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Mathematical Modelling for Performance Prediction of Ex-mining Lake Water Phytoremediation by *Scirpus Grossus*

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ABSTRACT

This study explores the use of *Scirpus grossus* for phytoremediation of ex-mining lake water, offering a potential low-cost alternative to conventional wastewater treatment. The focus is on removing contaminants such as total iron, total nitrate, total sulfate, total phosphorus, electrical conductivity, chemical oxygen demand, turbidity, and pH. Over 28 days, the ex-mining lake water was treated with *S. grossus* to assess contaminant removal, with the results analyzed using a mathematical model in Microsoft Excel. The model simulated exponential reductions in pollutants and increases in pH, with absorption coefficients calculated for each parameter. The study found that *S. grossus* effectively reduced contaminants, with the most significant removal of total iron at 95.45%. The pH of the water increased from 2.61 (acidic) to 6.29 (neutral), improving its suitability for aquatic life. The predicted removal rates closely matched the observed data, suggesting that the model is reliable for forecasting phytoremediation outcomes. Overall, the study confirms that *S. grossus* is a highly effective species for cleaning ex-mining lake water, offering a sustainable and cost-effective solution for industrial wastewater treatment. The findings encourage further research into the scalability, long-term effectiveness, and integration of this technique with other wastewater management strategies.

Keywords: Abandoned mine lake water, mathematical computing, plant-based remediation, *Scirpus grossus*, simulation

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INTRODUCTION

Phytoremediation, using plants to remove, degrade, or stabilize contaminants from soil and water, has emerged as a promising, eco-friendly approach for environmental

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cleanup. This technique leverages the natural abilities of plants and their associated microorganisms to absorb, transform, and detoxify pollutants, including heavy metals, radionuclides, and organic compounds (Almaamary et al., 2017). Despite its potential, the practical application of phytoremediation poses several challenges, including variability in contaminant removal efficiency, environmental conditions, and plant species performance. Mathematical modeling has become invaluable in optimizing and predicting the outcomes of phytoremediation efforts to address these complexities (Tangahu et al., 2022).

S. grossus (locally known as *Rumput Menderong*), as shown in Figure 1, holds great promise as a phytoremediation agent for contaminated water bodies, particularly those affected by industrial activities. Its robust growth, high tolerance to pollutants, and ability to enhance microbial degradation of contaminants make it a valuable tool in sustainable and effective water quality management (Almaamary et al., 2022). As research continues to explore and optimize the use of *S. grossus* in phytoremediation, this plant may become an integral part of efforts to restore and protect our water resources.

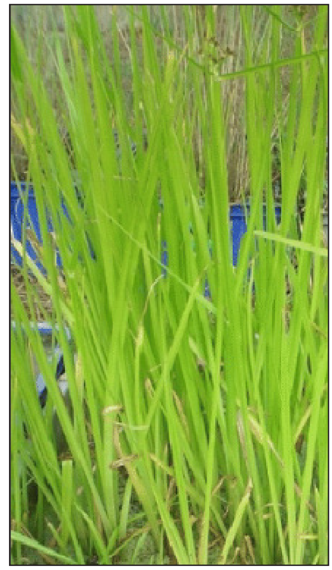

Figure 1. Scirpus grossus (Rumput Menderong) (Tangahu et al., 2015)

Sordes et al. (2023) reported that mathematical modeling in phytoremediation involves the development of theoretical frameworks and computational algorithms to simulate the interactions between plants, contaminants, and environmental variables. These models can predict the behavior of contaminants in different scenarios, evaluate the effectiveness of various plant species, and optimize the design and management of phytoremediation projects. By integrating data from laboratory experiments, field studies, and environmental monitoring, mathematical models provide insights into the dynamics of phytoremediation processes, allowing for more precise and efficient remediation strategies (Alvarez-Vazquez et al., 2019).

The use of mathematical models offers several advantages in phytoremediation. They can reduce the need for extensive and costly field trials by simulating different remediation scenarios, thus saving time and resources. According to Darajeh et al. (2016), models can also identify the most effective plant species for specific contaminants and environmental conditions, enhancing the overall efficiency of phytoremediation. Furthermore, they help understand the complex interactions between plants and contaminants, providing a deeper insight into pollutant uptake, transformation, and stabilization mechanisms.

