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Mathematical Modeling of the growth of *Acinetobacter baumannii* YNWH 226 on Azo dye Congo red

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ABSTRACT

Industrial effluents (Azo dyes) are brightly coloured, making their disposal into receiving waters undesirable not only because many Azo dyes and their breakdown products are toxic to aquatic life and mutagenic to humans, but also because many Azo dyes and their breakdown products are harmful to aquatic life due to the presence of aromatics and metals, chlorides, and other chemicals. Various kinetic models, including modified Gompertz, Baranyi-Roberts, modified Richards, Von Bertalanffy, modified Logistics, modified Schnute, Buchanan three-phase, and the most recently presented Huang, were used in this study. Based on statistical tests, the modified Schnute model provided the best fit, with the lowest values for RMSE and corrected Akaike Information Criteria (AICc), the greatest value for adjusted R^2, and the closest to unity for both Accuracy and Bias Factor. The Modified Schnute parameters such as λ (lag time), μ_{max} (maximum specific bacterial growth rate) and curve fitting parameters α and β (Constant), were found to be -4.39 (95% confidence interval of -77.58 to 68.79), 57.00 (95% confidence interval of -2854.30 to 2968.30), 0.78 (95% confidence interval of -0.34 to 1.89) and 0.96 (95% confidence interval of -0.85 to 2.78, respectively.

INTRODUCTION

The use of dyestuffs has risen steadily as a result of rapid industrialization and man's desire for colour [1]. Industrial effluents are highly coloured, and their disposal into receiving waters harms the environment as a result of the limited light penetration, it may disrupt photosynthetic activity in aquatic life and may also be harmful to some aquatic species due to the presence of aromatics and metals, chlorides, and other chemicals [1–3]. The biological oxygen demand (BOD), chemical oxygen demand (COD), total suspended solids (TSS), and metal pollution due to the presence of dye and additives have all been observed to be high in these sorts of effluents [4]. As a co-pollutant, the azo dye Congo red is common. Annually, nearly one million tons of basic and diazo direct dye are produced. The Ecological and Toxicological Association of the Dyestuff Manufacturing Industry (ETAD) reports that it has the highest levels of toxicity [5]. In the tannery, textile, paper, food, cosmetics, and pharmaceutical industries, dye is used as a colorant during the dyeing process. It is also used in printing and dyehouses [1,2,6]. It tends to pass through traditional water treatment systems unscathed because it is brightly coloured and water-soluble. As a result, the textile finishing industry is well known for contributing to one of the highest levels of water pollution, as 10-15% of dyes are lost in the effluent during the dyeing process [5].

Azo dye is a major source of concern because dye precursors or its biotransformation products, such as aromatic amines, has been linked to cancer and mutation [7]. The azo dye has a chromophore azo group (N=N) that gives the materials colour. Based on the number of azo groups present, azo dyes can be classified as monoazo, diazo, or polyazo dyes [8]. Azo dyes are characterised as direct, reactive, dispersion, metalized, cationic, and anionic azo dyes based on their applications [9]. The removal of dyes from wastewater effluent has been utilized by a variety of physical and chemical treatment processes, including ozonation, photooxidation, electrocoagulation, froth flotation

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reverse osmosis, ion exchange, membrane filtering, and flocculation. These procedures, on the other hand, have the disadvantages of being expensive and commercially unviable, less efficient, producing difficult-to-dispose wastes, and potentially causing additional environmental problems. Biodegradation is a cost-effective and dependable method for removing pollutants from wastewater [1,6,8,10]. Using bacteria and other microorganisms such as *Acinetobacter* sp., White rot fungi, *Shewanella oneidensis*, and *Aspergillus ochraceus*, azo dyes can be degraded. During the process, the azo-bonds (–N=N–) present in the dye are reductively cleaved, releasing aromatic amines and removing the effluent's colour [2,3]. Mathematical modeling analysis were employed where data from fig 2 of Xun-an Ning, et. al. was used [2]. A variety of models for pollutant biodegradation have been published in several research [9,11–15].

MATERIALS AND METHODS

Data Origin

The graphical data from Fig. 2. of the published work by Xun-an Ning et al. [2] of decolorization and biodegradation of the azo dye congo red by an isolated *Acinetobacter baumannii* YNWH 226 was processed using the software Webplotdigitizer [16], which digitises the scanned graph and has been used and acknowledged by many researchers because of its precision and reliability [9,15,17,18]. After processing the data, it was modelled using the CurveExpert Professional software (Version 2.6.5).

