Modeling Biodegradation Kinetics using MatLab®

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Abstract

A major objective of the Junior/Senior Engineering Clinics at Rowan University is to introduce students to open-ended engineering projects. All engineering students from the four engineering disciplines, namely Civil, Chemical, Electrical and Mechanical share a common engineering *clinic* class. This class is a major hallmark of the Rowan engineering program for all students throughout their eight semesters of study. The purpose of the clinic classes is to provide engineering students with hands-on, multidisciplinary experience throughout their college education. The junior and senior clinics emphasize multidisciplinary projects of progressive complexity. This paper focuses on the use of MATLAB for modeling biodegradation kinetics of organic compounds. A multidisciplinary team of students and faculty participated in this project. Environmental engineering students conducted experiments on biodegradation of organic pollutants and set up the model equations for determining biodegradation kinetics. Electrical and computer engineering students assisted in using MATLAB for the mathematical modeling studies. The entire study can be also be used in various core environmental, chemical and electrical engineering classes. This type of multidisciplinary interaction is of great value not only for students but faculty too. It provides first hand experience as to how relevant skills of engineers from various disciplines can be brought together for efficient creative solutions to problems.

Introduction

Rowan University is a regional state university committed to teaching and community service. The enrolment is approximately 9,000 students. The College of Engineering at Rowan University was initiated in 1996 as a result of a $100 million donation in 1992 from the Rowan Foundation. The engineering faculty use innovative methods of teaching and learning to better prepare students for entry into a rapidly changing and highly competitive marketplace[1-4]. The Rowan Engineering curriculum encourages innovative integration of course work, topics and research within the four engineering programs Chemical, Civil and Environmental, Electrical and Computer, and Mechanical Engineering [5-6]. To best meet these objectives, the four engineering programs of Chemical, Civil, Electrical, and Mechanical Engineering have common engineering clinic classes throughout their programs of study, in which undergraduates work in teams on hands-on open-ended projects. The descriptions of the Rowan Engineering Clinics are well documented[1-6].

This experimental work was conducted over two semesters of the Junior/Senior

Engineering Clinic and the modeling work as part of two courses: Wastewater Treatment and Design and Nonlinear Control. The Civil and Environmental Program offer the first course while the Electrical and Computer Engineering Program offer the latter. The experimental work was funded through the Northeast Hazardous Substance Research Center located in Newark, New Jersey.

Biodegradation Studies

Literature indicates that the metabolites of NPEs especially nonylphenol adsorbs to soils and sludges[7-9]. *Nonylphenol is persistent, lipophilic and tends to bioaccumulate. It has also been shown to be mildly estrogenic*. Sewage sludge thus applied to agricultural land may contain nonyphenol. European studies indicate high concentrations of nonylphenol in treated sewage sludge thereby indicating sludge disposal as a source of aquatic contamination [7-9]. Nonylphenol biodegradation has been studied by a number of researchers[7-9]. However very little information is available on the biodegradation kinetics of nonylphenol. Kinetic information is important for predicting fate of pollutants using mathematical models. Studies by Grady et al.[10], Dang et al.[11] have demonstrated that it is possible to determine intrinsic kinetics of single organic compounds by using oxygen uptake data from electrolytic respirometry. With the use of computer simulation techniques and non-linear curve fitting methods, intrinsic kinetic parameters are obtained from oxygen consumption data. The model predictions agree with data obtained from traditional measurements of subtrate removal and cell growth. This makes oxygen uptake data very attractive as it can eliminate monitoring of substrate removal and cell growth. Nonyphenol concentration measurements require an exhaustive steam distillation extraction procedure before using HPLC for analyses. Oxygen uptake using respirometry gives fast, accurate and reliable data.

The justification for using respirometry to obtain intrinsic biodegradation kinetics lies in the concept of oxygen consumption as an energy balance[10]. This concept states that all of the electrons available in a substrate undergoing biodegradation must either be transferred to the terminal acceptor or be incorporated into new biomass or soluble products. Since biomass growth and product formation are proportional to substrate removal, this suggests that an oxygen uptake curve can provide with the same information as either a substrate removal curve or a cell growth curve.

Experimental Method

Nonylphenol biodegradation was monitored through electrolytic respirometery. Nonylphenol (99% pure) was obtained from Fluka Chemical Corporation, Milwaukee, WI. An acclimated culture capable of degrading nonylphenol was developed from a local wastewater treatment plant. Enrichment cultures were developed in batch reactors incubated at room temperature with nonylphenol as the sole carbon source. All solutions were prepared in deionized water. Oxygen uptake measurements were recorded with time through electrolytic respirometry (N-CON Systems Comput-OX 244, Crawford, GA). All experiments were conducted in duplicate at 20^{o}C.

Model Development

A model addressing nonylphenol biodegradation was developed. The model was based on the rates of biodegradation and oxygen utilization in terms of three coupled differential equations. The equations describe:

(a) the cumulative mass of oxygen utilized for growth, substrate oxidation and endogenous respiration

(b) the rate of growth of cell mass (which also accounts for endogenous decay) due to utilization of soluble substrate

(c) the time dependent changes in concentration of soluble substrate.

Some basic assumptions of the model are: the microorganisms are preacclimated and utilize soluble substrate for growth.

In order to simulate this model numerically we used MATLAB. This powerful software package offers an array of numerical methods that can be used for simulation of nonlinear differential equations. Among the main functions in MATLAB that we used are `ode15s`, which implements a variation of the Runge-Kutta numerical method to solve stiff differential equations, and `leastsq`, which we used to perform nonlinear optimization to determine the parameters in the bacterial growth model that best match the experimental data sets.

