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# Batch Degradation Of Thiocyanate And Kinetic Modelling.

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## ABSTRACT

Bacillus brevis was isolated from carbonization wastewater soil suspension of Briquetting and Carbonization Plant, NLC Limited, Neyveli. Batch degradation of Thiocyanate by Bacillus brevis was carried out using optimized Moving-Bed Biofilm Sequencing Batch Reactor. This model was suitable and resulted in a good correlation ($R^2 > 0.99$) at all thiocyanate concentration variations. This revealed that the predicted data was in good agreement with the experimental data for the batch degradation of thiocyanate.

**Keywords:** Batch Degradation, *Bacillus brevis*, Thiocyanate, Kinetic Modelling, Moving-Bed Batch Reactor.

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## INTRODUCTION

Briquetting and Carbonization Plant wastewater with high organic loading causes a lot of environmental problems and increased treatment cost[1,2]. Hence the best solution is to adopt a low cost bio-reactor with efficient treatment [3,4]. Moving-bed biofilm sequencing batch reactor (MBSBR) is obtained by combining Moving-bed biofilm reactor (MBBR) and sequencing batch reactor (SBR) processes for treating industrial discharges[5]. Advantages of this process are: Attached growth, suspended growth, stable performance, operation simplicity and flexibility, reactor volume reduction, no sludge return and strong resistance to impact [5-8]. SBR is one among the most common activated sludge modifications, which greatly enhance the treatment process.

### Kinetic Modelling

Kinetic modelling is an analytical method to predict and optimize the reactor performance. Various mathematical modelling have been used to predict the performance [9,10]. Monod model was used to assess performance of reactor efficiency in wastewater treatment and to calculate kinetic constants [11,12].

“ Fig . 1”

The Batch reactor, shown in Fig. 1, is a simple device reported earlier and is adaptable to a small scale set up [13]. In the biological process the experimental batch reactor is operated isothermally and at constant volume. The kinetic parameters estimated for a batch reactor are to be used for the determination of kinetic data of largescale continuous flow reactors. This data is utilized for the design of largescale reactors and also to predict the performance in industries[13].

We have isolated a novel strain of *Bacillus brevis* from the Briquetting and Carbonization Plant wastewater and reported its fatty acid profile [14].This microbe was utilized for the degradation of thiocyanate. In the present paper, the results of batch degradation of thiocyanate obtained experimentally and by mathematical modelling are compared and discussed.

## EXPERIMENTAL

A bacterium from the soil suspension of Briquetting & Carbonization Plant effluent was isolated and identified as *Bacillus brevis* according to its morphological, physiological, and biochemical properties. Medium used for growth of bacterium, its isolation and identification are detailed in our earlier publication [14]. The consortium was found to assimilate thiocyanate as a dietary source. Thus the bacterium used thiocyanate as a carbon and nitrogen source and sulphate transformation for energy [15].

### Analysis Of Thiocyanate

Thiocyanate was estimated by its reaction with iron (III) to form orange-red color complex. The thiocyanate concentration was determined photometrically from the absorbance at 465 nm using a spectrophotometer. Biomass concentration was found from the absorbance at 600 nm and correlated by the standard biomass concentration [16].

### Experimental Design To Study Degradation

A sample of 100 ml was taken in each 250 ml conical flask. Each sample contained the minimal medium with different thiocyanate concentrations as the sole carbon, nitrogen source. The flasks were kept at 34±0.1 ◦ C with the shaker speed at 150 rpm.

## RESULTS AND DISCUSSION

The thiocyanate degradation was studied with different initial concentrations of thiocyanate using the cells immobilized on lignite carbon under optimum conditions in a batch reactor. The concentrations of thiocyanate determined at different time intervals are given in Table. 1.

**Table 1: Thiocyanate concentrations (ppm) at different time intervals using Batch Reactor.**

| Initial Concentration of Thiocyanate (ppm) | Hours | | | | | % of Thiocyanate remaining (after 20th hour) |
|---|---|---|---|---|---|---|
| | 4 | 8 | 12 | 16 | 20 | |
| 200 | 160 | 100 | 60 | 40 | 10 | 5 |
| 400 | 300 | 220 | 152 | 96 | 44 | 11 |
| 600 | 550 | 460 | 370 | 290 | 200 | 33.3 |
| 800 | 760 | 640 | 510 | 390 | 280 | 35 |

The percentage of degradation decreases from 95 to 65 (at 20th hour) when the concentration changes from 200 to 800ppm. The activity of the cells are affected above 200ppm. But there is no significant change in percentage decrease above 400ppm. In the study of culture growth and degradation of thiocyanate under different conditions, it was found that the thiocyanate degradation matched with the growth of the culture [17]. This indicates that the reaction is simple and can be written as

$$S \rightarrow P \text{ -------------(1)}$$

in the presence of Biomass –x, S - Thiocyanate, P – Product

## MATHEMATICAL MODELLING

A mathematical model can be obtained for the above reaction (1) The degradation was carried out under isothermal conditions with uniform sized lignite carbon particles.The following assumptions are made.