Fitting of the data

Nonlinear regression utilizing the Marquardt algorithm was used to fit the bacterial growth curve using several growth models (**Table 1**) using CurveExpert Professional software (Version 2.6.5). The algorithm seeks the most efficient approach for reducing the sum of squares between predicted and measured values. The software can be manually or automatically coded to estimate parameter initial values and the sharpest gradient search of the curve between the four datum points was used to estimate the μ_{max}.

Statistical analysis

The statistically significant difference between the models was calculated using several approaches such as the adjusted determination coefficient (R2), accuracy factor (AF), bias factor (BF), root-mean-square error (RMSE), and AICc (Akaike Information Criterion) corrected as previously [5,15,18,19]. Ross and McMeekin [20] were the first to suggest BF and AF.

RESULTS AND DISCUSSION

Modified Schnute was shown to have the best performance based on the bacterial growth modelling (**Figs. 1-8**), with the lowest AICc, RMSE, and modified R2 values. The AF and BF values for the model were also good, with their values being the closest to 1.0. Modified Richards with the highest AICc and RMSE values had the worst result, failing to model the growth curve (**Table 2**). The Modified Schnute model coefficients parameters are shown in **Table 3**.

Table 1. Growth model used in this research.

Model	Equation
modified Logistic	$y=\frac{A}{\left\{1+\exp\left[\frac{4\mu_m}{A}(\lambda-t)+2\right]\right\}}$
modified Gompertz	$y=A\exp\left\{-\exp\left[\frac{\mu_m e}{A}(\lambda-t)+1\right]\right\}$
modified Richards	$y=A\left\{1+v\exp(1+v)\exp\left[\frac{\mu_m}{A}(1+v)\left(1+\frac{1}{v}\right)(\lambda-t)\right]\right\}$
modified Schnute	$y=\left(\mu_m\frac{(1-\beta)}{\alpha}\right)\left[\frac{1-\beta\exp(\alpha\lambda+1-\beta-\alpha t)}{1-\beta}\right]^{\frac{1}{\beta}}$
Baranyi-Roberts	$y=A+\mu_m x+\frac{1}{\mu_m}\ln\left(e^{-\mu_m x}+e^{-h_0}-e\right.$ $\left.-\ln\left(1+\frac{e^{\mu_m x+\frac{1}{\mu_m}\ln\left(e^{-\mu_m x}+e^{-h_0}-e^{-\mu_m x-h_0}\right)}-1}{e^{(y_{max}-A)}}\right)\right)$
von Bertalanffy	$y=K\left[1-\left[1-\left(\frac{A}{K}\right)^3\right]\exp^{-\left(\mu_m x/3K^{\frac{1}{3}}\right)}\right]^3$
Huang	$y=A+y_{max}-\ln\left(e^{A}+\left(e^{Y_{max}}-e^{A}\right)e^{-\mu_m B(x)}\right)$ $B(x)=x+\frac{1}{\alpha}\ln\frac{1+e^{-\alpha(x-\lambda)}}{1+e^{\alpha\lambda}}$
Buchanan three-phase linear model	Y = A, IF X < LAG Y=A + K(X–λ), IF λ ≤ X ≥ X_{MAX} Y = Y_{MAX}, IF X ≥ X_{MAX}

Note:
A= Bacterial growth lower asymptote;
μ_{max}= maximum specific bacterial growth rate;
v= affects near which asymptote maximum growth occurs.
λ=lag time
y_{max}= Bacterial growth upper asymptote;
e = exponent (2.718281828)
t = sampling time
α,β, k = curve fitting parameters
h_0 = a dimensionless parameter quantifying the initial physiological state of the reduction process. The lag time (h^{-1}) can be calculated as $h_0=\mu_{max}$

Table 2. Statistical tests for the various models used in modelling the growth curve of *Acinetobacter baumannii* YNWH 226

Model	*p*	RMSE	adR^2	AF	BF	AICc
Huang	4	0.136	0.975	3.084	2.57	44.14
Baranyi-Roberts	4	0.090	0.989	3.004	2.47	38.29
modified Gompertz	3	0.136	0.977	3.175	2.73	2.12
Buchanan-3-phase	3	0.200	0.951	3.175	2.78	7.53
modified Richards	4	0.157	0.965	3.100	2.73	46.14
MS	3	0.082	0.992	3.026	2.48	-4.93
modified Logistics	3	0.192	0.952	3.140	2.85	6.98
von Bertalanffy	3	0.113	0.984	3.076	2.63	-0.40

