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A Comparative Accuracy of Regularized and Tension Spline Methods to Estimate and Model the Surface Water pH of Pulau Tuba, Langkawi, Kedah

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ABSTRACT

This research is conducted to assess the accuracy of spline interpolation methods to predict and model the surface water pH of Pulau Tuba, Langkawi, Kedah, Malaysia. *In-situ* sampling activities using pH-meter and Geographic Positioning Systems (GPS) were carried out during high tides and at noon in November 2018. The development of spatial models was constructed using Regularized and Tension spline methods. Then, validation of models was carried out to compare the observed and predicted values of pH using correlation analysis, regression analysis, and error analysis. The accuracy of the developed map was calculated using the overall accuracy equation. This research found that the regularized spline method had more accuracy in estimating surface water pH variability than the tension spline method. Pearson correlation coefficient (r), Coefficient of determination (R^2), Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) were reported at 0.896, 0.803, 0.0265 and 0.0344 for the regularized spline method,

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respectively. The developed spatial model was then transformed into a map by adding map elements such as legend, title, north arrow, and scales for effective visualization. The developed map has an accuracy of 87.50%. The surface water pH was found at the range of 7-8. Low reading of pH is expected due to the addition of rainwater to the coastal water of Pulau Tuba, Langkawi, Kedah. The research outcomes would benefit government and non-government agencies to monitor the coastal and ocean acidification and the development of strategic policies and rules to reduce the impact of anthropogenic activities and climate changes for this area.

Keywords: *pH, Pulau Tuba, Spline, GIS, Interpolation*

INTRODUCTION

Increasing public perception of global warming phenomena has become a major concern in many geographical areas [1]. Delicate but complex ecologies such as coastal and estuarine areas should be sustained effectively and efficiently as there are many social and economic activities carried out in these areas [2]. The impacts of global warming have a significant effect on ocean acidification and the global food chain [3]. The climatic changes over the years have been studied by environmentalists and scientists to monitor the changes in ocean pH to sustain the coastal and marine resources [4]. Tourism areas especially Pulau Langkawi, consist of valuable marine resources and increasing revenue is expected due to the opportunity in tourism activities and social-economic interests [5].

Increasing anthropogenic activities in Pulau Langkawi, Kedah, has a great potential to expose its coastal and marine water to various contamination that could affect its marine ecosystem in the short term and long-term perspective. Human activities such as sewage discharge and land use can cause degradation of surface water quality [6]. To date, research on ocean acidification and climate change effects in Pulau Langkawi, Kedah are limited [7].

One way of understanding the variability of pH in water is by using the Geographic Information System (GIS). GIS provides many applications to help users to model and map the attribute data and visualize the geo-data efficiently especially when dealing with environmental modelling and sciences. One way of mapping and visualizing the water pollutants in the study area is by using a spline mathematical model [8]. The spline tool interpolates known values using a mathematical function that minimizes the overall surface curvature by producing a smooth surface that passes exactly the input points [9]. Researchers used the spline interpolation method to generate a model that exhibits gently varying surfaces such as pollution concentration [10].

Based on the query using Scopus, Web of Science and other journal search engines, there has been no model of pH developed for Pulau Tuba, Langkawi, Kedah using spline interpolation methods. Thus, a study is required to address the research gap to develop baseline data on water

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pH to monitor its effects toward marine life in Pulau Tuba, Langkawi, Kedah. The research questions that were developed for this research are (1) could the regularized and tension spline methods able to estimate the pH level and (2) which of the methods has a minimal error in estimating the pH level.

The aim of this research is to compare the accuracy of spline interpolation methods to estimate and model the surface water pH over coastal water of Pulau Tuba, Langkawi, Kedah. To achieve the aim of this study, several objectives are outlined: (1) to estimate the pH level using regularize and tension spline methods and (2) to compare the accuracy of regularized and tension spline to estimate the pH level.

This research is significant for the government and non-government organization to monitor the coastal water of Pulau Tuba and Pulau Dayang Bunting, Langkawi. Langkawi Development Authority (LADA) for instance, can use this information to formulate sustainable eco and marine tourism in these areas. The Department of Environment (DOE, Malaysia) can also help to plan an efficient rule or act to control point source and non-point source of pollution that may affect these locations. Fisheries Research Institute (FRI) and Department of Fisheries (DOF) may help local operators of marine culturist and fishermen to increase their catch and revenue by efficiently selecting areas that are not polluted by extreme pH readings.

