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MDS of Plasmepsin II

Molybdenum Blue Production from *Serratia* sp. strain DRY5: Secondary Modeling

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ABSTRACT

In this work, kinetic growth models such as Luong, Yano, Teissier-Edward, Aiba, Haldane, Monod, Han and Levenspiel were used to model molybdenum blue production from *Serratia* sp. strain DRY5. Based on statistical analyses such as root-mean-square error (RMSE), adjusted coefficient of determination ($adjR^2$), bias factor (*BF*), and accuracy factor (*AF*), the Monod model was chosen as the best. The calculated values for the Monod constants q_{max} (the maximum specific substrate degradation rate (h^{-1}), and K_s (concentration of substrate at the half maximal degradation rate (mg/L)) were found to be 3.86 (95% confidence interval of 2.29 to 5.43), and 43.41 (95% confidence interval of 12.36 to 74.46) respectively. The novel constants discovered during the modelling exercise could be used in further secondary modelling.

INTRODUCTION

Heavy metals are necessary for the biological processes of plants and animals, but at high quantities, they can disrupt metabolic reactions in organisms' systems. Toxic heavy metals, such as molybdenum, which is beneficial to plants, can impair plant development by lowering photosynthetic activities, plant mineral nutrition, and necessary enzyme function [1]. Metals are used in a wide range of industrial processes. As a result, many Malaysian environmental systems have been contaminated with heavy metals [2]. Due to indiscriminate dumping and unlawful discharge, heavy metal pollution has become a public health concern in Malaysia [3]. Toxic heavy metals, such as molybdenum, can build up in the body after being absorbed in contaminated food and pose a health danger to living organisms [1]. Molybdenum is a heavy metal with a wide range of industrial applications. It's a dangerous contaminant, with thousands of parts per million levels found in soils and aquatic bodies [2] . Molybdenum has also been shown to suppress spermatogenesis in drosophila and fish [4]. Molybdenum is a common metal that is frequently contaminated by mining operations and human sources. Molybdenum is becoming a global contaminant at an alarming rate. Its contamination levels have been measured in water and soils across the world, including Terengganu in Malaysia, Tokyo Bay, Tyrol in Austria, and the Black Sea, where molybdenum levels have reached dangerously high levels [3,5,6]. It is non-toxic to humans; however, it is lethal to ruminants at concentrations of many parts per million [5]. Molybdenum is used in the production of steel, corrosion-resistant steel components, engine anti-freeze additives, and molybdenum disulfide in lubricants, among other things. The usage of molybdenum in the industry has resulted in several examples of soil and water contamination [7]. In general, the reduction mechanism in molybdenum-reducing bacteria has been shown to involve an enzymatic reaction rather than a chemical one.

There have been reports of molybdenum-reducing bacteria from agricultural soil, with a second molybdenum-reducing bacterium capable of degrading pollutant [4]. Molybdenum reduction to molybdenum blue is a mechanism related to bacterial growth and, like bacterial growth, exposes a peculiar stage in which the true growth rate begins at zero and quickly accelerates to a maximum value (max), resulting in a lag period (λ) [6]. Microbes have an incredible ability to resist the toxicity of heavy metals, which is useful in bioremediation. Ruminants are highly poisonous to it, and bioremediation has been reported in previous research [5]. Microbes have been responsible for

molybdate decrease for over a century. In 1985, E. coli K12 was used in the first comprehensive study of molybdate reduction to Mo-blue. T. *ferrooxidans, Enterobacter cloacae* strain 48 (EC 48), and *Serratia marcescens* strain Dr.Y6 followed in 1988, 1993, and 2008 respectively [3,8].

MATERIALS AND METHODS

Data acquisition

The graphical data from Fig. 1. of the published work by Shukor et al. [6] of Mathematical Modeling of the Molybdenum Blue Production from Serratia sp. strain DRY5 was processed using the software Webplotdigitizer 2.5 [9], which helps to digitizes the scanned figure and has been widely used and acknowledged by many researchers because of its precision and reliability [3,5,6,10]. CurveExpert Professional software (Version 2.6.5) was used to model the data after been processed.

Fitting of the data

Employing CurveExpert Professional software (Version 2.6.5), nonlinear regression using the Marquardt algorithm was utilised to fit the bacterial growth curve using multiple growth models (**Table 1**). The algorithm looks for the most efficient way to lower the sum of squares between predicted and measured values. The sharpest gradient search of the curve between the four datum points was used to estimate the growth rate(max), while the line crossing the X-axis was used to estimate the lag time (λ). The highest growth rate was picked for the modelling exercise.

Table 1. Mo-blue production models employed in this research.

