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Numerical Study on Microbial Depolymerization Process of Xenobiotic Polymer

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Abstract

This study demonstrates mathematical analysis of biodegradation processes of xenobiotic polymers. A model for microbial population is based on the fact that growth rate of microorganisms is proportional to the microbial population and consumption rate of parts of carbon sources. The model is paired with a model for weight distribution. Those models lead to inverse problems for a molecular factor and a time factor of degradation rate. Solution of the inverse problems allows us to simulate the biodegradation process.

Keywords

Biodegradation, Polymer, Mathematical Model, Inverse Problem, Numerical Simulation

1. Introduction

Microbial depolymerization processes are classified into exogenous type and endogenous type. Molecules liberate their parts to reduce in an exogenous type depolymerization process. Polyethylene (PE) and polyethylene glycol (PEG) are polymers subject to exogenous type depolymerization processes. Studies showed utilization of PEG of average molecular weight 20,000 by *Psedomonas aeruginosa* [1], degradation of PEG 20,000 by anaerobic bacteria isolated from sludge of a municipal anaerobic digester [2], and efficient biodegradation of PEG by *Pseudomonas stutzeri* was documented [3]. A mathematical model was proposed and numerical techniques were developed for PE biodegradation [4]. The mathematical techniques were reapplied to a biodegradation process of PEG [5].

Random breakdown of molecules is the primary factor of endogenous type depolymerization processes. Polyvinyl alcohol (PVA) and polylactic acid (PLA)

are polymers subject to endogenous depolymerization processes. A mathematical model was proposed and numerical techniques were developed for an enzymatic degradation of PVA [6]. Those mathematical techniques were reapplied to an enzymatic hydrolysis of polylactic acid (PLA) [7]. Techniques originally developed for endogenous type processes were replied to exogenous type depolymerization processes of PE and PEG [8].

This study revisits an exogenous type depolymerization process of PEG to demonstrate mathematical techniques. Experimental outcomes before and after cultivation of microbial consortium E-1 in culture media were incorporated into a computational analysis based on a mathematical model. Inverse problems for a molecular factor and a time factor of a degradation rate were formulated. Solutions of those inverse problems allow us to simulate a biodegradation process of PEG.

2. Formulation of Exogenous Type Depolymerization Process

Consider an exogenous type depolymerization process in a culture medium. Let $w(t, M)$ [mg] be the weight distribution of a polymer with respect to the molecular weight M at time t, and $v(t)$ [mg] be the total weight of polymer molecules with molecular weight between A and B at time t. The total weight $v(t)$ over the interval $[A, B]$ is expressed in terms of the integral

$$v(t) = \int_A^B w(t, M)\, dM \tag{1}$$

The total weight $v(t)$ of the residual polymer at time t is expressed in terms of the integral

$$v(t) = \int_0^\infty w(t, M)\, dM \tag{2}$$

Integral (1) well approximates the integral (2) with suitable choices of A and B. In this study, integrals with the lower limit were replaced with integrals with the lower limit $A = 10^{3.0}$, and integrals with the upper limit ∞ were replaced with integrals with upper limit $B = 10^{4.2}$.

Let $\sigma(t)$ be the population of viable cells at time t. Equations (3) for the weight distribution $w(t, M)$ and the microbial population σ(t) was proposed in previous studies [8] [9] [10].

$$\frac{\partial w}{\partial t} = \sigma(t)\left[-\lambda(M)w + c(M)\int_M^\infty \lambda(K)d(K)w(t,K)\,dK\right] \tag{3}$$

$$c(M) = Me^{\rho M},\ d(K) = \frac{\rho e^{-\rho K}}{K\left(1-e^{-\rho K}\right)},\ \rho = \frac{\log 2}{L},$$

Parameter L is the molecular weight of a monomer unit, e.g. PE: 28 (CH_2CH_2), PEG: 44 (CH_2CH_2O), and k and h are positive parameters. The function $\lambda(M)$ corresponds to a molecular factor of degradation rate.

This study proposes the equation

$$\frac{d\sigma}{dt} = ku(t)\sigma - h\sigma, \tag{4}$$

where $u(t) = -v'(t)$. Note that $u(t)$ is the rate of consumption of total weight. System of Equations (3), (4) is associated with the initial conditions

$$w(0, M) = f_0(M), \tag{5}$$

$$\sigma(0) = \sigma_0, \tag{6}$$

where $f_0(M)$ and σ_0 are the initial weight distribution and the initial microbial population, respectively.