EXPERIMENTAL

Description of Study Area

Pulau Tuba is situated in the southern part of the main island of Pulau Langkawi, Kedah. Pulau Tuba is remarkably closed to Pulau Dayang Bunting. The strait between both islands is surrounded by a complex mangrove ecosystem that houses many marine and coastal communities [11]. Varied species of mangrove can be found and have been reported along the strait between both islands [12]. Collection of villages can also be observed along the coastal line such as community of Kampung Selat Bagan Nyior etc. In term of potential sources of marine pollution, human activities such as boating, mariculture and surface runoff from agriculture farming can be expected. This island is chosen because of its increasing popularity among tourism and business players and the importance of the coastal and mangrove communities that flourish in these areas that required sustainable protection and monitoring plans.

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Sampling Area and Sampling Design

In this research, the coastal water and the strait of Pulau Tuba are chosen as sampling areas. A total of 40 sampling points denoted as SP01 – SP40, have been planned and distributed randomly. The pH reading was performed using a pH-meter and the sampling activities were carried out during high tide and at noon. Sampling activities were carried out twice during the monsoon seasons (the first week and the third week of November 2018). The first sampling data was used to develop the spatial model while the second sampling data was used to validate the developed models. The sampling design follows the research conducted by [7]. Figure 1 shows the sampling area and sampling points established for this research.

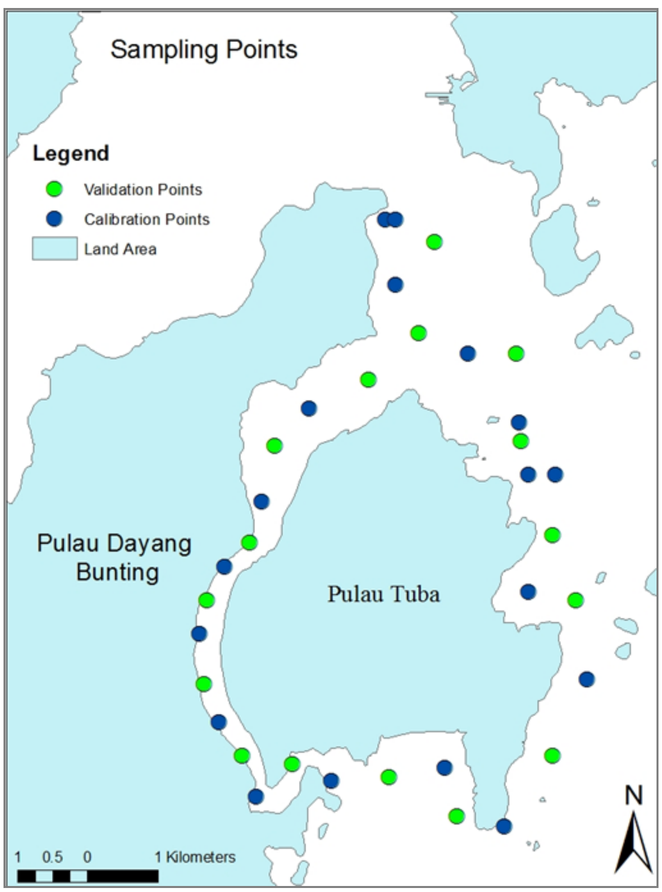

Figure 1: A total of 34 sampling points were established over the coastal water of Pulau Tuba

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Sampling Procedure

Handheld pH-meter was used to read the pH level of the surface water. The sensor is lowered under the surface water at 1 meter. For every point, 3 replications were taken to avoid bias. Prior to using the instrument, the pH meter was calibrated carefully. The data presented in this research has been converted into the mean (average) reading of pH. The data were then transferred into the excel worksheet. During the first sampling activities, a total of 20 sampling points was sampled, however, pH readings of 18 sampling points are used for this research. During the second sampling activities, a total of 16 out of 18 sampling points were extracted and valid to be used. The invalid reading of pH was rejected to avoid outlier during model development and validation stages. Outliers were determined using literature analysis and reading of pH at other sampling areas. Figure 2 shows the overall methodology in the form of a flow chart.