Kamalu et al. (2017) mentioned that mathematical modeling can play a crucial role in managing and mitigating environmental risks in the context of contaminated sites, particularly those affected by mining activities. For instance, ex-mining lake waters often contain high concentrations of heavy metals and other pollutants, posing significant ecological and human health risks. Modeling the phytoremediation processes in such environments can help predict the long-term behavior of contaminants, assess the potential impact of remediation activities, and design effective remediation plans (Simha & Achyuth, 2015).

Jaskulak et al. (2020) stated that mathematical modeling is crucial in optimizing and predicting the effectiveness of phytoremediation processes, providing valuable insights into the interactions between plants, contaminants, and environmental conditions. However, many limitations in this field still hinder the full realization of phytoremediation's potential. Therefore, it is essential to explore the various aspects of mathematical modeling in phytoremediation, including model development, validation, and application in real-world scenarios, as studied by Shi et al. (2023). By harnessing the power of computational techniques to develop a suitable predictive system, we can enhance the effectiveness of phytoremediation and contribute to sustainable environmental management. Mathematical modeling in phytoremediation lies in its ability to enhance the efficiency, precision and applicability of phytoremediation techniques. The models can simulate contaminant uptake, translocation, and degradation over time, providing accurate remediation rates and time frame predictions.

MATERIALS AND METHODS

Experimental Setup

Seedling *S. grossus* collected from the natural pond at Bukit Besi was thoroughly washed with tap water to remove any surface contamination and then placed in a plastic vessel containing tap water. Two constructed wetland (CW) chambers were set up for two replicates, each approximately 50 cm in length (L), 35 cm in width (W), and 34 cm in depth (D), as shown in Figure 2. Each chamber was filled with approximately 13 cm height of river sand and lake water (approximately 28 liters). The CWs were placed in a greenhouse exposed to ambient conditions but shielded from direct sunlight to prevent water evaporation. Twelve plants were allowed to grow in each tub for 28 days (Sidek et al., 2020).

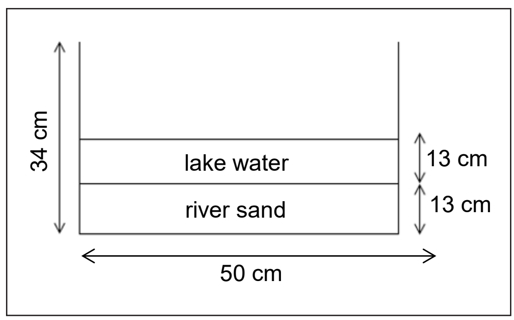

Figure 2. CW setup dimension

Plant Physical Observation

Plant physical observation was also recorded on each monitoring date, as reported by Ismail et al. (2017). Visual stress symptoms, including chlorosis, wilting, necrosis and stunted growth, were observed on each of the sampling days. This is crucial for assessing plant health, growth and tolerance during remediation.

Lake Water Analysis

Analysis of total iron (TI), total nitrate (TN), total sulfate (TS), total phosphorus (TP), electrical conductivity (EC), chemical oxygen demand (COD), turbidity and pH. of the lake water drawn from experimental treatments was done on 0^{th}, 7^{th}, 14^{th}, 21^{st} and 28^{th} of sampling days using standard methods outlined in APHA11 (Kumari et al., 2015; Kutty & Al-Mahaqeri, 2016). All selected parameters considered the possible characteristics of contaminants in the ex-mining lake water.

Mathematical Modelling Hypothesis

The parameter variation is attributed to the phytoremediation of ex-mining lake water by *S. grossus*, which contains high organic and inorganic compounds. This study assumes that the concentration of pollutants and/or effectiveness decreases over time as aquatic plants decrease inorganic and some organic compounds from wastewater (Jyotsna et al., 2015). However, once equilibrium is reached (when the plants' capacity for pollutant sequestration is maximized), the plants no longer contribute to pollution removal—noted that the parameter variation due to the phytoremediation of ex-mining lake water is limited and reaches its peak on the first day of the experiment.