1. Homogenous distribution of reactivity in the particles.
2. Perfect homogeneity of concentration within the particle.

For the reaction

$$S \rightarrow P \text{ -------------(1)}$$

The rate of production of cell mass is given by Monod's equation.

$$\mu = \frac{1}{X} \frac{dx}{dt} = \frac{\mu_{max}\ S}{K+S} \qquad \ldots\ldots \quad (2)$$

$$\frac{dx}{dt} = \frac{\mu_{max}\ .\ SX}{K+S} \qquad \ldots\ldots \quad (3)$$

In a batch reactor no liquid is added or removed, then the material balance for the reactant 'S' is given by the equation

[18](James E Bailey et al., 1986).

$$\frac{dC_s}{dt} = r_{fs}$$

ie., The rate of the reaction is

$$\frac{dC_s}{dt} \text{ or } \frac{dS}{dt}$$

$\frac{dS}{dt}$ can be written in terms of $\frac{dx}{dt}$

$$\frac{dS}{dt} = \frac{1}{y} \frac{dx}{dt} \qquad \ldots\ldots \quad (4)$$

$$\mathrm{Y} = \frac{dx}{ds} = \frac{\Delta x}{\Delta s} = Y_{x/s}$$

$$= \frac{gms\ of\ cell\ mass\ produced}{gms\ of\ substrate\ \ consumed} = \text{Yield factor}$$

The equation (3) $\dfrac{dx}{dt} = \dfrac{\mu_{max}\ .\ SX}{K+S}$

can be solved for getting kinetic parameters $\mu_{max}$and K using experimental values (set of values for which the error is minimum for curve fitting)[15,19] . Rearranging the equation and substituting different values of K and $\mu_{max}$ in a systematic manner, the optimum values are obtained. For this the equation is transformed by defining the following dimensionless terms.

$$y_1 = \frac{S}{S_0}$$

$$y_2 = \frac{X}{X_0}$$

$$\tau = \mu_{max} t$$

The resulting equations are:

$$\frac{dy_1}{d\tau} = -G_1 \frac{dy_2}{d\tau}$$

$$\frac{dy_2}{d\tau} = \frac{y_1 y_2}{G_2 + y_1}$$

$$\text{At } \tau = 0$$

$$y_1 = 1$$

$$y_2 = 1$$

Substituting the equation (3) in equation (4), we get

$$\frac{dS}{dt} = \frac{1}{y} \frac{\mu_{max}\, S\, X}{K + S}$$

The experimental results were fitted with this equation and the values of parameters were estimated with a tolerance limit of $10^{-6}$

The optimum values obtained for the following terms are

K = 0.1, y = 0.01, $X_0$ = 0.005, $\mu_{max}$ = 0.04

Using these values, the concentrations of thiocyanate at different times were computed. The stiff 3 (differential equation solver) programme was used to solve the model equations for fixed parameter value.

## Validation And Testing

Fig. 2-5 gives the comparison of experimental and predicted data for different concentrations of thiocyanate.