3. Numerical Solutions of Inverse Problems for Molecular Factor and Time Factor

The initial value problem (3), (4), (5) (6) is solvable for $w(t, M)$ and $\sigma(t)$ provided the molecular factor $\lambda(M)$ and values of parameters σ_0, k, and h are given beforehand. In order to obtain the function and values of parameters, consider change of variables from t to τ defined by the equation

$$\tau = \int_0^t \sigma(s)ds. \tag{7}$$

Denote by by $w(\tau, M)$, $S(\tau)$, and $V(\tau)$ functions that correspond to $w(t, M)$, $\sigma(t)$, and $v(t)$ according to the change of variables (7), respectively.

Note that

$$\frac{\partial W}{\partial \tau} = \frac{dt}{d\tau}\frac{\partial w}{\partial t} = \frac{1}{\sigma(t)}\frac{\partial w}{\partial t}, \quad \frac{dS}{d\tau} = \frac{dt}{d\tau}\frac{d\sigma}{dt} = \frac{1}{\sigma(t)}\frac{d\sigma}{dt}, \quad \frac{dV}{d\tau} = \frac{dt}{d\tau}\frac{dv}{dt} = \frac{1}{\sigma(t)}\frac{dv}{dt}$$

and that Equations (3) and (4) lead to

$$\frac{\partial W}{\partial \tau} = -\lambda(M)W + c(M)\int_M^\infty \lambda(K)d(K)W(\tau, K)dK, \tag{8}$$

$$\frac{dS}{d\tau} = kU(\tau)S - h, \tag{9}$$

respectively, where $U(\tau) = -V'(\tau)$.

Suppose that $F_1(M)$ is the weight distribution for $\tau = T_1$, that is,

$$W(T_1, M) = F_1(M), \tag{10}$$

and that $F_2(M)$ is the weight distribution for $\tau = T_2$, that is,

$$W(T_2, M) = F_2(M). \tag{11}$$

Equation (8), the initial condition (10), and the final condition (11) form an inverse problem for the molecular factor $\lambda(M)$, for which the solution of the initial value problem (8), (10) also satisfies the final condition (11).

Numerical techniques to solve the inverse problem for $\lambda(M)$ were developed in previous studies. Weight distributions of PEG 6000 before and after cultivation of microbial consortium E-1 for one day, three days, five days, seven days, and nine days $f_0(M)$, $f_1(M)$, $f_2(M)$, $f_3(M)$, $f_4(M)$, and $f_5(M)$ were introduced into analysis. Note that $w(t_i, M) = f_i(M)$ for $i = 0, 1, 2, 3, 4$, and 5, where $t_0 = 0$, t_1

= 1, t_2 = 3, t_3 = 5, t_4 = 7, and t_5 = 9. Weight distributions after cultivation of the microbial consortium E-1 for one day and three days were the functions $F_1(M)$ and $F_2(M)$, respectively, and the inverse problem (8), (10), (11) was solved numerically for $T_1 = 0$ and $T_2 = 1.0$ [10]. Note a positive scalar multiple of a molecular factor is also a molecular factor.

Once the molecular factor $\lambda(M)$ was obtained, Equation (10) was solved for $W(\tau, M)$ with the initial condition

$$W(0, M) = f_0(M). \tag{12}$$

A previous study shows the exponential function

$$V(\tau) = v_0 e^{-\mu\tau} \quad \left(v_0 = \int_0^\infty f_0(M)\, dM\right), \tag{13}$$

well approximates function $V(\tau)$ so that $V'(\tau) = -\mu v_0 e^{-\mu\tau}$. In this study, function $V(\tau)$ was approximated by the exponential function (13) with $\mu \approx 0.878$.

Once the function $V(\tau)$ was obtained, Equation (9) was solved with the initial condition

$$S(0) = \sigma_0. \tag{14}$$

Denote by $S(\tau, \sigma_0, k, h)$ the solution of the initial value problem (9), (14). In view of the Formula (7), $t = q(\tau, \sigma_0, k, h)$, where

$$q(\tau, \sigma_0, k, h) = \int_0^\tau \frac{dr}{S(r, \sigma_0, k, h)}.$$

Given m pairs of values of t and τ, $(t_i, \tau_i)(i = 1, 2, 3)$, consider the system of equations

$$g_i(\sigma_0, k, h) = 0 \quad (i = 1, 2, 3) \tag{15}$$

where $g_i(\sigma_0, k, h) = q(\tau_i, \sigma_0, k, h) - t_i$. Here τ_i is the value of τ that satisfy $v(t_i) = V(\tau_i)$. In particular,

$$t_1 = 1,\ \tau_i \approx 0.024275,\ t_2 = 3,\ \tau_2 \approx 0.288317,\ t_3 = 5,\ \tau_3 \approx 2.62864.$$