Phytoremediation Prediction Model

According to Jyotsna et al. (2015), let *P* (phytoremediation parameter) be at the time of the initial day of the experiment for the phytoremediation potential of the *S. grossus*. The rate of change in *P* from the first day of the experiment until the plants reach equilibrium is directly proportional to *P*; then,

$$\frac{dp}{dt}\alpha P = \mu P \qquad [1]$$

Where μ is a constant. Integrating Equation 1.

$$\ln P = \mu t + C \qquad [2]$$

Where *C* is the constant of integration. To determine the value of *C*, apply the initial condition to Equation 2 by setting t=0 on the starting day of the experiment, where *P* will be at its maximum value, denoted as P_0. Then,

$$\ln P_0 = \mu 0 + C$$

Or $C = \ln P_0$

Putting the value of *C* in Equation 2,

$\ln P = \mu t + \ln P_0$

Or $\ln P - \ln P_0 = \mu t$

Or $\ln(P/P_0) = \mu t$

Or $P/P_0 = exp(\mu t)$

Or $P = P_0 \exp(\mu t)$ [3]

Now, when the plant reaches equilibrium after 28 days, the change in *P* with respect to *t* approaches zero.

$\frac{dp}{dt} = 0$

This indicates that,

$P = b$ [4]

Where *b* is a constant. Now, merging Equations 3 and Equation 4,

$P = P_0 \exp(\mu t)$ (before reaching steady-state)

$= b$ (after reaching steady-state) [5]

For the condition before reaching equilibrium, Equation 3 should be applied and denoted as Equation 5 to find the *P* values at the interval. At the same time, *P* is equal to *b* (constant) after reaching equilibrium.

Now consider *t* at an identical interval, let these be $t_{1,} t_{2,} t_{3,}$….., t_N.

$\mu = \{ \ln(P_i / P_0 \} / t_i$, where $i = 1, 2, 3, \ldots N$

$$\mu = \frac{\sum_1^N \mu_i}{N}$$

The activity can be predicted by substituting the value of μ into Equation 3 (Kumar et al., 2005).

Mathematical Model Application

The method previously discussed was used to apply the model to the observed data. Observations were taken at three equidistant time intervals: on the 0th, 7th, 14th, 21st, and 28th days. The value of μ was calculated using these observations, and the predicted value of P for *S. grossus* was compared with the observed values (Figures 3–10) (Jyotsna et al., 2015). The prediction simulation task was performed using the developed predictive system in Microsoft Excel.

RESULTS AND DISCUSSION

Plant Growth Observation

The plants show symptoms of yellowing leaves, root impairment, brown spots, and reduced metabolic activity. According to Sidek et al. (2018), this initial plant behavior (up to 28 days) for nutrient absorption from the lake water could be due to the plants reaching their carrying capacity, as all binding sites in the root zone were occupied. Additionally, the high elemental concentration in the plant bodies may have negatively impacted plant growth, resulting in relatively poor growth beyond 28 days (Table 1). This stunted growth likely halted the absorption of organic and inorganic contents from the lake water (Ismail et al., 2020).

Table 1
Scirpus grossus *physical observation*

Observation day	**Initial day (0th day)**	**Final day (28th day)**
Observation result	 All healthy	 A few withered and dead

Lake Water Parameters Analysis

All parameters showed an exponential decrease in P of *S. grossus* from the start of the experiment up to 28 days, after which the decrease became negligible until the experiment's conclusion. A comparison between the estimated and observed values of a given parameter of the lake water (Figures 3–10) shows minimal variation. This finding strongly agrees with previous studies by Jyotsna et al. (2015) and Kumar et al. (2005), evident from the values of μ and the percentage reduction of different parameters with respect to the observed and estimated values. However, some inconsistency between observed and estimated values can be attributed to the subjectivity inherent in the experiment (Darajeh et al., 2016). Additionally, as the duration of phytoremediation increases, the pH values rise exponentially towards neutral.

