Modeling and Simulation of Biodegradation Process in a Batch Reactor

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Abstract: **The objectives of this study is to find the kinetic constants and then to simulate the data using the constants. In this work, the experimental data obtained from atrazine biodegradation and starch biodegradation were used. From the experimental data, the kinetic constants were calculated. Using the values the degradation data were simulated and compared with the experimental values. High correlation value more than 0.99 value show the simulation values fits the experimental values.**

Keywords —Atrazine, biodegradation, modeling, Kinetic constant, substrate utilization and simulation

I. INTRODUCTION

The world practice of using agro-chemicals for long periods, in an indiscriminated and abusive way, has been a concern of authorities involved in public health and sustainability of natural resources, as a consequence of environmental contamination. Atrazine is widely used in sugarcane, corn and sorghum cultures. Researchers have demonstrated that atrazine has toxic effects in algae, aquatic plants, aquatic plants, aquatic insects, fishes and mammals. Due to the toxicity and persistence of atrazine in the environment, the search of microbial strains capable of efficient degradation it is fundamental to the development of bioremediation processes, as corrective tools to solve the current problems of the irrational use of atrazine [1-5]. Atrazine removal is carried out by physical, chemical, and biological methods. In general, biological treatment processes have advantages over physical and chemical treatment methods. It is cost effective and environmental friendly. Few works are available on biodegradation of atrazine [6–8].

The process of extracting starch from tapioca tubers require large quantities of water and significant quantum of wastewater is generated during the process, which ultimately is the major contributor of pollutants. The effluent generated from tapioca based sago industry is acidic with high organic and solid content. It poses a serious threat to environment and quality of life in rural areas, where these factories are situated. The impacts of the pollution problems created by starch industries are well explained [9-10].

In the present study, a model was used to describe the behavior of biodegradation system. The model can provide insights to the analysis conducted during the course of operation of the bioreactor. In this study, the kinetic model was used since these types of models are much easier to apply and they are accurately proved that the model can express many biodegradation processes.

II. MATERIALS AND METHODS

Atrazine was locally procured from the market. Sludge from an anaerobic pond treating pharmaceutical wastewater, was used as inoculum for the present study. 500cc Erlenmeyer flasks were used as batch reactors. 100 cc of 100 mg atrazine /L was taken in the batch reactor and seed sludge 2g/L is added to it. The pH of the wastewater is adjusted to 7 by adding acid or base as required. The COD of the wastewater in each batch reactor are measured at regular time intervals.

The wastewater is collected from the small-scale tapioca based starch industries located near Athur in Tamilnadu, India. The combined wastewater is stored at 5^0 C in a freezer. The seed sludge for the batch degradation study is brought from the aerobic pond treating the starch wastewater. 250cc Erlenmeyer flasks are used as a batch reactor. 100 cc of wastewater obtained from the starch industry is taken in the batch reactor and seed sludge 4g/L is added to it. The pH of the wastewater is adjusted to 7 by adding acid or base as required. The COD of the wastewater in each batch reactor are measured at regular time intervals. The initial concentration of the wastewater is approximately 2250 mg COD/L.

III. KINETIC MODELS

The simplest kinetic model expresses the stoichiometric relation for product formation and substrate utilization is

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unstructured model. In this study, the unstructured model was used. The rate equation is expressed by the biomass concentration (X), removal efficiency (P) and substrate concentration (S) to describe the degradation process.

A. Microbial growth

Based on the rate of cell growth, the biomass can be calculated using the logistic equation representing both the exponential and stationary phase, is written as [11]:

$$X = \frac{X_m e^{\mu_m t}}{1 - \left(\frac{X_O}{X_m}\right)\left(1 - e^{\mu_m t}\right)} \qquad (1)$$

Where X - Biomass concentration (g/L)

X_o - Initial maximum biomass concentration (g/L)

X_m - Maximum biomass concentration (g/L)

μ - Specific growth rate

μ_m - maximum specific growth rate (h^{-1})

k - promotion or decline of cell population in the batch culture

To predict the biomass concentration, the following equation is used [11].

$$X = \frac{X_m e^{\mu_m t}}{1 - \left(\frac{X_O}{X_m}\right)\left(1 - e^{\mu_m t}\right)} \qquad (2)$$

B. Substrate uptake

A carbon source, is used to support cell viability. The substrate consumption equation used is as follows (Mohammad Pazouki1 et al 2008).

$$S = S_o - \frac{X_o e^{\mu_m t}}{Y_{X/S}\left[1 - \left(\frac{X_O}{X_m}\right)\left(1 - e^{\mu_m t}\right)\right]} + \frac{X_o}{Y_{X/S}} - \frac{X_m m_s}{\mu_m} \ln\left[1 - \left(\frac{X_o}{X_m}\right)\left(1 - e^{\mu_m t}\right)\right] \qquad (3)$$