Intervals $[\sigma_{0,0}, \sigma_{0,1}]$, $[k_0, k_1]$, $[h_0, h_1]$ were divided into n_1, n_2 and n_3 intervals, respectively, and the initial value problem (9), (14) was solved for

$$\sigma_0 = \sigma_{0,0} + i\Delta\sigma_0,\ \Delta\sigma_0 = \frac{\sigma_{0,1} - \sigma_{0,0}}{n_1},\ i = 0, 1, \ldots, n_1,$$

$$k = k_0 + j\Delta k,\ \Delta k = \frac{k_1 - k_0}{n_2},\ j = 0, 1, \ldots, n_2,$$

$$h = h_0 + l\Delta h,\ \Delta h = \frac{h_1 - h_0}{n_3},\ l = 0, 1, \ldots, n_3,$$

$$\sigma_{0,0} = 0.0015,\ \sigma_{0,1} = 0.0016,$$

$$k_0 = 0.0045,\ k_1 = 0.0055,$$

$$h_0 = 0.35,\ h_1 = 0.45,$$

$$n_1 = 100, n_2 = 100, n_3 = 100.$$

The value of σ_0, k, and h that minimize the error

$$\sqrt{\sum_{i=1}^{5}\left[g_i(\sigma_0,k,h)\right]^2}$$

were approximately 0.00156, 0.00518, and 0.404, respectively.

Given $\lambda(M)$ and $\sigma(t)$, the initial value problem (3), (5) was solved numerically. **Figures 1-5** show some numerical results. **Figures 1-4** show comparison between experimental results and numerical results for weight distribution after cultivation of microorganisms for one day, three days, five days, and seven days, respectively. **Figure 5** shows the graph of the function $\sigma(t)$.

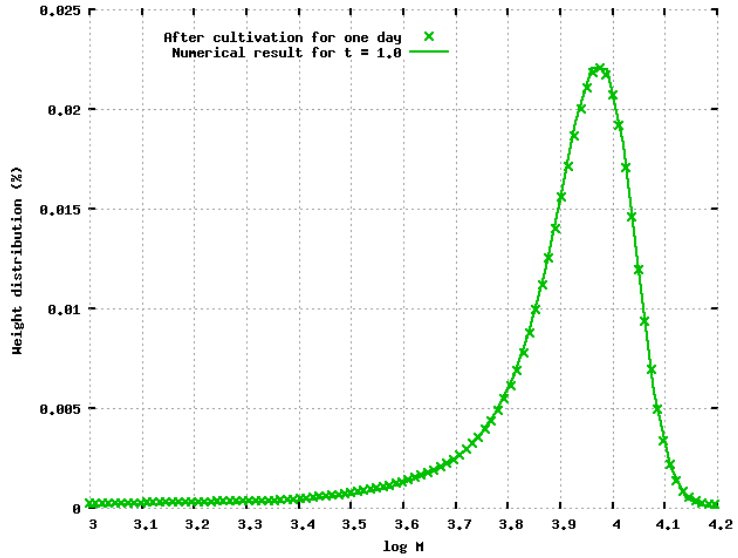

Figure 1. Weight distribution after cultivation of microbial consortium E-1 for one day. An experimental result and numerical results are shown.

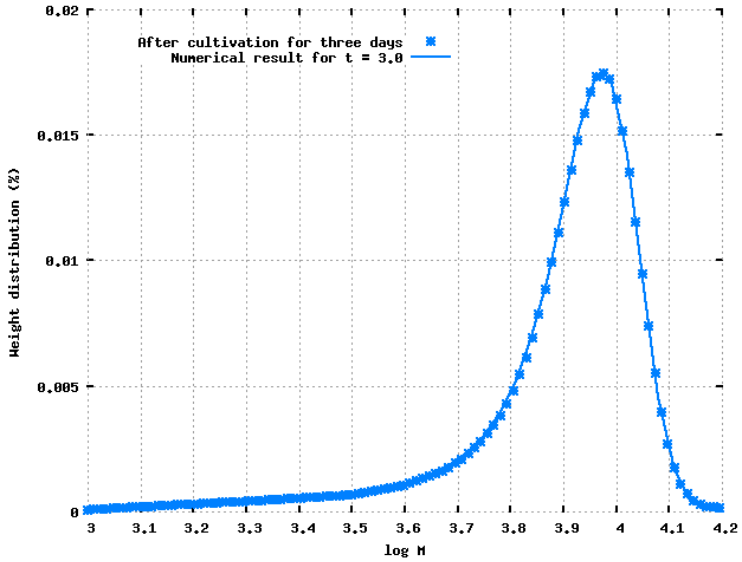

Figure 2. Weight distribution after cultivation of microbial consortium E-1 for three days. An experimental result and numerical results are shown.