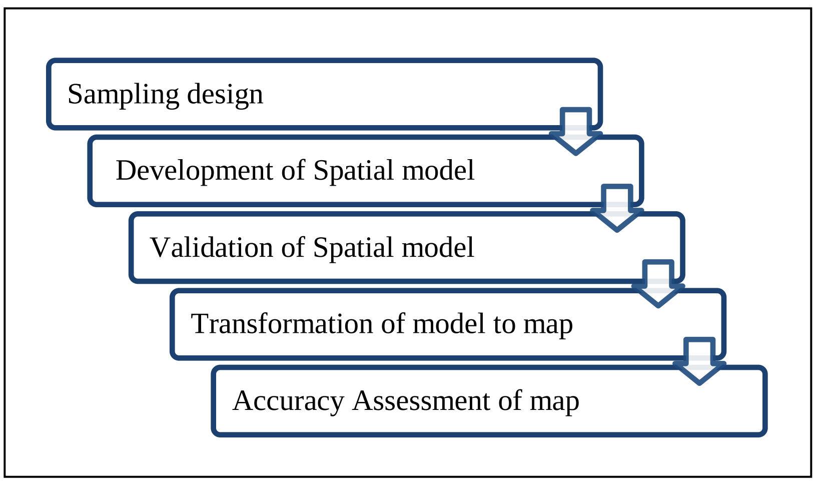

Figure 2: Flow chart of developing and validating model of surface water pH

Development of Spatial Model

Spline tool from ArcGIS version 10.1 was used to generate spatial models. 2 methods of spline interpolation methods: regularized and tension spline were employed with the default weight is 0.1. The developed spatial model is stored as a shapefile for further use. The mathematical equations of spline (A), tension spline (B) and regularized spline (C) are explained in Equation 1 until 5 [13].

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A. Splines Equation

$$S(x,y) = T(x,y) + \sum_{j=1}^{N} \lambda j\, R(r_j) \quad (1)$$

Where:

J =1,2, ……… N
N =Number of points
λj =Coefficients found by the solution of a system of linear equations.
r_j =Distance from the point (x, y) to the jth point.

B. Tension Spline Method

$$T(x, y) = a_1 \quad (2)$$

Where:

a_1 = coefficients found by the solution of a system of linear equations.

And,

$$R(r) = \frac{1}{2\pi\varphi^2}[1n\left(\frac{r\varphi}{2}\right) + c + K_o(r\varphi)] \quad (3)$$

Where:

φ^2= Weight parameter
K_o=Modified Bessel function
C=constant equal to 0.0577215

C. Regularized Spline Method

$$T(x, y) = a_1 + a_2x + a_3y \quad (4)$$

Where:

a_1 = coefficients found by the solution of a system of linear equation.

And,

$$R(r) = \frac{1}{2\pi}\{\frac{r^2}{4}\left[1n\left(\frac{r}{2\pi}\right) + c - 1\right] + \tau^2\left[K_o\left(\frac{r}{\tau}\right) + c + 1n\left(\frac{r}{2\pi}\right)\right]\} \quad (5)$$

Where:

r = Distance between the point and the sample, τ^2= Weight parameter and K_o=Modified Bessel function.

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Validation of Model

Validation of spatial models was carried out using correlation analysis, regression analysis and error analysis. For correlation and regression analyses, Pearson correlation coefficient and coefficient of determination were used, respectively. For the error analysis, Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) were applied to the spatial model to indicate error between the observed and predicted pH value. The equations for each statistical analysis were explained in Equation 6 until 9.

A. Pearson correlation coefficient, r

$$r = \frac{\sum_{i=1}^{n} (x_i - \underline{x})(y_1 - \underline{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \underline{x})^2 \sum_{i=1}^{n} (y_i - \underline{y})^2}} \quad (6)$$

Where:

$\underline{X}$ and $\underline{Y}$ are the sample means of x_i and y_i.

B. Coefficient of determination, R^2

$$R^2 = r^2 \quad (7)$$

Where:

r = Pearson correlation coefficient

C. Mean Absolute Error, MAE

$$Mean\ Absoulte\ Error\ (MAE) = \frac{1}{n}\sum_{j=1}^{n} |y_j - \hat{y}_j| \quad (8)$$

Where:

y_j is the observed value and $\hat{y}_j$ is the predicted value.

D. Root Mean Square Error, RMSE

$$Root\ Mean\ Square\ Error\ (RMSE) = \left[\sum_{i=1}^{N} (z_{fi} - z_{0i})^2 / N\right]^{\frac{1}{2}} \quad (9)$$

Where:

z_{fi} is the observed value and z_{0i} is the predicted value.

