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Kinetics Modeling on the Biosorption of Remazol Black B Dye by *Aspergillus flavus*

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ABSTRACT

Azo dyes, such as Remazol Black B, are different from conventional dyes in that they establish covalent bonds with textile fibers like cotton. They are widely utilized in the textile industry because of their favorable properties of bright color, water resistance, simple application procedures, and low energy consumption. Their discharge into receiving streams has major environmental consequences, such as reducing photosynthesis in aquatic life due to lower light penetration. The biosorption isotherm data of Remazol Black B dye biosorption by *Aspergillus flavus* were investigated using two models—pseudo-1st order and pseudo-2nd order—and fitted using non-linear regression. The pseudo-1st order model was found to be the best by statistical analysis using root-mean-square error (RMSE), adjusted coefficient of determination ($adjR^2$), bias factor (BF), accuracy factor (AF), corrected AICc (Akaike Information Criterion), Bayesian Information Criterion (BIC), and Hannan–Quinn information criterion (HQC). At 250 mg/L, kinetic analysis using the pseudo-1st order model yielded an equilibrium sorption capacity q_e of 4.61 mg/g (95 % confidence interval from 4.54 to 4.68) and a pseudo-1st-order rate constant, k_1 of 0.15 (95% C.I. from 0.128 to 0.164).

INTRODUCTION

Dyes are one of the most important hazardous compounds found in industrial effluents that must be treated because their presence in water bodies reduces light penetration, preventing photosynthesis of aquatic flora as well as being aesthetically objectionable for drinking and other purposes [1]. Azo dyes, such as Remazol Black B, are different from conventional dyes in that they establish covalent bonds with textile fibers like cotton. They are widely utilized in the textile industry because of their favorable properties of bright color, water resistance, simple application procedures, and low energy consumption [2]]. The correct assignment of the kinetics study is critical in understanding the mechanism of biosorption of Remazol Black B dye. The use of linearization on an obviously nonlinear curve disrupts the error structure of the data. This makes estimating the uncertainty of the kinetics parameters, which are commonly displayed as a 95 percent confidence interval range, even more difficult [3]. Furthermore, the weight assigned to each data point can be changed, which usually results in differences in the fitted parameter values between the linear and nonlinear versions of the kinetics model [4]. In this study, the published data (figure 6) from Biosorption of Remazol Black B dye (azo dye) by growing *Aspergillus flavus* [[5] is remodelled using different kinetic models, then regressed using nonlinear regression approach, and the best model was determined using various error function analyses. The purpose for this modeling analysis is that in the original paper, there was no modeling exercise for the kinetics.

MATERIALS AND METHODS

Data Acquisition

The software Webplotdigitizer 2.5 [6] was used to digitize data from Figure 6 from a published work [5]. The accuracy of digitization using this program has been used and acknowledged by many researchers [7–9]. The data was then nonlinearly regressed using multiple models in the curve-fitting software CurveExpert Professional (Version 2.6.5) (Table 1).

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Table 1. Kinetics Models used in the study

Model	Equation	Reference
Pseudo-1st order	$q_t = q_e(1 - e^{-K_1 t})$	[9]
Pseudo-2nd order	$q_t = \frac{K_2 {q_e}^2 t}{(1 + K_2 q_e t)}$	[10]

Statistical analysis

Corrected AICc (Akaike Information Criterion), Bayesian Information Criterion (BIC), Hannan and Quinn's Criterion (HQ), Root-Mean-Square Error (RMSE), bias factor (BF), accuracy factor (AF), and adjusted coefficient of determination (R2) are some of the most widely used statistical discriminatory methods.

The RMSE was determined using Eq. (1) [11] and it is expected that a lesser number of factors will result in a lower RMSE value. The number of experimental data is n, the experimental and projected data are Obi and Pdi, and the number of parameters is p.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(Pd_i - Ob_i)^2}{n - p}} \qquad \text{(Eqn. 1)}$$

Because R2, or the coefficient of determination, does not take into account the number of parameters in a model, the adjusted R^2 is used to overcome this limitation. The total variance of the y-variable is given by S_y^2 in the equation (Equations 2 and 3), where RMS is the Residual Mean Square.

$$Adjusted\left(R^2\right) = 1 - \frac{RMS}{s_Y^2} \qquad \text{(Eqn. 2)}$$

$$Adjusted\left(R^2\right) = 1 - \frac{\left(1 - R^2\right)(n-1)}{(n-p-1)} \qquad \text{(Eqn. 3)}$$

The Akaike Information Criterion (AIC) is an information theory-based criterion. It strikes a balance between a model's goodness of fit and its complexity [12]. The corrected Akaike information criterion (AICc) is used to manage data with a large number of parameters or a small number of values (Burnham and Anderson 2002). The AICc is calculated as follows (Eqn. 4), where p represents the number of parameters and n represents the number of data points. A model with a lower AICc value is thought to be more accurate (Burnham and Anderson 2002).

$$AICc = 2p + n\ln\left(\frac{RSS}{n}\right) + 2(p+1) + \frac{2(p+1)(p+2)}{n-p-2} \qquad \text{(Eqn. 4)}$$

