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Mathematical Modelling of Azo Blue Dye Degradation by *Streptomyces* DJP15

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ABSTRACT

Azo dyes are the most well-known synthetic dyes. They have been widely utilized as colorants in various sectors, including textiles, photography/printing, food, medicines, etc. This industry has produced a massive quantity of solid waste, soil slurry, and effluents which are mostly passed into the water bodies or the environments. These dyes tend to compromises the physical, chemical and biological nature of the environments. More so, they have significant health risks on the aquatic life, livestock and the whole environmental biodiversity. Furthermore, they are known to be carcinogenic. In this research, seven (7) different kinetics models, Huang, modified Richards, modified Logistics, modified Gompertz, Buchanan-3-phase, Baranyi-Roberts and von Bertalanffy, were utilized in modeling the growth of *Streptomyces* DJP15 growth in the degradation of azo blue dye. While all the models show good curve fitting, the von Bertalanffy model was found to be the best model with the lowest RMSE (0.410), AICc (0.58) and has the highest $adjR^2$ (0.983). Thus, this study indicated that the growth of *Streptomyces* DJP15 on azo blue dye could be described mathematically. Notably, the parameters obtained can be utilized to predict the bioremediation of azo blue dye in the future.

INTRODUCTION

Azo dyes are the most broadly used and adaptable synthetic dyes; they account for more than half of all synthetic dyes produced yearly [1–3]. Based on the number of the azo groups, the azo dyes are classified as monoazo dyes, diazo dyes, triazo dyes and poly azo dyes [4,5]. Example of theses dyes includes reactive yellow 201, disperse blue 399, acid black 1, reactive brown 1, direct black 19, direct red 80, etc. based on applications, azo dyes are classified as direct, reactive, disperse, metalized, cationic and anionic azo dyes [6,7]. Most azo dyes are light and temperature stable and as well very resistant to degradation. Reactive dyes are the only azo dyes designed to bond covalently with cellulosic fibers and are therefore widely utilized in the textile industry [8,9]. Because of their high sulphonation, reactive dyes are highly water-soluble and non-degradable in normal aerobic conditions [10,11]. The presence of the sulfo and the azo groups is the main reason for the persistence and recalcitrant of the azo dyes [12]. Azo dyes pollution in the environment can persist for a very long time without appropriate treatment [13,14]. These compounds are carcinogenic, mutagenic and tend to bioaccumulate in the environment [15]. The release of dyes into the marine environment reduces the dissolved oxygen level, resulting in death from aquatic species [2].

Bioremediation has been viewed as a successful, less energy-intensive, ecologically friendly method that results in partial or total bioconversion of contaminants to stable harmless end products [12]. The process of microbial remediation involves the increasing of microorganism's natural degradation capacity. The use of microorganisms for biodegradation is gaining popularity because it is cost-effective, environmentally friendly and result in nontoxic byproducts. Several microorganisms from different taxonomic groups, such as fungi, bacteria, actinomycetes and algae, have been found to decolorize azo dyes [16–20]. Environmental variables are known to have a significant impact on microorganism decolorization activity. The stability of the enzyme system involved in dye degradation may be affected by physicochemical factors, resulting in reduced decolorization activity at extreme pH and temperature, which may compromise the strain's survival [1,21]. The decolorization efficiency of the bacteria is influenced by variables such as carbon source, nitrogen source, aeration, temperature, dye concentration, pH, inoculum size [13].

Pillai [19] investigate the optimization of the biodegradation process conditions of azo blue dye by Streptomyces DJP15 at different concentrations of the dye (50, 100, 150, 200, 250 and 300 mg/L). The decolorization percentage was quantified after taking the absorbance using a spectrophotometer. It was noted that the degradation of the dye was found to be concentration-dependent. The percentage of dye decolorization increased with time, regardless of the initial dye concentration [19]. Furthermore, the dye degradation rate dropped with an increase in dye concentration, meaning the lower the dye concentration, the better the degradation efficiency. The effect of initial dye concentration on biodegradation has been previously modelled using different kinetics inhibition models [22–24]. This study aims to model the effect of initial dye concentration on the bio decolorization rate of azo blue dye by *Streptomyces* DJP15 using other primary kinetics models.