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Evaluation of Model

A robust interpolation model should yield [7]:

- The positive and strong correlation between the observed and predicted value.
- High percentage of variation in the observed value that the predicted value could explain.
- Minimal error between the observed and predicted value.

The Transformation of a Spatial Model into a Spatial Map

The chosen spatial models are transformed into spatial maps. Map elements such as title, legend, scale, and north arrow were inserted into the model for effective presentation and communication.

Map accuracy assessment

The map accuracy assessment was carried out to determine the precision of the developed map. Comparison between the predicted and the observed pH readings was carried out. The research used the Overall Accuracy (OA) which reported the accuracy in percentage form as described in the Equation 10.

$$Overall\ Accuracy\ (OA) = \frac{Number\ of\ Correct\ Occurrences}{Total\ Occurrences} \times 100\% \tag{10}$$

RESULTS AND DISCUSSION

Spatial models developed using regularized and tension spline were successfully developed. Figure 3 shows the spatial interpolation of pH developed using regularized spline method (left) and tension spline method (right). The range of estimated pH interpolated by regularized and tension spline methods was projected at 7.41532 – 8.06038 and 7.57234 – 8.05068, respectively. The black colour represents the lowest value while the white signifies the highest value of estimated pH level. Both images show rather similar patterns generally. The bottom left corner of the images indicated the highest reading of estimated pH while the top-right corner shows the lowest reading of estimated pH levels.

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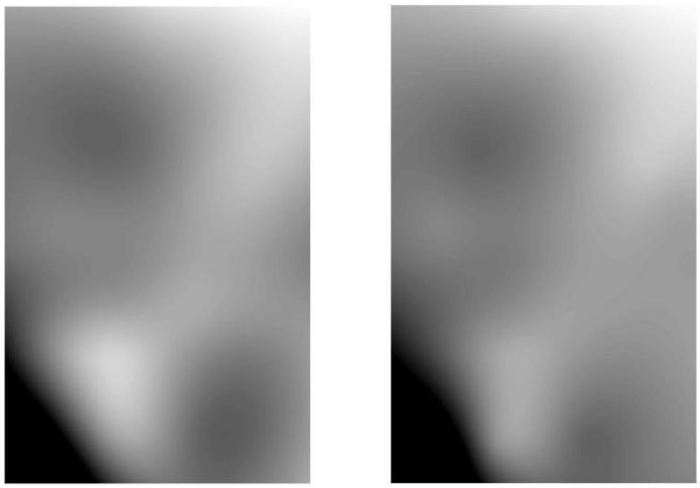

Figure 3: Spatial interpolation of pH developed using regularized spline method (Left) and tension spline method (Right)

The research found that the regularized spline method overestimated the level of pH at SP002, SP004, SP006, SP008, SP012, SP014, SP016, SP018, SP028 and SP032. The method also underestimated the level of pH at SP010, SP020, SP024 and SP030. Regularized splines had been estimated correctly at SP022 and SP026. Overall, the spline regularized method recorded 62.5%, 25% and 12.5% of overestimated, underestimated, and correct value of pH, respectively. Conversely, the research found that that the tension spline method overestimated the level of pH at SP002, SP004, SP006, SP008, SP012, SP014, SP016, SP018, SP026, SP028 and SP032. The method also underestimated the level of pH at SP010, SP020, SP022 and SP024. The tension spline method was estimated correctly at SP030. Overall, the spline regularized method recorded 68.75%, 25%and 6.25% of overestimated, underestimated, and correct value of pH, accordingly. Table 1 shows a list of observed and predicted values of pH estimated by both methods.

A Pearson product-moment correlation coefficient was computed to assess the correlation between the observed and predicted value of pH based on regularized and tension spline methods at 2-tailed correlation analysis (alpha =0.05). For estimation made by regularized spline method, there was a positive correlation between the 2 variables, $r = 0.896$, $n = 16$, $p < 0.001$. On the other hand, for the prediction made by tension spline method there was a positive correlation between the 2 variables, $r = 0.877$, $n = 16$, $p < 0.001$. Overall, there was a strong, positive correlation between the observed and predicted value of pH for both methods. Increases in observed pH value were correlated with increases in predicted pH value. Table shows the correlation analysis among the observed and predicted pH values. Further analysis using *Kendall's* Tau and Spearman's rank correlation coefficient also indicate significant positive correlations. Table 2 shows the correlation coefficient tabulated using Pearson correlation, *Kendall's* Tau and Spearman's rank correlation at 2-tailed significance.