**Fig. 1: Moving-Bed Biofilm Sequencing Batch Reactor**

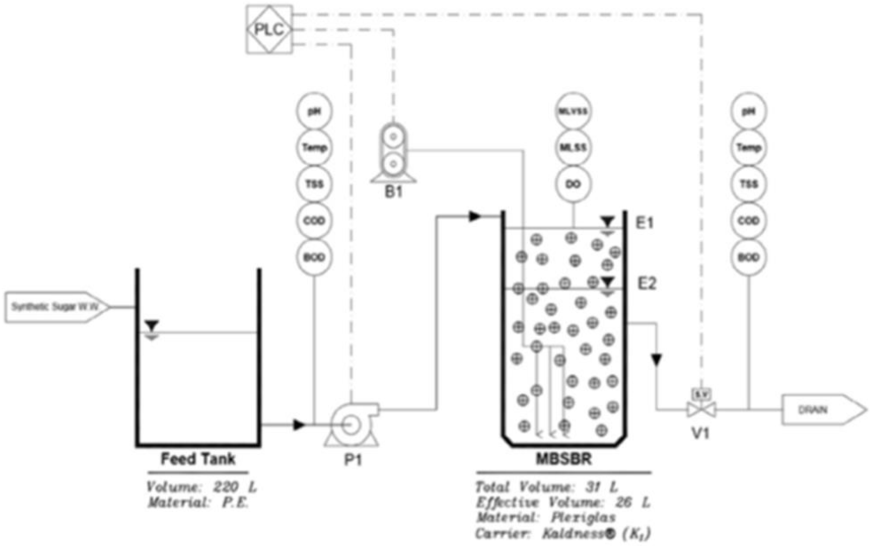

**Fig. 2: Batch Degradation of Thiocyanate(200ppm)**

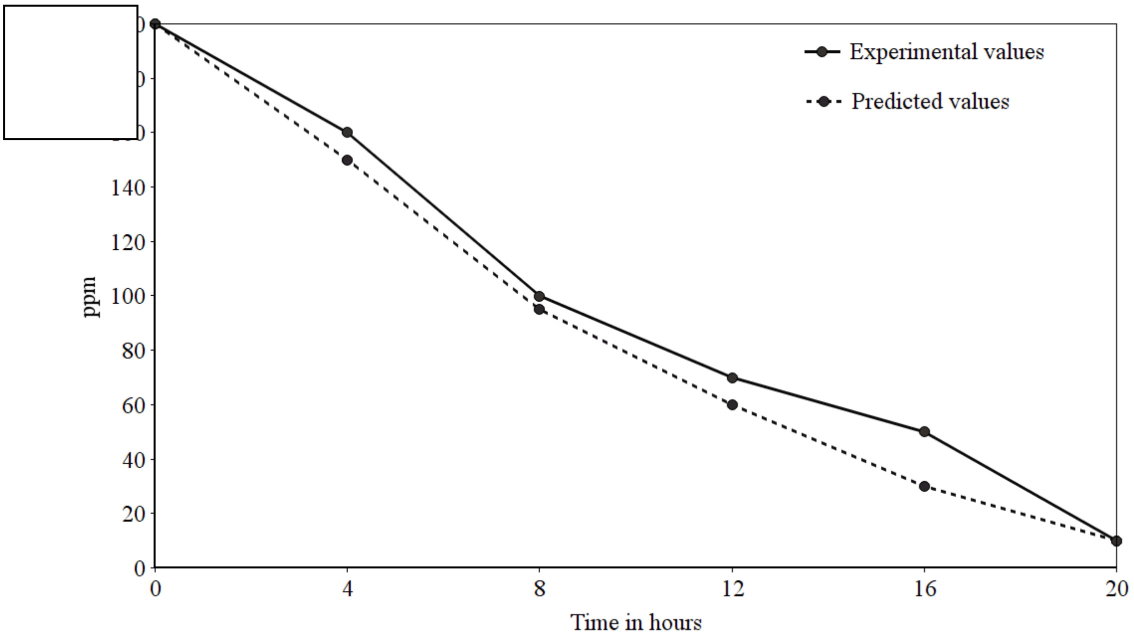

Fig. 3: Batch Degradation of Thiocyanate(400ppm)