MATERIALS AND METHODS

Data source

Data from Pillai [19] Figure 2 was scanned and processed using Wetplotdigitizer 2.5 [25]; this is a program that digitizes figures and has been widely employed and praised for its reliability [22,26–28].

Fitting of the data

CurveExpert Professional software (version 1.6) was used to fit the nonlinear equations using the Marquardt algorithm [29,30]. The algorithm seeks the most efficient method for reducing the sum of squares between measured and predicted values. It calculates the initial values automatically through the steepest ascent method. The models for inhibition of the dye decolorization shows in **Table 1**.

Statistical analysis

As previously reported, different statistical approaches were used in selecting the best model; these include the corrected AICc (Akaike Information Criterion), Root-Square Error (RMSE), bias factor (BF), accuracy factor (AF) and adjusted coefficient of determination (R^2) [22,26,31].

RESULTS AND DISCUSSION

Among the seven (7) different models examined, it was discovered that all the models show good fitting (**Fig 1 to 7**). Thus, the models were both practical and relevant to the biodegradation of azo blue dye by *Streptomyces* DJP15. The lowest RMSE, AICc, and highest adjusted R^2 values were used to determine the best performance of the model fitting. The AF and BF values for the model were likewise good, with the closest values near 1.0 [32]. Statistical analysis revealed that the von Bertalanffy model was the best because of its lowest value for RMSE and AICc [33]. The model also has the highest adjusted correlation coefficient (adR^2) and the values for AF and BF were close to unity (**Table 2**).

Table 1. Kinetic models were used in this study.

Model	p	Equation
Modified Logistic	3	$y=\frac{A}{\left\{1+\exp\left[\frac{4\mu_m}{A}(\lambda-t)+2\right]\right\}}$
Modified Gompertz	3	$y=A\exp\left\{-\exp\left[\frac{\mu_m e}{A}(\lambda-t)+1\right]\right\}$
Modified Richards	4	$y=A\left\{1+v\exp(1+v)\exp\left[\frac{\mu_m}{A}(1+v)\left(1+\frac{1}{v}\right)(\lambda-t)\right]\right\}^{\left(\frac{-1}{v}\right)}$
Baranyi-Roberts	4	$y=A+\mu_m x+\frac{1}{\mu_m}\ln\left(e^{-\mu_m x}+e^{-h_0}-e^{-\mu_m x-h_0}\right)$ $-\ln\left(1+\frac{e^{\mu_m x+\frac{1}{\mu_m}\ln\left(e^{-\mu_m x}+e^{-h_0}-e^{-\mu_m x-h_0}\right)}-1}{e^{(y_{\max}-A)}}\right)$
Von Bertalanffy	3	$y=K\left[1-\left[1-\left(\frac{A}{K}\right)^3\right]\exp^{-\left(\mu_m x/3K^{\frac{1}{3}}\right)}\right]^3$
Huang	4	$y=A+y_{\max}-\ln\left(e^A+\left(e^{Y_{\max}}-e^A\right)e^{-\mu_m B(x)}\right)$ $B(x)=x+\frac{1}{\alpha}\ln\frac{1+e^{-\alpha(x-\lambda)}}{1+e^{\alpha\lambda}}$
Buchanan Three-phase linear model	3	Y = A, IF X < LAG $Y=A+K(X-\lambda)$, IF $\lambda \le X \ge X_{MAX}$ $Y = Y_{MAX}$, IF $X \ge X_{MAX}$

Note:
A= maximum no of death cases lower asymptote;
y_{max}= maximum no of death cases upper asymptote;
μ_m = maximum specific growth rate of death;
v= affects near which asymptote maximum no of death cases occurs.
λ=lag time
e = exponent (2.718281828)
t = time after first death case is reported
α,β,δ and k = curve fitting parameters
h_0 = a dimensionless parameter quantifying the initial physiological state of the reduction process. The lag time (h^{-1}) or (d^{-1}) can be calculated as $h_0=\mu_m$

Table 2. Error function analysis of the effect of increasing concentrations of Azo Blue dye to the degradation by *Streptormyces* DJP15 as fitted to various primary models.