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Table 1: The list of observed and predicted values of pH estimated by regularized and spline method

No	Sampling Point	Observed Value (unit)	Predicted Value (unit)	
			Regularized Spline	Tension Spline
1	SP002	7.98	8.02	8.01
2	SP004	7.95	7.96	7.96
3	SP006	7.97	8.01	8.01
4	SP008	7.91	7.92	7.92
5	SP010	7.96	7.93	7.93
6	SP012	7.92	7.93	7.93
7	SP014	7.86	7.88	7.88
8	SP016	7.78	7.80	7.80
9	SP018	7.70	7.74	7.73
10	SP020	7.94	7.88	7.85
11	SP022	7.96	7.96	7.95
12	SP024	7.96	7.91	7.91
13	SP026	7.93	7.93	7.94
14	SP028	7.94	7.96	7.96
15	SP030	7.96	7.95	7.96
16	SP032	7.92	7.99	7.99

Table 2: Correlation coefficient tabulated between the observed and predicted pH value.

			Observed pH	Predicted Regularized pH	Predicted Tension pH
Pearson Correlation	Observed pH	Correlation Coefficient	1	0.896**	0.877**
		Sig. (2-tailed)		0.000	0.000
		N	16	16	16
Kendall's tau_b	Observed pH	Correlation Coefficient	1.000	0.578**	0.555**
		Sig. (2-tailed)		0.003	0.004
		N	16	16	16
Spearman's rho	Observed pH	Correlation Coefficient	1.000	0.689**	0.672**
		Sig. (2-tailed)		0.003	0.004
		N	16	16	16

**Correlation is significant at the 0.01 level (2-tailed).

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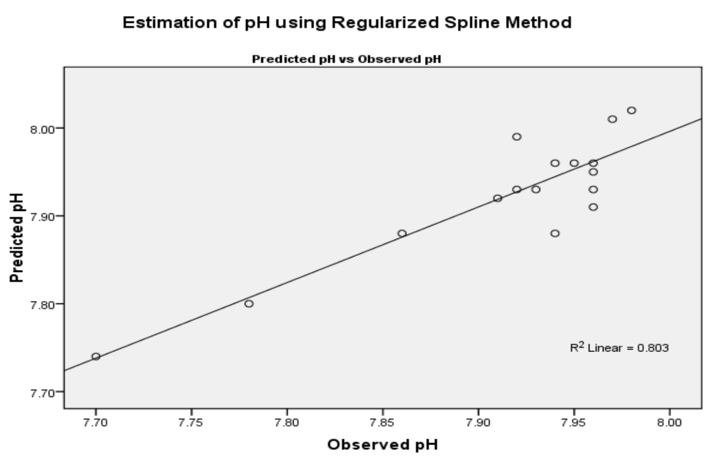
A simple linear regression analysis was used to predict the relationship between the observed and predicted values of pH based on the regularized and tension spline methods at 95% confidence level. Prediction value of pH estimated by the regularized spline method did explain a significant amount of variance in the observed value of pH, F (1,14) =56.958, p <0.001, R^2= 0.803, $R^2_{adjusted}$= 0.789 (Figure 4A). Similarly, prediction value of pH estimated by the tension spline method did explain a significant amount of variance in the observed value of pH, F (1,14) =46.453, p <0.001, R^2= 0.768, $R^2_{adjusted}$= 0.752 (Figure 4B). A simple scatter plots with a regression line between the predicted and observed pH reading produced by both methods were shown in Figure 4.



(B)

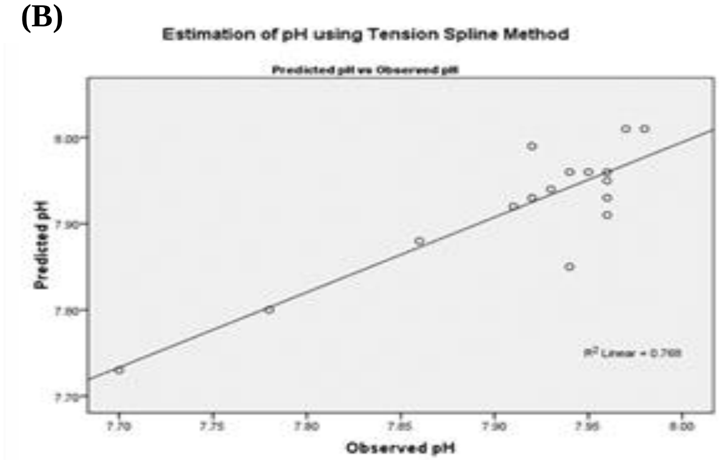


Figure 4: A regression line between predicted (A) and observed pH (B) estimated using regularized spline and tension spline method.