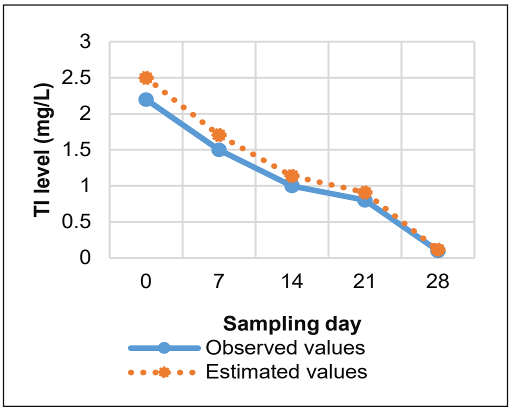

Figure 3. Comparison between the estimated value and observed value of TI

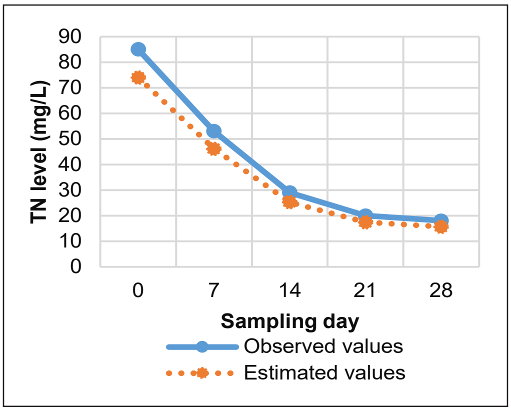

Figure 4. Comparison between the estimated value and the observed value of TN

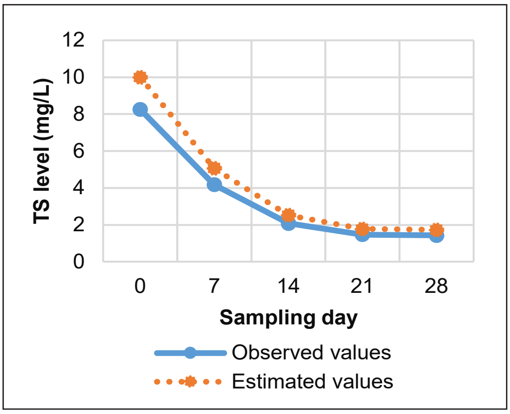

Figure 5. Comparison between the estimated value and the observed value of TS

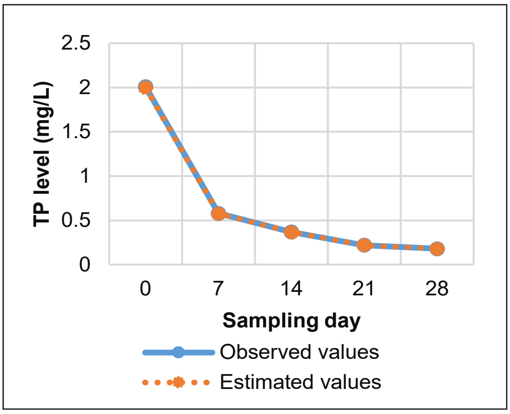

Figure 6. Comparison between the estimated value and the observed value of TP

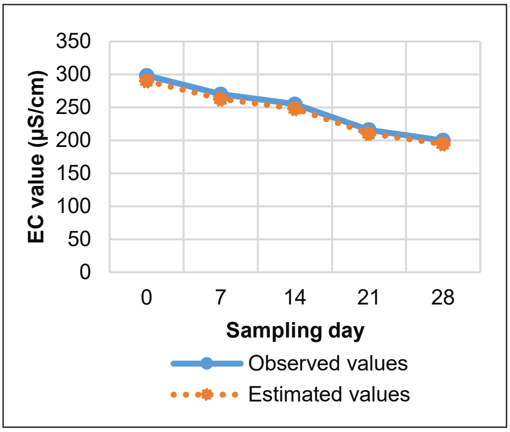

Figure 7. Comparison between the estimated value and the observed value of EC

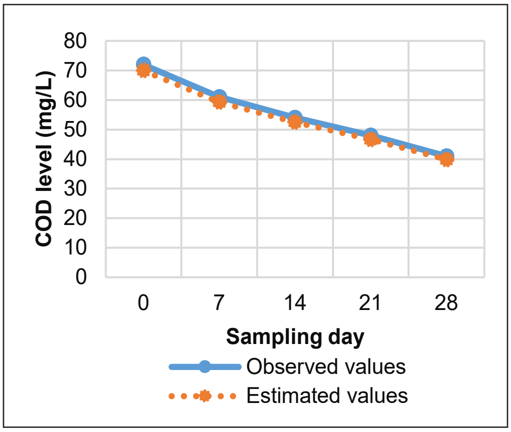

Figure 8. Comparison between the estimated value and the observed value of COD

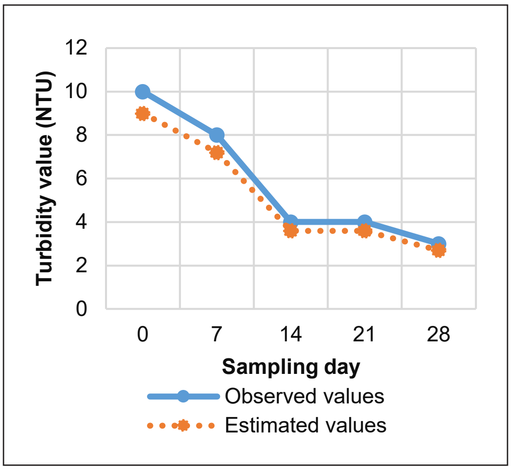

Figure 9. Comparison between the estimated value and observed value of turbidity

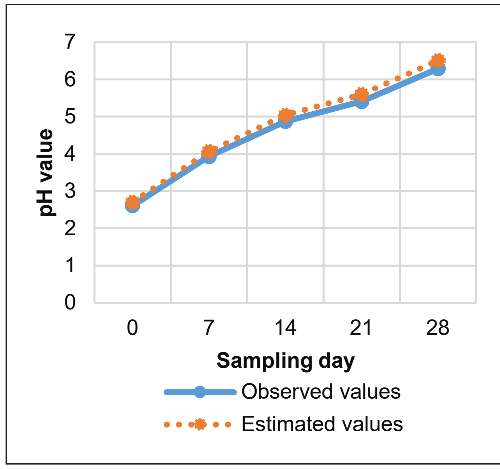

Figure 10. Comparison between the estimated value and observed value of pH

Mathematical Modelling

The trend of contaminant reduction is dependent on the value of μ (equilibrium constant) calculated using the mathematical model and the developed predictive system as shown in Table 2 as the highest value is 0.19358 (R=95.45%) for TI and the lowest is 0.02949 (R=32.89%) for EC neglecting the (-ve) signs which exhibit decrement values. This indicates that with extended phytoremediation, the phytoremediator reaches an equilibrium level of absorption and/or degradation of the pollutants in the lake water, resulting in a halt in the reduction of the studied parameters beyond that point (Wang & Delavar, 2024). Figure 11 displays the window of the phytoremediation predictive system, which consists of the observed values, estimated values and contaminants removal graphs developed in Microsoft Excel.