Model	*P*	RMSE	R^2	adR^2	AF	BF	AICc
Huang	4.00	0.502	0.986	0.974	1.029	1.002	14.10
Baranyi-Roberts	4.00	0.502	0.986	0.974	1.029	1.002	14.10
modified Gompertz	3.00	0.435	0.987	0.981	1.030	1.103	1.77
Buchanan-3-phase	3.00	0.465	0.986	0.978	1.030	1.003	3.11
modified Richards	4.00	0.470	0.987	0.977	1.133	1.103	12.78
modified Logistics	3.00	0.463	0.986	0.978	1.076	1.047	3.05
von Bertalanffy	3.00	0.410	0.989	0.983	1.122	1.093	0.58

Note:
p no of parameter
adR^2 adjusted correlation coefficient
RMSE Root mean square error
AF Accuracy factor
BF Bias factor

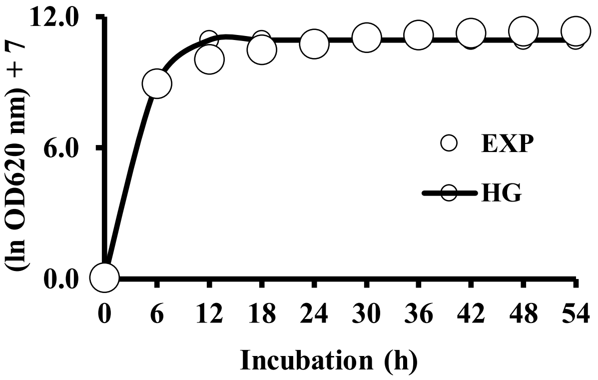

Fig. 1. Growth of *Streptomyces* DJP15 as modelled using the Huang model

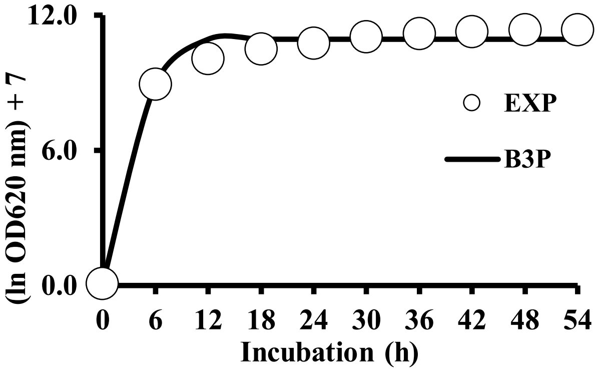

Fig. 4. Growth of *Streptomyces* DJP15 as modelled using the Buchanan-3-phase model

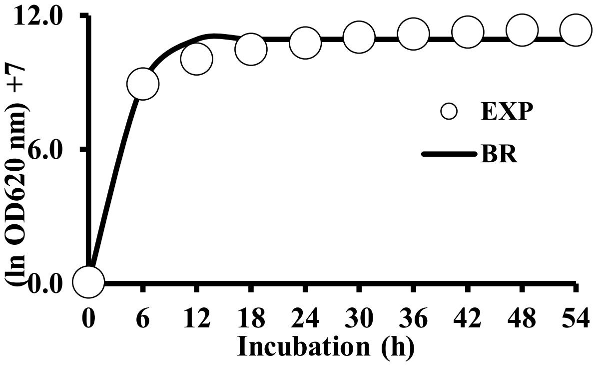

Fig. 2. Growth of *Streptomyces* DJP15 as modelled using the Baranyi-Roberts model.

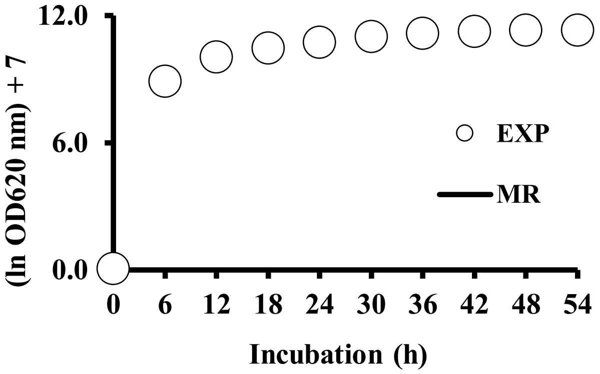

Fig. 5. Growth of *Streptomyces* DJP15 as modelled using the modified Richards model.