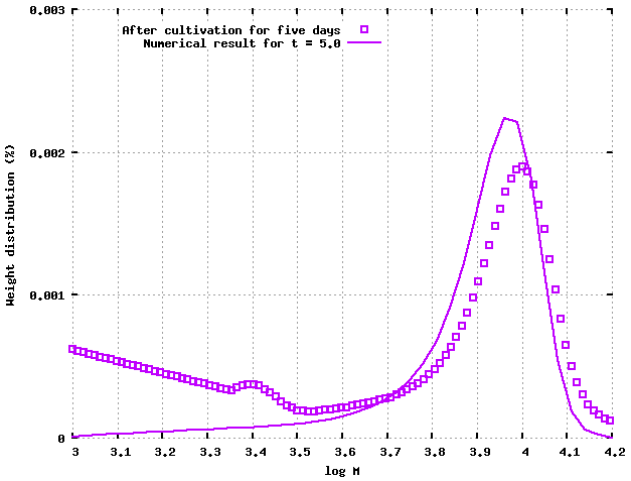

Figure 3. Weight distribution after cultivation of microbial consortium E-1 for five days. An experimental result and numerical results are shown.

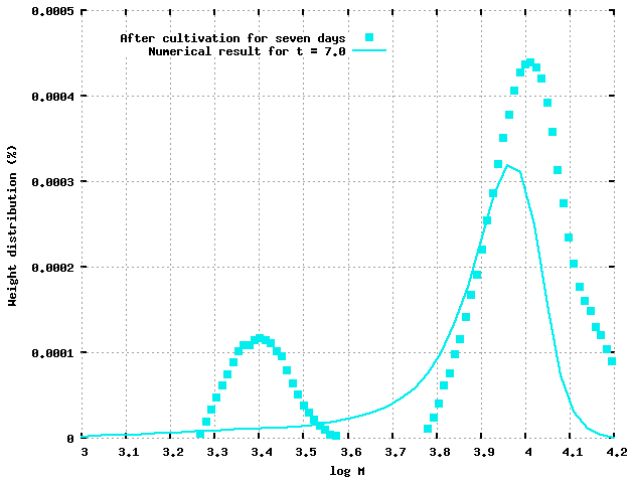

Figure 4. Weight distribution after cultivation of microbial consortium E-1 for seven days. An experimental result and numerical results are shown.

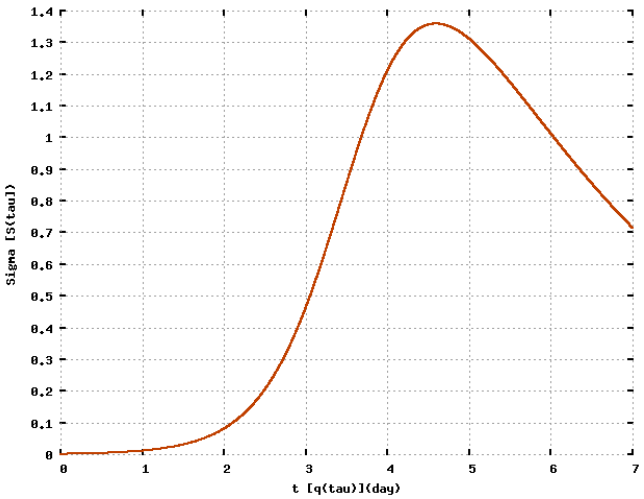

Figure 5. Transition of microbial population over seven days.

4. Discussion

Equation (4) is based on the fact that the increasing rate of the microbial population is proportional to both the consumption rate and the microbial population. Parameter k is the conversion rate from the carbon source to the microbial population per unit population, It is also based on the fact that the decreasing rate of the microbial population is proportional to the microbial population. Parameter h is the rate of loss of active microorganisms. Our analysis shows that the microorganisms convert approximately 0.5% of carbon source consumed per day to their growth, and that approximately 40% of microorganism loses degradability per day. The numerical results show that our model is appropriate.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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