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The Modified Schnute parameters such as λ (lag time), μ_{max} (maximum specific bacterial growth rate) and curve fitting parameters α and β (Constant), were found to be -4.39 (95% confidence interval of -77.58 to 68.79), 57.00 (95% confidence interval of -2854.30 to 2968.30), 0.78 (95% confidence interval of -0.34 to 1.89) and 0.96 (95% confidence interval of -0.85 to 2.78, respectively (**Table 3**).

Table 3. Growth coefficients as predicted by the Modified Schnute model.

	μ_{max} (h^{-1})	β	α	λ
Value	57.001004	0.965313	0.776127	-4.396026
Std Err	914.799833	0.570316	0.350422	22.999094
Range (95% Confidence)	-2854.30 to 2968.30	-0.84 to 2.78	-0.33 to 1.89	-77.58 to 68.79

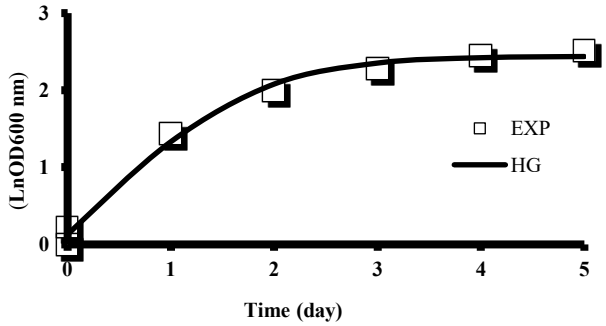

Fig. 1. Growth of *Acinetobacter baumannii* YNWH 226 modeled using the Huang model.

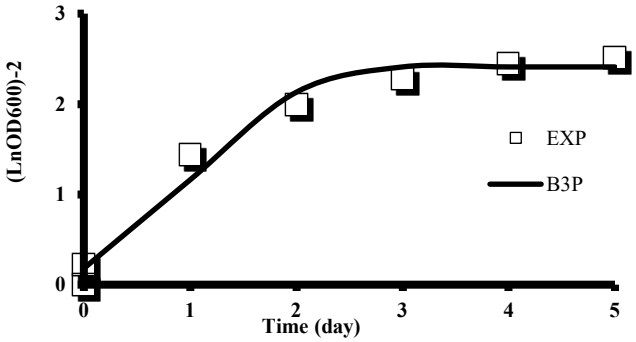

Fig. 2. Fiq.1. Growth of *Acinetobacter baumannii* YNWH 226 modeled using the Buchanan-3-phase model.

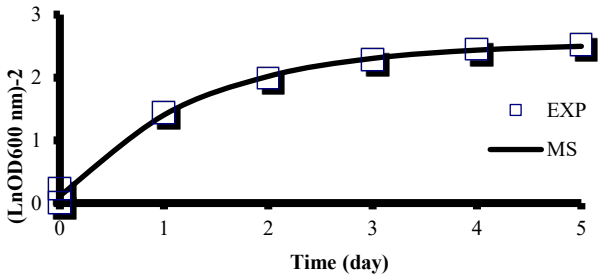

Fig. 3. Growth of *Acinetobacter baumannii* YNWH 226 modeled using the Modified Schnute model

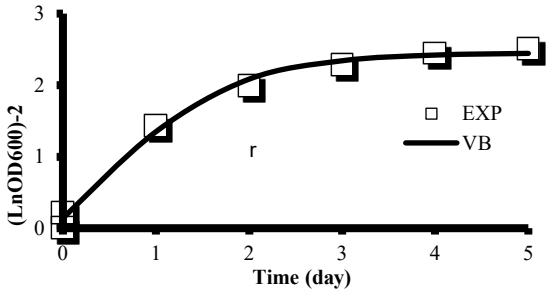

Fig. 4. Growth of *Acinetobacter baumannii* YNWH 226 modeled using the von Bertalanffy model.