S – Substrate Concentration, g/L

S_o – Initial Substrate Concentration, g/L

$Y_{X/S}$ – Yield of Biomass

C. Atrazine degradation

The product formation rate, dP/dt allows a correlation between the cell mass and product concentration. For the growth associated product formation (Mohammad Pazouki1 et al 2008):

$$P = K + bX \qquad (4)$$

In this study, equations 1,2,3,4 were used to simulate the experimental results

IV. RESULTS AND DISCUSSION

Batch study has been performed in a bio reactor at an initial substrate concentration of 100 mg of atrazine/L. The performance of the bioreactor for the biodegradation of atrazine is illustrated in Figure 1. The atrazine concentration decreased from 100 mg/L to 19 mg/L on ten days of operation. The figure shows that a maximum of 81% removal efficient occurs on the tenth day of operation. Also a maximum biomass concentration of 6.5 g/L was attained at the end of tenth day of operation. Similarly in Fig.2, the performance of bioreactor for starch industry wastewater was depicted. The results show that as the time progresses the substrate concentration decreases and reaches a final value of 265 mgCOD/L. The maximum percentage COD removal of 88.3%, is obtained for the initial concentrations of 2250 mg COD/L.

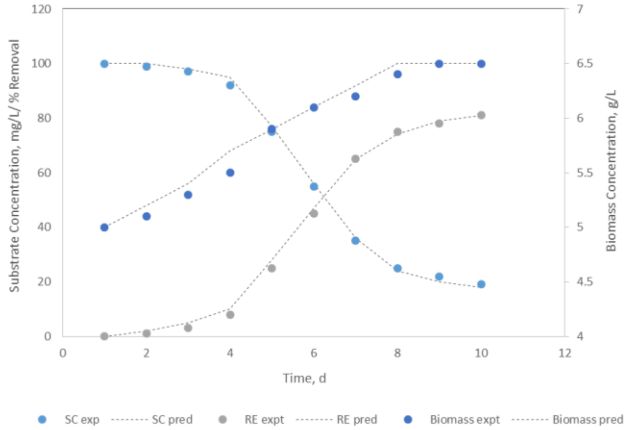

Fig.1 Comparison of experimental and simulated values for the degradation of atrazine

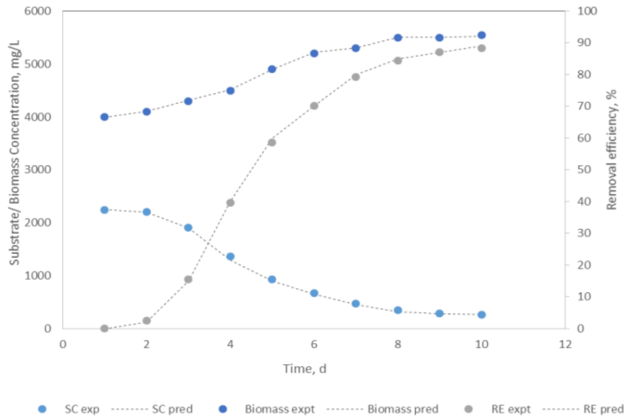

Fig.2 Comparison of experimental and simulated values for the degradation of Starch industry wastewater

The kinetic constants in the equation were calculated and they were given in the Table 1. These calculated values were used to simulate the data.

Table 1. Constants estimated using the equation from experimental data

Parameters	Atrazine	Starch wastewater
μ_m, h^{-1}	0.089	0.74
X_m, g/L	6.6	5.4
X_o, g/L	5.0	4.0
K	-19.5	-42
B	10.2	18.5
$Y_{X/S}$	0.65	0.9
m_s	0.0006	0.0008

The simulation results were also given in Fig.1 and 2. The dotted line in the figure shows the simulated values of substrate concentration (SC), removal efficiency (RE) in %,

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and biomass concentration. From the figures it is clear that the model predict the data well. The R^2 value in the Table 2 shows that, for all the parameters the R^2 value was found to be more than 0.99. This indicates that the model predict the biodegradation process well. This is clearly depicted in Fig. 3-8 also.