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For the regularized spline method, the regression coefficient (*B*= 0.933) indicated an increase in the predicted value of pH corresponded to an increase in the observed value of 0.933. The simple linear regression equation was reported as *observed value = 0.523 + 0.933 (predicted value)*. On the other hand, for the tension spline method, the regression coefficient (*B*= 0.882) indicated that an increase in predicted value of pH corresponded to an increase in the observed value of 0.882. The simple linear regression equation was reported as *observed value = 0.927 + 0.882 (predicted value)*. Table 3 shows the coefficient and t-statistics after the regression analysis was carried out between the observed and predicted pH value for both methods.

Table 3: The coefficients and t-statistics after the regression analysis was carried out between the observed and predicted pH value for regularized (model 1) and tension (model 2) methods.

	Unstandardized Coefficients		**Standardized Coefficients**		
Model	**B**	**Std. Error**	**Beta**	**t**	**Sig.**
1 (Constant)	0.523	0.979		0.534	0.602
Predicted Regularized pH	0.933	0.124	0.896	7.547	0.000
2 (Constant)	0.927	1.025		0.904	0.382
Predicted Tension pH	0.882	0.129	0.877	6.816	0.000

a. Dependent Variable: Observed pH

In the error analysis, the Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) calculated for the regularized spline model was at 0.0265 and 0.0344, each respectively. On the other hand, the Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) calculated for the tension spline model was determined at 0.0290 and 0.0379, accordingly. Table 4 shows the residual and squared residual for the Observed (O), Regularized (R) and Tension (T) spline model for all sampling points (SP).

To choose the optimal interpolation method, the lowest RMSE among the methods is chosen. Based on the error analysis, the regularized spline method estimated the value of pH at minimal error compared to the tension spline method. Transformation process from spatial model into spatial map was carried out. Map elements are inserted for better visualization and communication. In the legend section, 3 classifications of pH ranges were chosen: <7, 7-8 and >8. Figure 5 shows the map of pH developed using regularized spline method.

An accuracy assessment was carried out to determine the accuracy of spline interpolation method. Correct occurrences were observed at all sampling points except for SP002 and SP006 due to overestimation effects. The overall accuracy of the developed map was calculated at 87.50%. Table 5 shows the comparison between the observed value and predicted value of pH in

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the form of ranges. The ranges were based on less than 7 pH reading (<7), between 7 to 8 pH reading (7-8), and more than 8 pH reading (>8).

Based on the map, the strait and the coastal water of Pulau Tuba, Langkawi shows the distribution of pH at between 7 to 8. The pH level reduced due to the rainy season that occurred during sampling activities. Addition to high quantities of rainwater contributes to the low salinity level and low reading of pH values [14]. There are several potential reasons of low value of pH in coastal water region which could be contribute by salinity effects, mixing effects between freshwater and saltwater, variation concentration of carbon dioxide, alkalinity, and hydrogen ion; photosynthetic consumption, decomposition of organic matter, acidity, or chemical spill [15].

Table 4: Results of squared residuals between the Observed (O), Regularized (R) and Tension (T) spline model for 16 sampling points

No	SP	Reading of pH			Residual		Squared residuals	
		O	R	T	(O-R)	(O-T)	$(O-R)^2$	$(O-T)^2$
1	SP002	7.98	8.02	8.01	-0.04	-0.03	0.0013	0.0011
2	SP004	7.95	7.96	7.96	-0.01	-0.01	0.0000	0.0001
3	SP006	7.97	8.01	8.01	-0.04	-0.04	0.0013	0.0013
4	SP008	7.91	7.92	7.92	-0.01	-0.01	0.0000	0.0002
5	SP010	7.96	7.93	7.93	0.03	0.03	0.0011	0.0012
6	SP012	7.92	7.93	7.93	-0.01	-0.01	0.0001	0.0001
7	SP014	7.86	7.88	7.88	-0.02	-0.02	0.0005	0.0005
8	SP016	7.78	7.80	7.80	-0.02	-0.02	0.0004	0.0004
9	SP018	7.70	7.74	7.73	-0.04	-0.03	0.0017	0.0008
10	SP020	7.94	7.88	7.85	0.06	0.09	0.0041	0.0089
11	SP022	7.96	7.96	7.95	0.00	0.01	0.0000	0.0001
12	SP024	7.96	7.91	7.91	0.05	0.05	0.0026	0.0027
13	SP026	7.93	7.93	7.94	0.00	-0.01	0.0000	0.0001
14	SP028	7.94	7.96	7.96	-0.02	-0.02	0.0002	0.0004
15	SP030	7.96	7.95	7.96	0.01	0.00	0.0001	0.0000
16	SP032	7.92	7.99	7.99	-0.07	-0.07	0.0056	0.0052