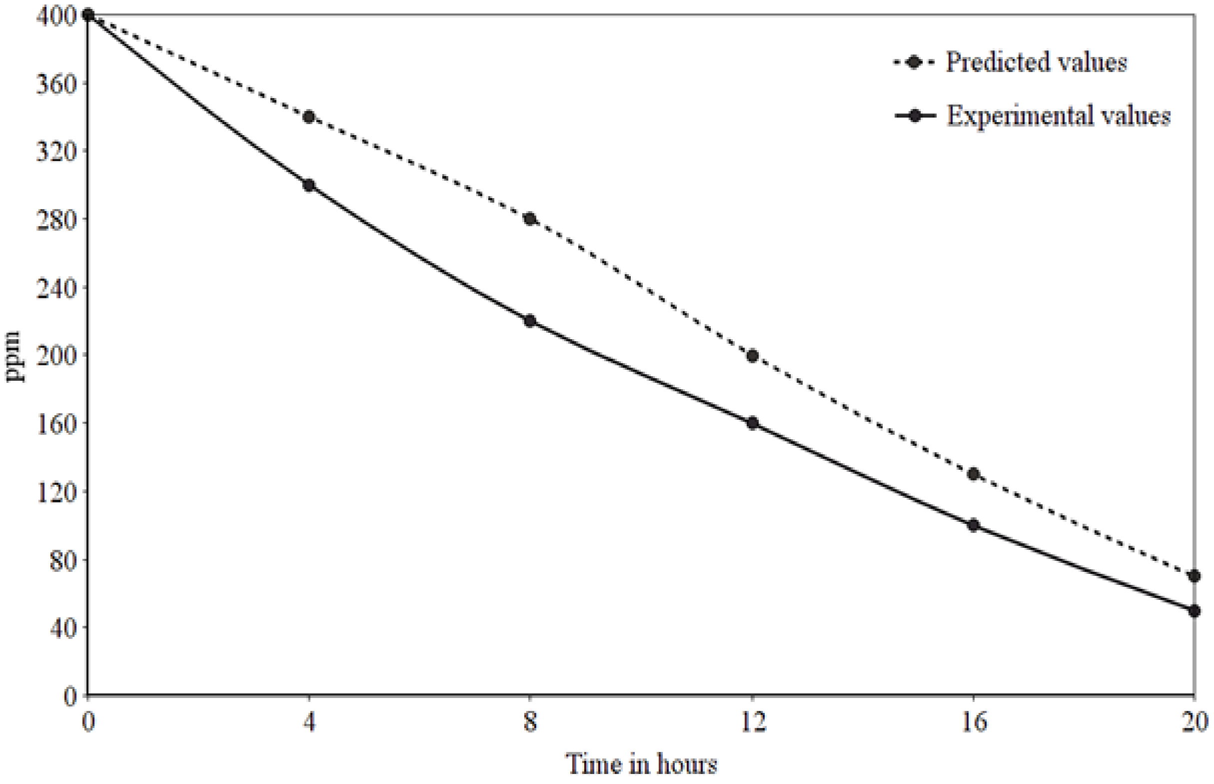

Fig. 4: Batch Degradation of Thiocyanate(600ppm)

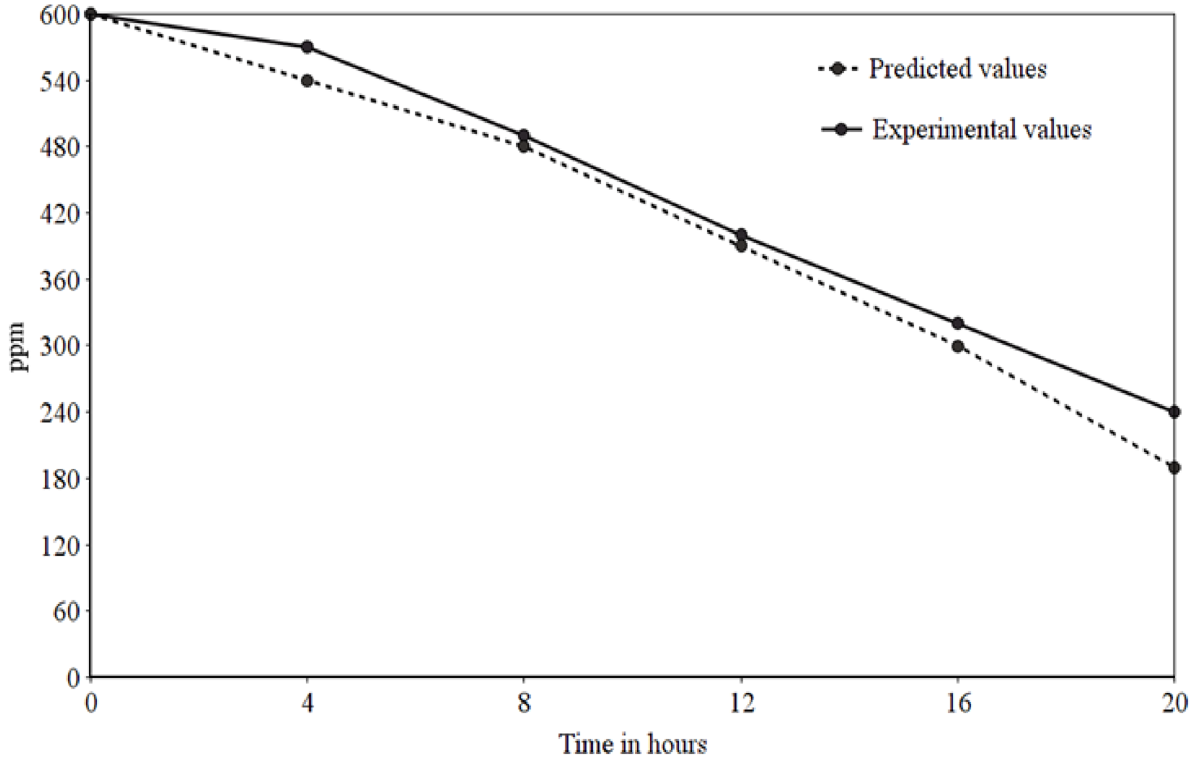

Fig. 5: Batch Degradation of Thiocyanate(800ppm)