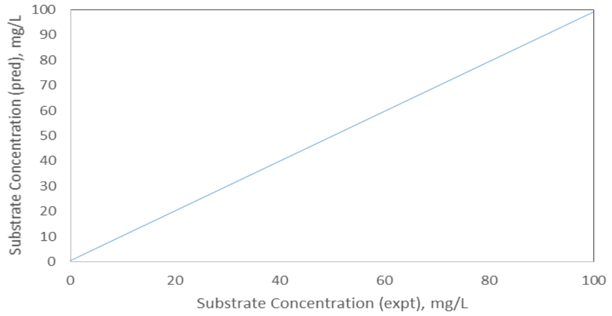

Fig.3. Comparison of experimental substrate concentration with predicted substrate concentration for atrazine degradation

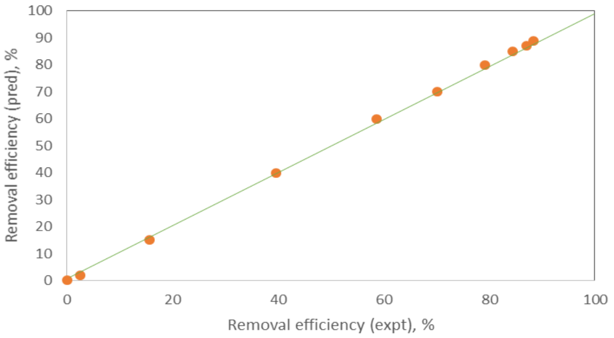

Fig.4. Comparison of experimental removal efficiency with predicted removal efficiency for atrazine degradation

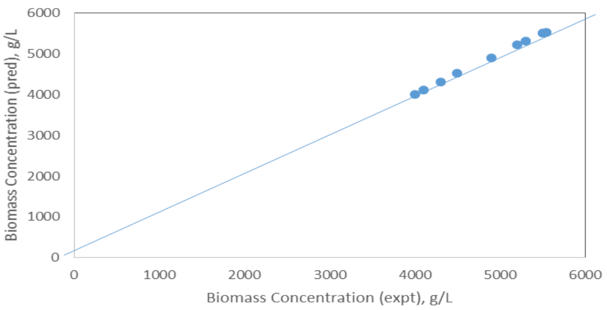

Fig.5. Comparison of experimental biomass concentrations with predicted biomass concentrations for atrazine degradation

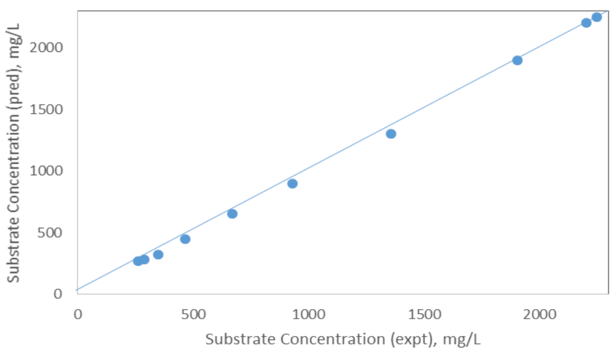

Fig.6. Comparison of experimental substrate concentration with predicted substrate concentration for starch wastewater degradation

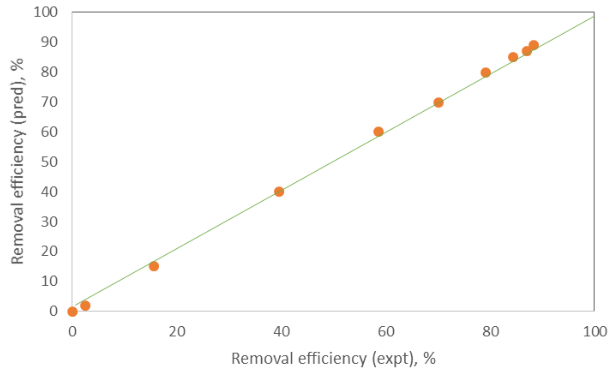

Fig.7. Comparison of experimental removal efficiency with predicted removal efficiency for starch wastewater degradation

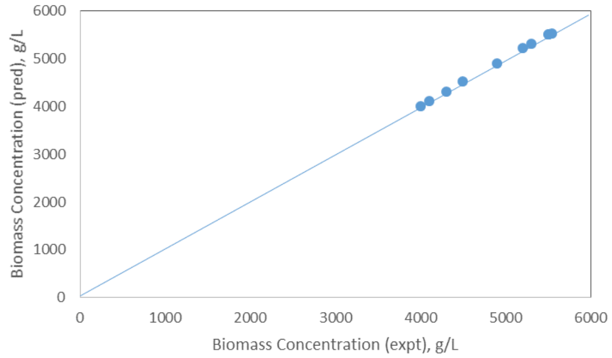

Fig.8. Comparison of experimental biomass concentrations with predicted biomass concentrations for starch wastewater degradation

Table 2 Correlation coefficient

Parameters	Atrazine	Starch wastewater
SC	0.9987	0.9992
RE	0.9978	0.9996
Biomass	0.9924	0.9995

V. CONCLUSION

In this work, the kinetic models has been utilized to study the biodegradation of atrazine and starch industry wastewater. The constants were evaluated and they were used to simulate the biodegradation process. The results shows that the model predicts the experimental data well. It is confirmed by high R^2 values. It shows that these kinetic models can be effectively utilized for various biodegradation process.

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