Aside from AICc, the Bayesian Information Criterion (BIC) is another statistical tool based on information theory (Eqn. 5). This error function penalises the number of parameters more precisely than AIC [13].

$$BIC = n.\ln\frac{RSS}{n} + k.\ln(n) \qquad \text{(Eqn. 5)}$$

The Hannan–Quinn information criterion (HQC) is another error function approach based on information theory (Eqn. 6). Because of the ln ln n term in the equation, the HQC is more consistent than the AIC [14].

$$HQC = n \times ln\frac{RSS}{n} + 2 \times k \times ln(\ln n) \qquad \text{(Eqn. 6)}$$

The Accuracy Factor (AF) and Bias Factor (BF) are two further error function analyses derived from the work of Ross[15] .These error functions assess the statistical evaluation of models for goodness-of-fit but do not penalise for a lot of parameters (Eqns. 7 and 8).

$$\text{Bias factor} = 10^{\left(\sum_{i=1}^{n}\log\frac{(Pd_i/Ob_i)}{n}\right)} \qquad \text{(Eqn. 7)}$$

$$\text{Accuracy factor} = 10^{\left(\sum_{i=1}^{n}\log\frac{|(Pd_i/Ob_i)|}{n}\right)} \qquad \text{(Eqn. 8)}$$

RESULTS AND DISCUSSION

The biosorption isotherm data from a published work [5] on the biosorption of Remazol Black B dye by *Aspergillus flavus* was examined using two models—pseudo-1st and pseudo-2nd—and fitted with non-linear regression (**Figs. 1-2**). The pseudo-first-order model was found to be the best using statistical analysis based on root-mean-square error (RMSE), adjusted coefficient of determination (adjR2), bias factor (BF), accuracy factor (AF), corrected AICc (Akaike Information Criterion), Bayesian Information Criterion (BIC), and Hannan–Quinn information criterion (HQC). At 250 mg/L, kinetic analysis using the pseudo-1st order model yielded an equilibrium sorption capacity q_e of 4.61 mg/g (95 % confidence interval from 4.54 to 4.68) and a pseudo-1st-order rate constant, k_1 of 0.15 (95% C.I. from 0.128 to 0.164).

The equilibrium sorption capacity q_e in the original published paper was 4.37 mg/g, which is close to the remodeled value. The pseudo-1st order model, due to its mathematical simplicity has found application together with the pseudo-2nd order model in modelling numerous dye sorption kinetics [16–30]. Some works has suggested mechanism of sorption only basing with the kinetics results, which should not be done, as numerous current works have indicated that more results from isotherm, diffusion and thermodynamics works should be obtained before arriving at the conclusion [31–38].

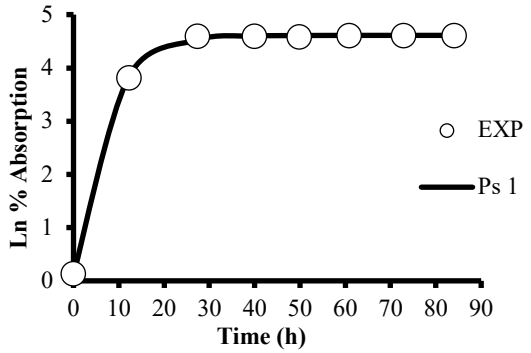

Fig. 1. Kinetic on the Biosorption of Remazol Black dye by *Aspergillus flavus* modelled using Pseudo-First order model.

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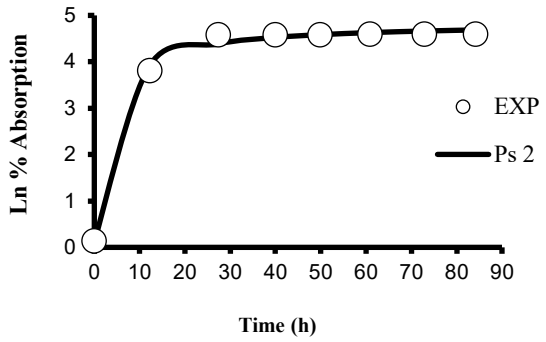

Fig. 2. Kinetic on the Biosorption of Remazol Black dye by *Aspergillus flavus* modelled using Pseudo-Second order model.

Table 2. Analysis of Error Functions for Regressed models.

Model	p	RMSE	adR^2	AICc	BIC	HQC	AF	BF
Pseudo-1st order	**2**	0.032	1.000	-32.41	-46.52	-47.75	1.026	0.978
Pseudo-2nd order	**2**	0.108	0.995	-15.52	-29.62	-30.85	1.025	0.986

CONCLUSION

In conclusion, kinetics modeling on the biosorption of remazol Black B dye by *Aspergillus flavus* was effectively modelled using two models—pseudo-1st and pseudo-2nd order models, which were fitted using non-linear regression.The pseudo-1st model was found to be the best by statistical analysis using root-mean-square error (RMSE), adjusted coefficient of determination (adjR2), bias factor (BF), accuracy factor (AF), and corrected AICc (Akaike Information Criterion). At 250 mg/L, kinetic analysis using the pseudo-1st order model yielded an equilibrium sorption capacity q_e of 4.61 mg/g which was similar to the original published paper of 4.37 mg/g.

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