Table 2
Calculated mean μ for eight physico-chemical parameters of Scirpus grossus

Parameters	Removal/Reduction	μ
TI	95.45%	-0.19358
TN	78.82%	-0.09256
TS	82.67%	-0.07106
TP	91.04%	-0.12235
EC	32.89%	-0.02949
COD	43.06%	-0.05247
Turbidity	70.00%	-0.06525
pH	+3.68	0.04591

Mathematical and computing techniques offer several advantages in phytoremediation technology, enhancing the efficiency, accuracy, and effectiveness of remediation processes. The advantages of this approach are beneficial for optimized plant selection, optimized plant selection, and cost and time efficiency (Jaskulak et al., 2020). Mathematical models can predict which plant species are most effective for specific contaminants, helping to select the best candidates for phytoremediation based on factors like growth rate, tolerance, and uptake capacity. Computational techniques enable the simulation of

PHYTOREMEDIATION PREDICTIVE SYSTEM

t	TI obs	TI est	TN obs	TN est	TS obs	TS est	TP obs	TP est	EC obs	EC est	COD obs	COD est	Turb obs	Turb est	pH obs	pH est
0	2.20	2.50	85.00	74.00	8.25	10.00	2.01	2.00	298.00	290.00	72.00	70.00	10.00	9.00	2.61	2.70
7	1.50	1.70	53.00	46.14	4.18	5.07	0.58	0.58	270.00	262.75	61.00	59.31	8.00	7.20	3.93	4.07
14	1.00	1.14	29.00	25.25	2.08	2.52	0.37	0.37	255.00	248.15	54.00	52.50	4.00	3.60	4.87	5.04
21	0.80	0.91	20.00	17.41	1.47	1.78	0.22	0.22	216.00	210.20	48.00	46.67	4.00	3.60	5.41	5.60
28	0.10	0.11	18.00	15.67	1.43	1.73	0.18	0.18	200.00	194.63	41.00	39.86	3.00	2.70	6.29	6.51