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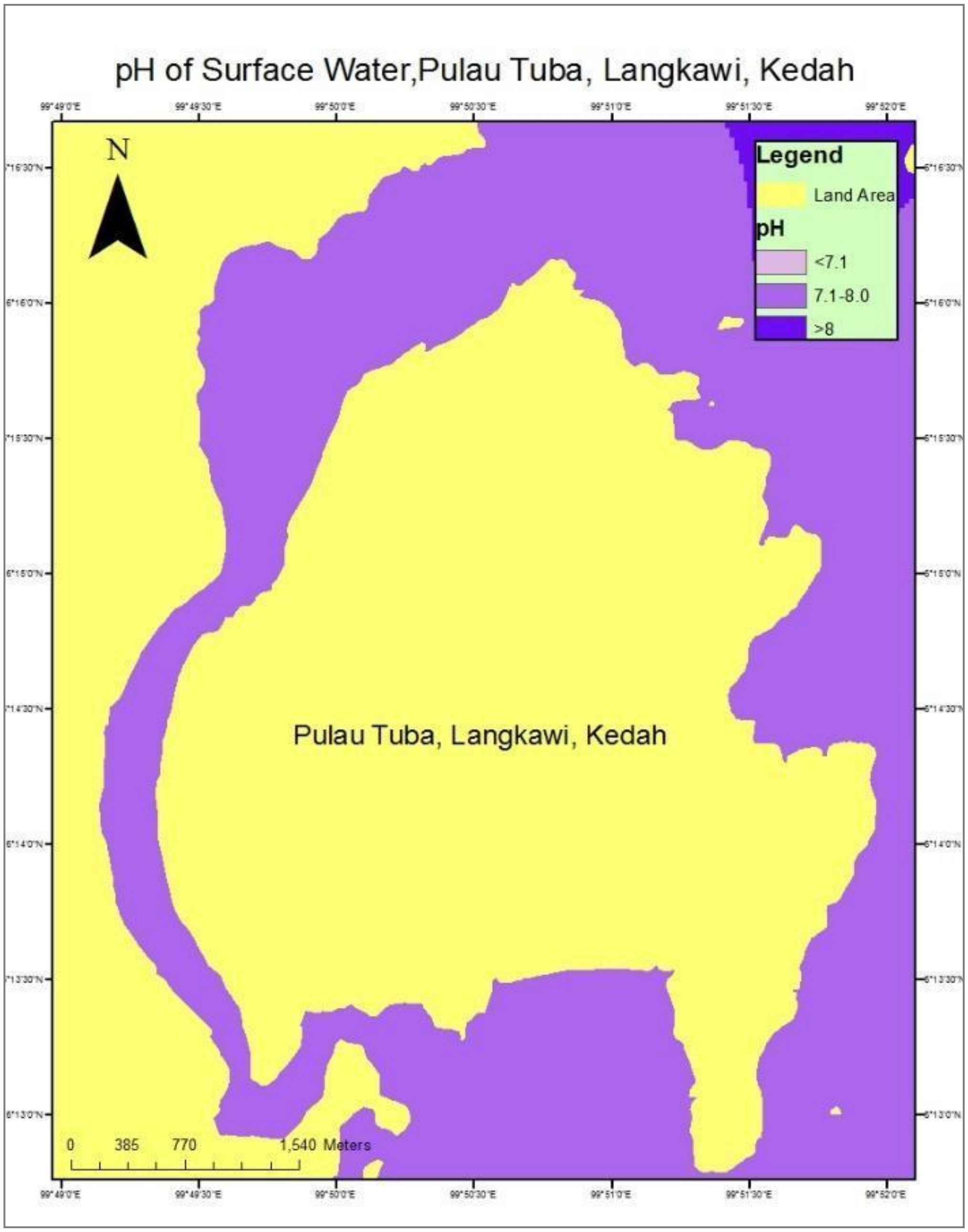

