Mathematical Modeling of The Biodegradation of Phenol from Industrial Effluents Using Immobilized Pseudomonas putida

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INTRODUCTION

Synthetic chemicals are extremely harmful, particularly those man-made ones. Models are used to describe the behavior of microorganisms under different physical or chemical conditions such as temperature, pH, and water activity. Phenol is one of the potentially hazardous synthetic industrial contaminants capable of causing deteriorating effects in humans. In this paper, for the first time we present different kinetics models such as Von Bertalanffy, Baranyi-Roberts, modified Schnute, modified Richards, modified Gompertz, modified Logistics and the most recent Huang were used to get values for the above kinetic constants or parameters from simultaneous biodegradation of phenol from industrial effluents using immobilized Pseudomonas putida. All the curves present the best models with highest adjusted \( R^2 \) value with the lowest RMSE and AICc value. The Accuracy and Bias Factors values were close to unity (1.0). Nearly all of the models best fit the curves indicating that Pseudomonas putida growth on phenol can be described mathematically the modelling parameters obtained can be utilized for predicting bioremediation of phenols in batch culture and perhaps in the future will be valuable in modelling growth on industrial effluent containing phenol.

Keywords
phenol
Pseudomonas putida
mathematical modelling
growth
Gompertz, modified logistics and Stannard [5]. They were compared statistically using a comprehensive model (Schunke model), which is a model that encompasses all other models. All sigmoidal functions have been updated to include all biologically important parameters. The Stannard, Schunke and Richards models appeared essentially to be the same [6]. The Gompertz equation was statistically adequate in the experiments to describe the growth data for caffeine [7]. The value of the growth curve is the maximum specified growth rate ($\mu_{max}$ or $\mu_0$), delay time and asymptotic values. For secondary models to analyze the effects of the substrate, temperature, pH, and product on growth rate, a maximum specific growth rate ($\mu_{max}$) value can be utilized. While the two categories can exist side by side, in fact, most bacterial growth models are between mechanistic and empirical features [8]. In this study, the use of primary models to model the phenol biodegradation of coke oven effluents using immobilized Pseudomonas putida is discussed for the first time.

**MATERIALS AND METHODS**

Data from Fig 1. from Singh et al [9] was processed using the software Webplotdigitizer 2.5 [10] which digitizes the scanned figure and has been utilized by many researchers and acknowledged for its reliability [11,12].

**STATISTICAL ANALYSIS**

Statistical significant difference between the models was calculated through various methods including the adjusted coefficient of determination ($R^2$), accuracy factor (AF), bias factor (BF), Root-Mean-Square Error (RMSE) and corrected AICc (Akaike Information Criterion) as before [11].

**FITTING OF THE DATA**

Fitting of the bacterial growth curve using various growth models (Table 1) was carried out using the CurveExpert Professional software (Version 1.6) by nonlinear regression utilizing the Marquardt algorithm. $\mu_{max}$ of estimation was carried out by the steepest ascent rifle of the curve while the crossing of this line with the x-axis is an estimation of $\lambda$. The highest growth was chosen for the modelling exercise.

**RESULTS AND DISCUSSION**

Out of the eight different models analysed it was shown that all the models show acceptable model fittings (fig 2 to 8) which were effective and relevant for the biodegradation of phenol present in coke-oven effluent using immobilized Pseudomonas putida. The best performance was measured using the lowest value for RMSE, AICc and the highest value for adjusted $R^2$. The AF and BF values were also excellent for the model with their values were the closest to 1.0.

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**Table 1: Growth models used in this study.**