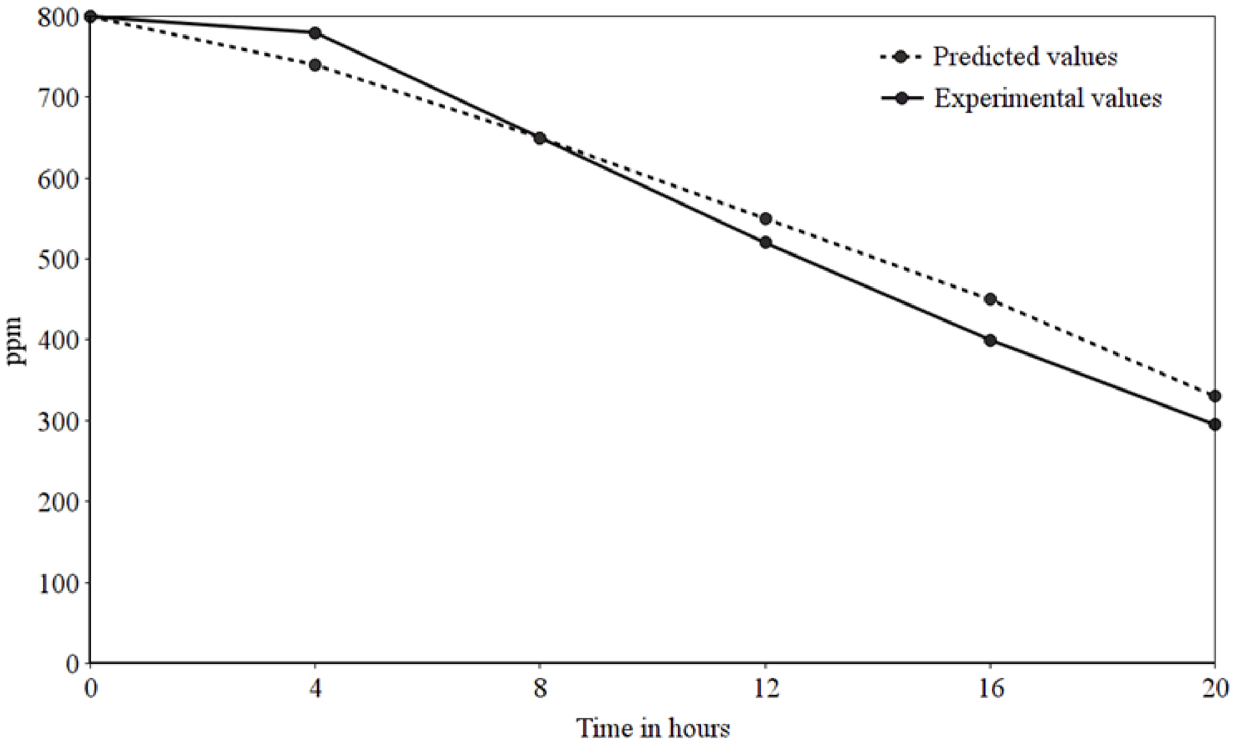

**Table 2: Accuracy of experimental and predicted data for different concentrations of thiocyanate**

| Initial Concentration of Thiocyanate(ppm) | Correlation Coefficient(R) | Co-efficient of Determination($R^2$) |
|---|---|---|
| 200 | 0.9945 | 0.989 |
| 400 | 0.9732 | 0.9471 |
| 600 | 0.9981 | 0.9962 |
| 800 | 0.9924 | 0.9849 |

From table. 2 the average value of Correlation Coefficient (R) was found to be 0.9896. This indicates that the predicted values are in good agreement with the experimental values. The average value of $R^2$ is 0.979, indicating the good performance of the applied model.

## CONCLUSION

This study demonstrates the utility of kinetic model as an useful optimization tool to treat industrial wastewater. Different concentrations of thiocyanate containing wastewater were treated by MBSBR. Monod's model showed accurate results. The agreement between the predicted and experimental results based on modelling and the real data, indicated that industries could apply optimized MBSBR to save the investment and meet environmental regulations.

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