($Algo_{New}$) which is the result of the development of this research has a mathematical form: $TSS(mg/L) = 4.453 - 8.777 * \rho_{BOA(b2)} - 29.839 * \rho_{BOA(b3)} + 227.654 * \rho_{BOA(b4)}$. The error value accuracy validated using in-situ data is MAPE = 3.315%, RMSE = 0.332 and R^2 = 0.845 or 84.5% where these results indicate that the $Algo_{New}$ algorithm has a smaller error, is more valid and has a stronger correlation than the existing algorithm (Parwati (2014) algorithm), so it is more representative and suitable for application in predicting the distribution of TSS in the Suwung estuary.

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Author Contributions

Conceptualization, I.M.Y. and N.N.R.; methodology and conductor of experiment, W.T.B.; data analyzer and data visualization, H.W.

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Conflicts of Interest

The authors declare no conflict of interest.

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