MODELING AND SIMULATION FOR MICROBIAL DEPOLYMERIZATION OF POLYETHYLENE GLYCOL

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Introduction

Microbial depolymerization processes are classified into exogenous type depolymerization processes and endogenous type depolymerization processes. In an exogenous type depolymerization process, molecules reduce their sizes by truncation of monomer units from their terminals. Polymer subject to exogenous depolymerization processes include polyethylene (PE). There are two essential factors in PE biodegradation, the gradual weight loss of large molecules due to the β-oxidation, and the direct consumption or absorption of small molecules by cells. A mathematical model based on those factors was proposed to study PE biodegradation processes. [4].

Polyethylene glycol (PEG) is another example of polymer subject to exogenous depolymerization processes. The mathematical techniques developed for the PE biodegradation were extended to studies of exogenous depolymerization processes of PEG [1]. Dependence of degradation rate on time was also considered in modeling and simulation of PEG depolymerization processes [2].

In this study, analysis of PEG biodegradation is continued. Model originally developed for endogenous depolymerization processes is applied to the exogenous depolymerization processes of PEG.

Modeling for depolymerization processes

Unlike exogenous depolymerization processes, molecules are cleaved at any positions in endogenous type depolymerization processes. In order to model endogenous depolymerization processes, let $w(t, M)$ be the weight distribution with respect to the molecular weight M at time t. Let $\gamma(t, M)$ be the loss of amount from $w(t, M)$per unit time and per unit weight. For $K \in [0, M]$, let $q(K, M)$ denote the increase in $w(t, K)$ per unit weight due to the weight loss in $w(t, M)$. Then

$$\frac{\partial w}{\partial t} = -\gamma(t, M)\, w + \int_M^\infty \gamma(t, K)\, q(M, K)\, w(t, K)\, dK. \tag{1}$$

holds. Equation (1) is a general case of models used in studies on degradation processes of polyvinyl alcohol (PVA) and polylactic acid (PLA) [5, 3]. Given an initial weight distribution in terms of a prescribed function $f(M)$, the equation (1) and the initial condition

$$w(0, M) = f(M). \tag{2}$$

form an initial value problem, provided the degradation rate $\gamma(t, M)$ is given.

Time averaged degradation rate

Time factors of degradability include temperature, dissolved oxygen, and microbial population. Those factors affect degradation of molecules regardless of molecular weight, the degradation rate $\gamma(t, M)$ is a product of a function of t, $\sigma(t)$, and a function of M, $\lambda(M)$, and Equation (1) becomes

$$\frac{\partial w}{\partial t} = -\sigma(t)\,\lambda(M)\, w + \sigma(t) \int_M^\infty \lambda(M)\, q(M, K)\, w(t, K)\, dK. \tag{3}$$

Let

$$\tau = \int_0^t \sigma(s)\, ds \quad \text{and} \quad W(\tau, M) = w(t, M).$$

Then Equation (3) becomes

$$\frac{\partial W}{\partial \tau} = -\lambda(M)\, W + \int_M^\infty \lambda(K)\, q(M,K)\, W(\tau,K)\, dK. \tag{4}$$

Equation (4) and the initial condition

$$W(0,M) = f(M). \tag{5}$$

form an initial value problem provided $\lambda(M)$ is known. Let

$$\mathcal{T} = \int_0^T \sigma(s)\, ds.$$

Then the equation (4) and the initial condition (5) and the condition

$$W(\mathcal{T},M) = g(M). \tag{6}$$

form an inverse problem to find the degradation rate $\lambda(M)$ for which the solution of the initial value problem (4) and (5) also satisfies the condition (6). The initial value problem (1), (2) corresponds to the initial value problem (4), (5).

High performance liquid chromatography (HPLC) patterns will be introduced into analysis as the weight distribution of PEG6000 with respect to the molecular weight before and after cultivation of a microbial consortium E1 (Figure 1). Numerical results based on the data shown in Figure 1 will be presented.

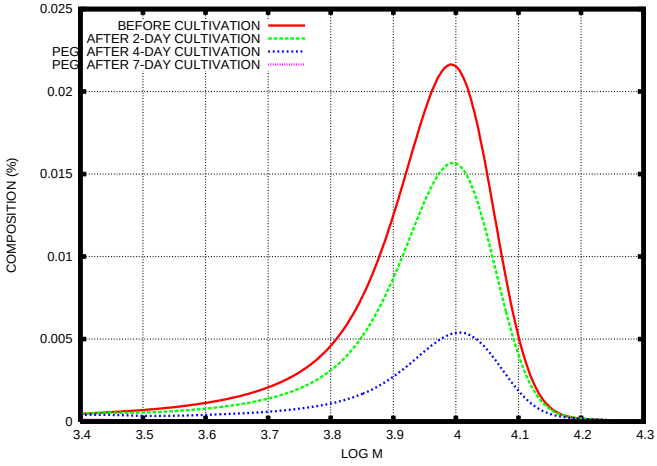

Figure 1: Weight distribution of PEG6000 before and after cultivation of a microbial consortium E1.

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