Model Equations

The Monod[12] model was used to describe biodegradation. Equations one and two represent cell growth and substrate removal:

$$\frac{dX}{dt} = \frac{\mu_m SX}{K_s + S} - K_d X \qquad (1)$$

$$\frac{dS}{dt} = -\frac{1}{Y}\frac{\mu_m SX}{K_s + S} \qquad (2)$$

An additional equation (3) was used to define oxygen uptake with time:

$$\frac{dO_x}{dt} = Y_{ox}\frac{\mu_m SX}{K_s + S} + Y_{oxd} K_d X \qquad (3)$$

The variables in the above equation are defined as follows:

X Cell mass concentration (mg/L)
S Substrate concentration (mg/L)
O_x Oxygen Uptake (mg/L)

μ_m specific growth rate ((1/day)
K_d endogenous decay coefficient (1/day)
Ks substrate utilization rate (mg/L)
Y cell yield
Y_{ox} oxygen consumption coefficient
Y_{oxd} oxygen consumption coefficient for endogenous respiration

Results

The main objective of modeling was to determine the curve that approximates experimental data points. Two methods were used for modeling the data. The nonlinear regression technique is an iterative process. This method requires some initial estimated values for the kinetic parameters. The parameter values are then adjusted at each iteration to find the curve closer to the actual data points. The initial estimate plays a key role in adjusting the value for the parameters, so the chosen initial values should be within the range of the real values. A second method, the least squares fit method, which minimizes the sum of the squares of the vertical distances between the data points and the predicted solution was also used.

Table 1: Initial Values of Kinetic Parameters

Range	μm	Ks	Y	Y_{ox}
Lower	0.1	0.005	0.1	1.5
Upper	1.0	1000	1.5	3.5

Sample modeling results are presented in Figure 1.

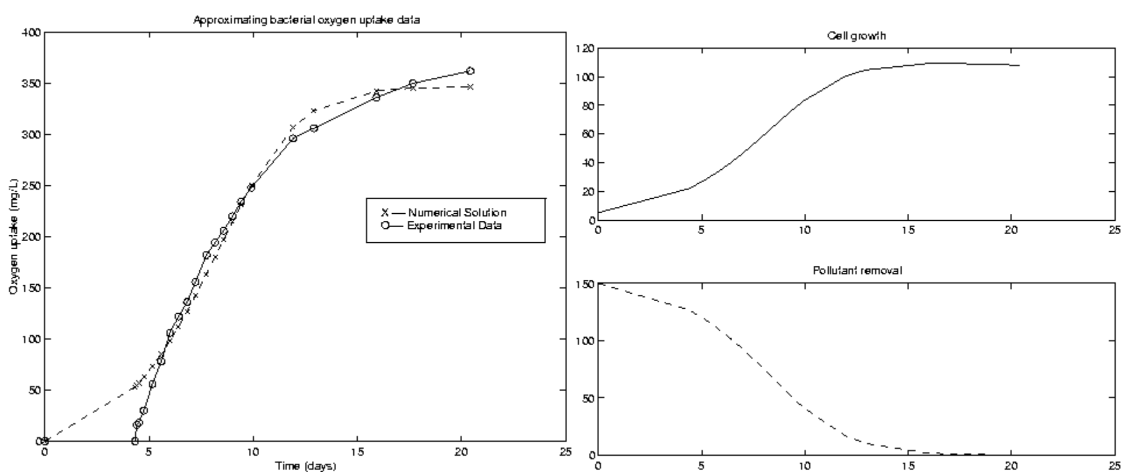

Figure 1: Fitted Respirometric Data for Nonylphenol and Model Predictions for Cell Growth and Nonyphenol Removal

The following coefficients in Table 2 were obtained for the above modeled data:

Table 2: Final Values of Kinetic Parameters

μm	Ks	Y	Y_{ox}
0.94	224	0.869	2.635

The model does not predict the acclimation phase or the initial part of the experimental data very accurately. More experiments are in progress to validate the values of the kinetic coefficients.

This paper has introduced the use of MATLAB for determining biodegradation kinetics. MATLAB is fast and powerful for this curve fitting process. It also allows the user to see the profiles of oxygen uptake, cell growth and nonylphenol removal simultaneously on the computer screen. The entire project is very successful in terms of interaction between students and faculty from various engineering disciplines.

Conclusions

This paper has presented the results of a multidisciplinary undergraduate project to conduct experiments on biodegradability and model the experimental data for predicting biodegradation kinetics. Benefits of such cooperative studies include efficient use of knowledge and resources from various engineering disciplines, enhanced broad based learning for students and a rewarding undergraduate research experience. Faculty also have an opportunity for introducing innovative approaches to teaching traditional core classes within their own disciplines.

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Biography

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Dr. Jahan is an Associate Professor of Civil and Environmental Engineering at Rowan University. She completed her Ph.D. studies in the Department of Civil and Environmental Engineering at the University of Minnesota, Minneapolis in 1993. Dr. Jahan has worked for Harza engineering as a water resources engineer and as an environmental engineer for the Nevada Division of Environmental Protection (NDEP).

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Ravi P. Ramachandran is an Associate Professor in the Department of Electrical and Computer Engineering at Rowan University. He received his Ph.D. from McGill University in 1990 and has worked at AT&T Bell Laboratories and Rutgers University prior to joining Rowan.