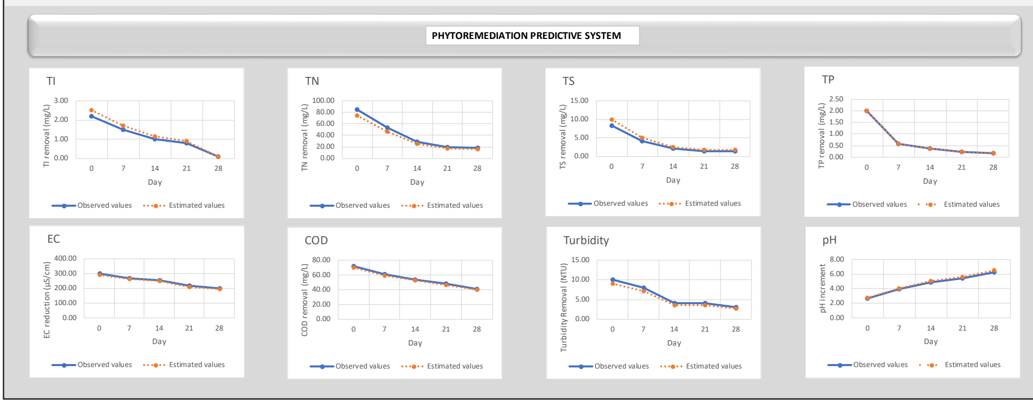

Figure11. Phytoremediation predictive system

different scenarios, predicting the outcomes of phytoremediation efforts under various conditions. This helps in planning and optimizing remediation strategies. By simulating different phytoremediation strategies, mathematical models can identify the most cost-effective and time-efficient approaches, reducing the need for extensive field trials, as reported by Mohammadi et al. (2019).

As a practical technique for further research, an integrated phytoremediation model should account for the influence of agronomic practices, soil amendments, and native plants (Alvarez-Vazquez et al., 2019). In real-world settings, industries and environmental agencies can use phytoremediation mathematical models to optimize the selection of plant species, predict pollutant uptake, scale remediation efforts, and ensure long-term sustainability. Proper calibration, monitoring, and consideration of site-specific conditions (like soil type, climate, and contaminant type) are essential for successfully implementing these models. With the right combination of data, models, and field validation, phytoremediation can become an effective and cost-efficient strategy for addressing environmental contamination (Jaskulak et al., 2020).

According to Wang and Delavar (2024), phytoremediation modeling is valuable for predicting and optimizing environmental cleanup using plants. However, its limitations can impact its accuracy, applicability, and scalability in real-world settings. These limitations stem from the inherent complexity of biological, ecological, and environmental systems.

Phytoremediation mathematical modeling can be highly applicable when certain conditions are met, ensuring that predictions and recommendations are robust and realistic. These conditions include access to site-specific data, knowledge of contaminant-plant interactions, the environmental and climatic context, and a solid understanding of soil-plant feedback mechanisms (Jaskulak et al., 2020). Additionally, the model should consider the economic feasibility and practical constraints of applying phytoremediation on a large scale, as well as include tools for uncertainty analysis to ensure that decision-makers can manage risks effectively. When these conditions are met, phytoremediation models can be a powerful tool for optimizing remediation strategies, ensuring sustainable and cost-effective environmental cleanup.

CONCLUSION

Based on the current investigation, the proposed model effectively predicts the phytoremediation potential of *S. grossus* for ex-mining lake water and similar industrial effluents over time. TI parameter shows the highest percentage removal at R=95.45% with μ value of -0.19358. This model is particularly useful for the fast observation of industrial pollution treatment. The mathematical model demonstrates a reasonably accurate remediation method for industrial wastewater pollution using plants such as *S. grossus*. This approach could be effectively utilized to remediate the effects of ex-mining lake water, at least on an experimental basis.

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