Model	Equation	No. Of parameters	Ref.
Monod	$\mu_{max}\frac{S}{K_s+S}$	2	[15]
Haldane	$\mu_{max}\frac{S}{S+K_s+\left(\frac{S^2}{K_i}\right)}$	3	[16]
Teissier	$\mu_{max}\left\{1-exp\left(\frac{S}{K_i}\right)-exp\left(\frac{S}{K_s}\right)\right\}$	3	[17]
Luong	$\mu_{max}\frac{S}{K_s+S}(1-\frac{S}{S_m})^n$	4	[18]
Aiba	$\mu_{max}\frac{S}{K_s+S}\,exp^{(\frac{S}{K_i})}$	4	[19]
Yano and Koga	$\frac{\mu_{max}S}{S+K_s+\left(\frac{S^2}{K_i}\right)\left(1+\frac{S}{K}\right)}$	4	[20]
Han and Levenspiel	$q=\frac{q_{max}S\left[1-\left(\frac{S}{S_m}\right)\right]^n}{K_s+S-\left[1-\left(\frac{S}{S_m}\right)\right]^m}$	5	[21]

Note:
μ_{max} = maximum cell growth and degradation rate (h^{-1})
K_s = Half saturation constant or half velocity constant (% v/v)
K_i = Inhibition constant (% v/v)
S = Substrate concentration (% v/v)
S_m = Maximum concentration of substrate tolerated (% v/v)
m, n, K = curve parameters

Statistical analysis

The adjusted determination coefficient (R^2), accuracy factor (AF), bias factor (BF), root-mean-square error (RMSE), and aicc (akaike information criterion) corrected were used to calculate the statistically significant difference between the models, as previously described [4,11–13]. The first to propose and suggest BF and AF were ross and McMeekin [14].

RESULTS AND DISCUSSION

Based on bacterial growth modelling (Figs 1-7), the Monod model was found to be the best model, with the lowest RMSE, AICc, and adjustedR^2 values. The model's AF and BF values were similarly excellent, with values close to 1.0. Except for the Tessier-Edward model, which shows poorest match (**Table 2**), the coefficients parameters for the Monod model were provided in **Table 3**.

Table 2. Statistical analysis of the various models used in this sturdy.

Model	P	RMSE	adR2	AICc	BF	AF
Luong	4	0.1503	0.952	-37	0.680	1.598
Yano	4	0.1364	0.959	-40	1.312	1.440
Tessier-Edward	3	0.4252	-0.941	-11	1.089	1.353
Aiba	3	0.1551	0.947	-41	0.764	1.460
Haldane	3	0.1457	0.954	-43	0.707	1.546
Monod	2	0.1595	0.944	-45	0.692	1.625
Han and Levenspiel	5	0.1586	0.9454	-29	0.687	1.625

Note:
P=number of parameters

Table 3. Growth coefficients as predicted by the Monod model.

	μ_m (h^{-1})	Ks (% v/v)
Value	3.86	43.41
Std err	0.7269	14.371
Range (95% confidence)	2.29 to 5.43	12.36 to 74.46

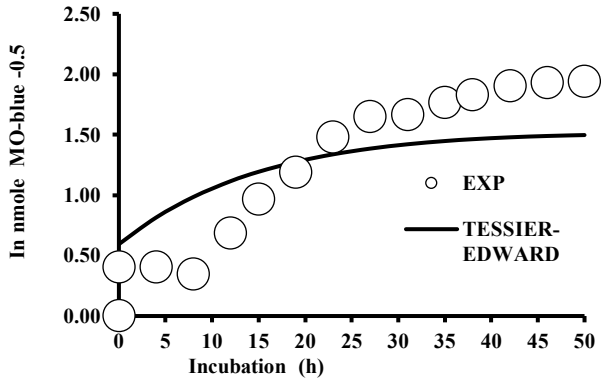

Fig. 1. Growth of ***Serratia*** **sp. strain DRY5** modeled using Tessier-Edward

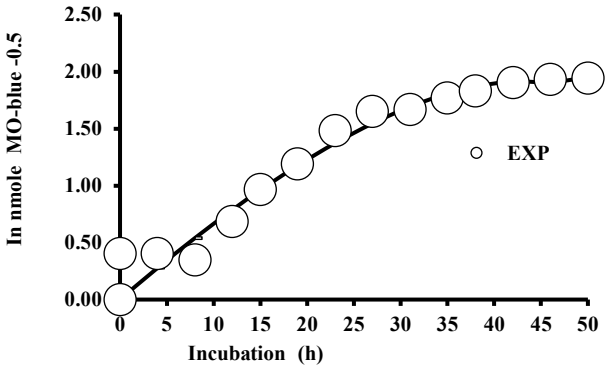

Fig. 3. Growth of ***Serratia*** **sp. strain DRY5** modeled using Han-levenspiel

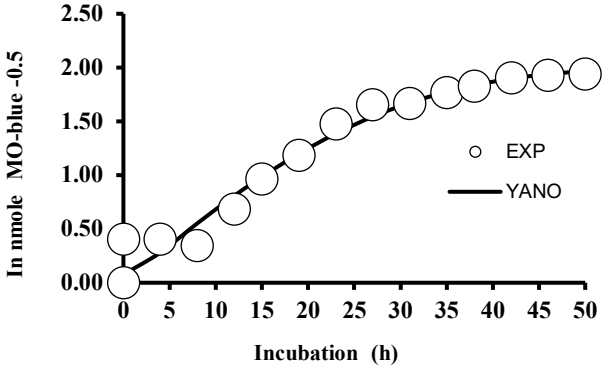

Fig. 5. Growth of ***Serratia* sp. strain DRY5** modeled using Yano.