Figure 5: Distribution of pH over coastal water of Pulau Tuba, Langkawi, Kedah

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Table 5: Correct occurrences based on the comparison between the observed and predicted values of pH readings for 16 sampling points

No	Sampling Point	Correct occurrences	Reading of pH	
			Observed value	Predicted value
1	SP002	NO	7-8	>8
2	SP004	YES	7-8	7-8
3	SP006	NO	7-8	>8
4	SP008	YES	7-8	7-8
5	SP010	YES	7-8	7-8
6	SP012	YES	7-8	7-8
7	SP014	YES	7-8	7-8
8	SP016	YES	7-8	7-8
9	SP018	YES	7-8	7-8
10	SP020	YES	7-8	7-8
11	SP022	YES	7-8	7-8
12	SP024	YES	7-8	7-8
13	SP026	YES	7-8	7-8
14	SP028	YES	7-8	7-8
15	SP030	YES	7-8	7-8
16	SP032	YES	7-8	7-8

Several studies have shown that the regularized spline method estimated the water parameter more accurate than the tension spline method. Regularized spline is shown to outperform tension spline when estimating surface water salinity in Sungai Merbok, Kedah [16]. Moreover, the regularized spline model also produces high accuracy estimating the surface water temperature over coastal water of Pulau Tuba, Langkawi [17]. Overall, spline has been known to be generating gently varying surfaces such as pollution concentrations [18]. GIS has been proven to be effective tools and software for visualizing and presenting the variation of water pollutants in a study area [19].

Many environments in the oceans could be ruined if the water pH changes drastically [20]. Coastal water and the ocean commonly exhibit high pH values because of alkalinity. The alkalinity of the seawater can also be called the hardness of the seawater [21]. The rocks and

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sand provided such element of calcium, magnesium and other minerals that transform the acidity of dissolved carbon dioxide into a basic solution and creates the hardness and alkalinity that all life process depends on. The ocean acidification process could reduce the amount of carbonate [22]. This makes it more difficult for many marine organisms, such as coral and some plankton, to form their shells and skeletons, thus, existing shells may begin to dissolve [23].

Today the pH of seawater is significantly variable, and a single living thing can cope with fluctuations of different pH levels during its lifetime. The setback with ocean acidification is the sustained nature of the change, as the menace comes from the lifetime exposure to lessen pH levels [24]. The fast leap of ocean acidification will influence the degree to which calcifying organisms will be able to adjust [25]. Sustainable approach should be carried out efficiently as society has become highly aware of the protection of environment [26]. The present research in Pulau Tuba has great significance for the government and non-government bodies to use this model to monitor, protect, and perform early detection of the impact of the ocean acidification process that could harm the marine and coastal biodiversity.

CONCLUSION

The research concludes that both methods can estimate the surface water pH. However, regularized spline method has been found to be superior to tension spline method in predicting variability of surface water pH as the method produces high correlation, high coefficient of determination and low values of mean absolute error and root mean square error. Transformation of spatial models into the map also contributes to high overall accuracy. There are two major limitations of this study that could be addressed in future research. First, for the methodology part, the study was conducted during the period of November and changes of pH level is expected and affected by monsoon season, tidal activities, and time of sampling activities. Water quality research is complex in nature due to every parameter having significant correlation to other water parameters. Secondly, limitation of time also contributes to the limited number of sampling frequency and number of sampling points. Lack of previous studies in this area also became a barrier for this research as there was a lack of baseline data for water pH. However, this limitation has been well analyzed and supported using literature and findings from other researchers. The limitation of this research has opened the opportunity for future research in the study area. The research proposed conducting the sampling activities for a longer period so that a robust model could be developed effectively. Furthermore, the effects of tidal activities, seasonal variation and time of sampling activities should be addressed as well. Nonetheless, the outcome of this research can be used by the government and non-government agencies for baselines data and help to monitor and sustain the coastal and marine water of Pulau Tuba, Langkawi effectively. The developed map can also be used for entrepreneurs on deciding on aquaculture or mariculture sites as pH has a crucial effect on fish growth and development.

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CONFLICT OF INTEREST STATEMENT

The authors declare that there is no conflict of interest regarding the publication of this article.

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