<table>
<thead>
<tr>
<th>Model</th>
<th>$p$</th>
<th>$A$</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Modified Logistic</td>
<td>3</td>
<td>$\frac{y}{A}$</td>
<td>$\frac{1}{1+\exp\left(\frac{4\mu_{max}(\lambda-1)+2}{A}\right)}$</td>
</tr>
<tr>
<td>Modified Gompertz</td>
<td>3</td>
<td>$y=\exp\left(\frac{-\mu_{max}t}{A}\right)$</td>
<td>$\frac{1}{1+\exp\left(\frac{4\mu_{max}(\lambda-1)+2}{A}\right)}$</td>
</tr>
<tr>
<td>Modified Richards</td>
<td>4</td>
<td>$y=\exp\left(\frac{-\mu_{max}t}{A}\right)$</td>
<td>$\frac{1}{1+\exp\left(\frac{4\mu_{max}(\lambda-1)+2}{A}\right)}$</td>
</tr>
<tr>
<td>Modified Schunke</td>
<td>4</td>
<td>$y=\left(\frac{1-\beta}{A}\right)$</td>
<td>$\frac{1}{1-\beta\exp\left(\alpha\lambda+1-\beta\alpha\lambda\right)}$</td>
</tr>
<tr>
<td>Baranyi-Roberts</td>
<td>4</td>
<td>$y=\left(\frac{1}{A}\right)$</td>
<td>$\frac{0.5}{\exp\left(\alpha\lambda-0.5\right)}$</td>
</tr>
<tr>
<td>Von Bertalanffy</td>
<td>3</td>
<td>$y=\left(\frac{1}{A}\right)$</td>
<td>$\frac{0.5}{\exp\left(\alpha\lambda-0.5\right)}$</td>
</tr>
<tr>
<td>Huang</td>
<td>4</td>
<td>$y=A+y_{max}\ln\left(1+e^{-\alpha\lambda}\right)$</td>
<td>$\frac{1}{\alpha\lambda}\ln\left(1+e^{-\alpha\lambda}\right)$</td>
</tr>
<tr>
<td>Buchanan</td>
<td>3</td>
<td>$Y=Y_{MAX}$</td>
<td>IF $X \geq X_{EFFECT}$</td>
</tr>
<tr>
<td>Three-phase linear</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>model</td>
<td>Y = $A_1X &lt; \lambda$</td>
<td>$Y = A + K(X-\lambda)$, IF $\lambda \geq X \geq X_{EFFECT}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Y = $Y_{MAX}$</td>
<td>IF $X \geq X_{EFFECT}$</td>
<td></td>
</tr>
</tbody>
</table>

Note:
- $A$ = Microorganism growth lower asymptote;
- $Y_{MAX}$ = Microorganism growth upper asymptote;
- $\mu_{max}$ = maximum specific microorganism growth rate;
- $\lambda$ = affects near which asymptote maximum growth occurs.
- $\lambda$ = lag time
- $e$ = exponent (2.718281828)
- $t$ = sampling time
- $\alpha,\beta,k$ = curve fitting parameters
- $\delta_0$ = a dimensionless parameter quantifying the initial physiological state of the reduction process. The lag time (h$^{-1}$) or (d$^{-1}$) can be calculated as $\delta_0 = \mu_{max}$.
Fig. 1. Growth of *Pseudomonas putida* (NAUN-16) in nutrient broth (NB) supplemented with various concentrations of phenol.

Fig. 2. Growth of *Pseudomonas putida* as modelled using the Huang model.

Fig. 3. Growth of *Pseudomonas putida* as modelled using the modified Gompertz model.

Fig. 4. Growth of *Pseudomonas putida* as modelled using the Buchanan-3-phase model.

Fig. 5. Growth of *Pseudomonas putida* as modelled using the modified Richard model.

Fig. 6. Growth of *Pseudomonas putida* as modelled using the modified Logistics model.

Fig. 7. Growth of *Pseudomonas putida* as modelled using the von Bertalanffy model.

Fig. 8. Growth of *Pseudomonas putida* as modelled using the Baranyi-Roberts model.
The Gompertz model is well-known and commonly used in many fields of biology. This has also been used to explain the growth of animals and plants, as well as the amount or volume of bacteria and cancer cells [13]. The logistic function also fits a sigmoid curve, but the modified model adds a lag time to account for a latency phase, as in the modified Gompertz model [14]. Huang’s model is compared with Baranyi and modified Gompertz model. Buchanan’s three-phase model also has acceptable practical identifiability properties in the presence of realistic data, which means that the confidence intervals on the parameter values are reasonable [16]. On the other hand, von Bertalanffy curve is used to model mean length from age in animals. The function is commonly applied in ecology to model fish growth, however it is now used in all organisms including biodegradation by bacteria [17].

Parameters obtained from the fitting exercise were maximum growth rate (μmax), lag time (θ) and maximal growth (Ymax). In basic research, these mechanistic models are used and are meant to reach a better understanding of the biological, chemical and physical processes that lead to the growth profile seen. All other things being equal, mechanistic models are more powerful since they tell you about the fundamental procedures driving patterns. They are more probable to work properly when concluding beyond the observed conditions [18].

CONCLUSION

In conclusion, the use of mathematical models to model the biodegradation of synthetic environmental chemical toxica tants is not very common, though very important. In our study the use of immobilized bacteria (*Pseudomonas putida*) for the biodegradation of phenol present in coke-oven was modelled, and all the models best fitted the curves.

REFERENCES