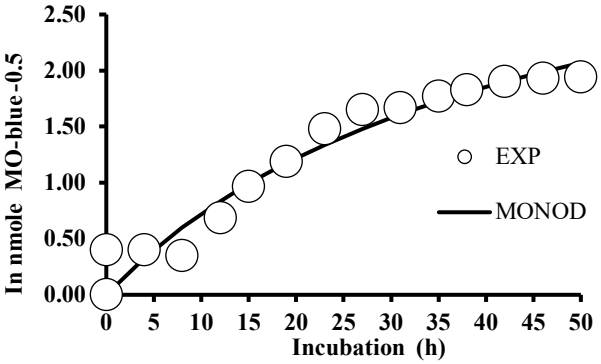

Fig. 6. Growth of ***Serratia* sp. strain DRY5** modeled using Monod.

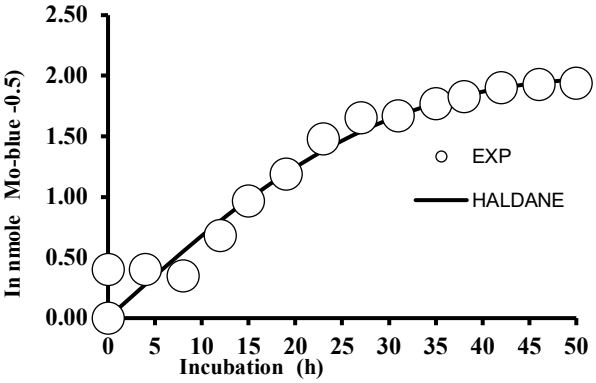

Fig. 2. Growth of ***Serratia* sp. strain DRY5** modeled using Haldane

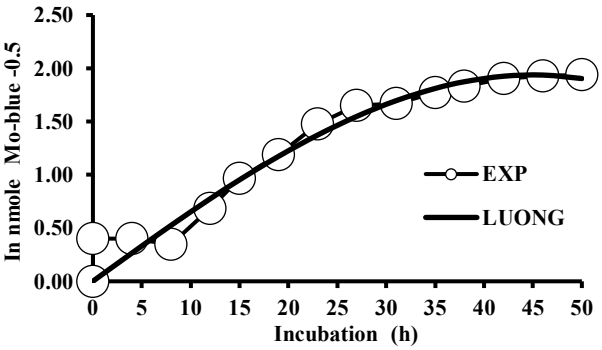

Fig. 7. Growth of ***Serratia* sp. strain DRY5** modeled using Luong.

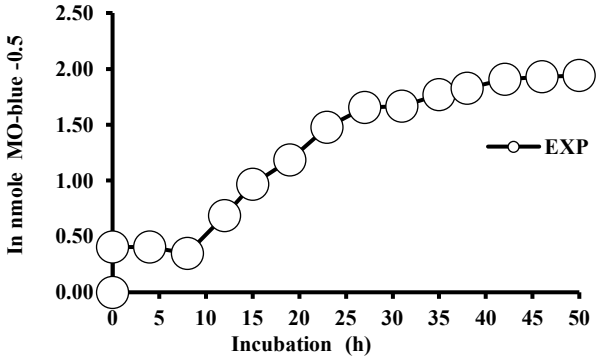

Fig. 4. Growth of ***Serratia* sp. strain DRY5** modeled using Aiba.

CONCLUSION

In conclusion, based on statistical analyses such as corrected AICc (Akaike Information Criterion), bias factor (BF), adjusted coefficient of determination ($adjR^2$), and root-mean-square error (RMSE), the Monod model was the best model in modelling the growth of *Serratia* sp in the production of Molybdenum Blue). Maximum specific growth rate (qmax) and Ks (concentration of substrate at half maximal specific growth rate (mg/L) were obtained from the fitting exercise, with values of 3.86 (95% confidence interval of 2.29 to 5.43) and 43.41 (95% confidence interval of 12.36 to 74.46), respectively. Under batch experiments, these biologically meaningful coefficients will be effective in predicting *Serratia sp*. strain DRY5 growth requirements in the production of Molybdenum Blue and therefore heavy metal will be remediated from the environment.

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