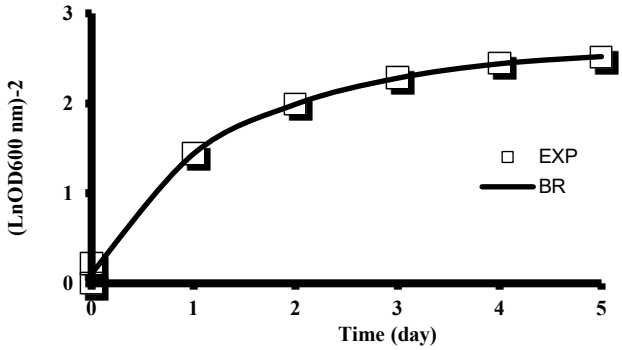

Fig. 5. Growth of *Acinetobacter baumannii* YNWH 226 modeled using the Baranyi-Roberts model.

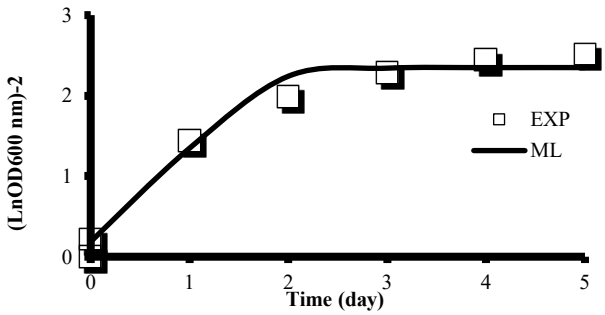

Fig. 6. Growth of *Acinetobacter baumannii* YNWH 226 modeled using the modified Logistics model

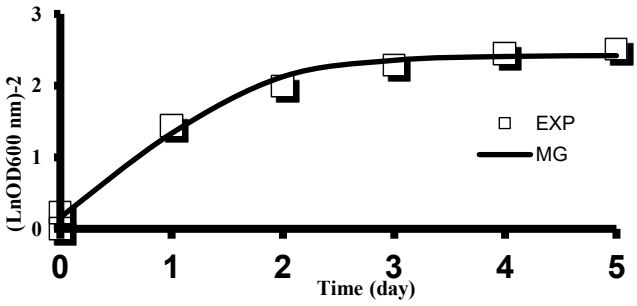

Fig. 7. Growth of *Acinetobacter baumannii* YNWH 226 modeled using the modified Gompertz model.

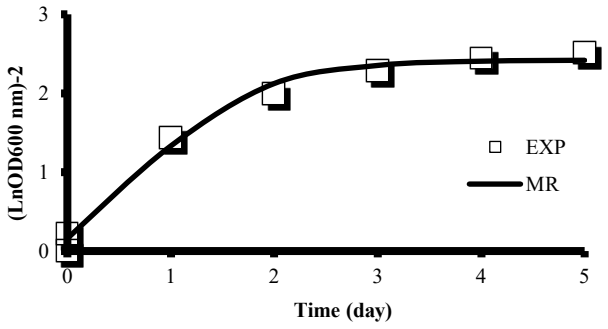

Fig. 8. Growth of *Acinetobacter baumannii* YNWH 226 modeled using the modified Richards model.

In contrast to bacterial growth, fish growth does not appear to achieve or is difficult to establish its asymptotes. The Schnute model was developed to model fish growth. Schnute's model is comparable to Richards' approach in many respects. Depending on the predicted coefficients for a given data set, both of these models can represent various shape relationships, such as concave, parabolic and sigmoidal-shape growths. The Schnute model was also utilized in modeling β-carotene production by *Dunaliella salina* in comparison to other models such as the modified Logistic, Gompertz, Richards, and Stannard models [21]. In a number of cases, the four-parameter Schnute model [22] was statistically better than the three-parameter Gompertz model in modelling the growth of *P. putida* and *E. agglomerans* [23]. The Schnute model was also a better model than other models such as von Bertalanffy, logistic, Gompertz and Schnute-Richards in modelling the growth of the Cortes geoduck *Panopea globosa* [24]. The Schnute model has also found application in modelling growth of forest species [25].

CONCLUSION

In conclusion the Modified Schnute model was the best model in modeling the growth curves of the bacterium under study, based on statistical tests such as corrected AICc (Akaike Information Criterion), bias factor (BF). The modified Schnute parameters obtained from fitting were λ (lag time), μ_{max} (maximum specific bacterial growth rate), α and β(Constant). As a result, the modified Schnute was found to be the best model for growing *Acinetobacter baumannii* YNWH 226 on Azo dye Congo red.

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