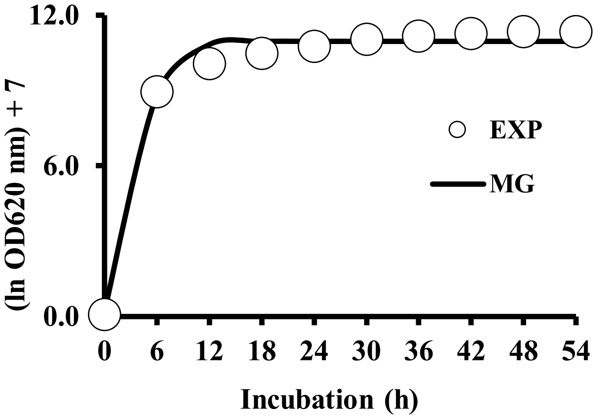

Fig. 3. Growth of *Streptomyces* DJP15 as modelled using the modified Gompertz model.

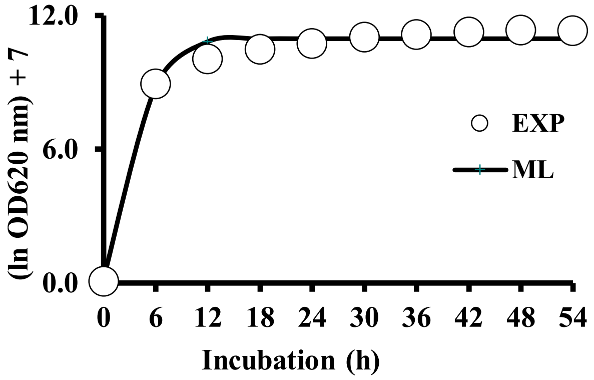

Fig. 6. Growth of *Streptomyces* DJP15 as modelled using the modified Logistics model.

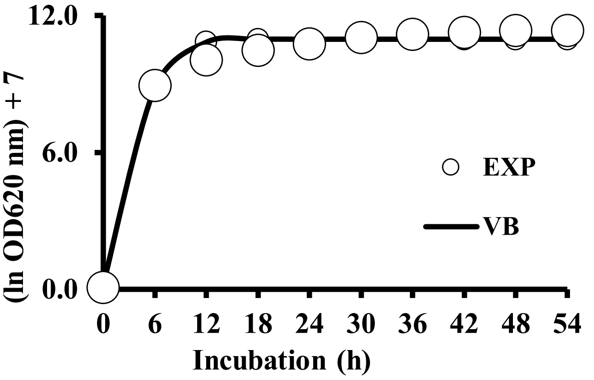

Fig. 7. Growth of *Streptomyces* DJP15 as modelled using the von Bertalanffy model.

The von Bertalanffy model is used to estimate mean length from age in animals. It was first used in ecology to model fish growth, but it is now employed in all organisms, including biodegradation by bacteria. The Gompertz model is famous and widely used in many disciplines of biology. This has also been used to explain the growth of animals and plants and the number or volume of bacteria and cancer cells. Regarding the capacity to estimate microbial growth under dynamic temperature circumstances, Huang's model is compared to Baranyi and Roberts's model using general estimate behavior, bias factor, precision, and root-mean-squared error. In realistic data, the Baranyi model also exhibits good practical identifiability properties, which implies that the confidence intervals on parameter values are reasonable. Although the logistic model fits a sigmoid curve, the modified model, like the modified Gompertz model, adds a lag time to account for a latency phase [24,32,33].

The fitting exercise yielded the following parameters: maximum growth rate (μ_{max}), lag time (δ), and maximal growth rate (*Ymax*). These mechanistic models are employed in fundamental research to understand better the biological, chemical, and physical processes that lead to the observed growth profile [34].

CONCLUSION

In conclusion, few studies apply mathematical modelling to the degradation of synthetic environmental chemical toxicants. In this present study, *Streptomyces* DJP15 was used to model the degradation of azo blue dye and all seven models were found to acceptably fit the curves.

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