SIMULATION FOR EXOGENOUS MICROBIAL DEPOLYMERIZATION OF POLYETHYLENE GLYCOL

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Introduction

Microbial depolymerization processes are categorized into two types, exogenous type and endogenous type. In an exogenous depolymerization process, molecules become small by truncation of monomer units from their terminals. Examples of polymers subject to exogenous depolymerization include polyethylene (PE) and polyethylene glycol (PEG). PE biodegradation is based on two essential factors: 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, and studies based on the model were conducted [1, 4].

The mathematical techniques originally developed for the PE biodegradation was extended to cover the biodegradation of PEG [2]. Dependence of degradation rates on time was also considered in modeling and simulation of microbial depolymerization processes of PEG [3].

Here the study on dependence of degradation rate in time in depolymerization processes of PEG is continued. The evolution of microbial population is taken into account in modeling of depolymezation processes. Experimental data are introduced into analysis, and the transition of weight distribution is simulated.

Modeling for exogenous depolymerization

Let t and M denote the time and the molecular weight, respectively. A molecule with molecular weight M is referred to as an M-molecule. Let L be the amount of weight loss due to the truncation of a monomer unit. In an exogenous depolymerization process of PEG, a molecule is first oxidized at its terminal, and then an ether bond is cleaved. Since the monomer unit CH_2CH_2O is truncated in one cycle of depolymerization, $L = 44$ for exogenous depolymerization processes of PEG. Let $w(t, M)$ represent the total weight of M-molecules present at time t. Equation (1) is analyzed to study exogenous depolymerization processes of PEG [2].

$$\frac{dx}{dt} = -\beta(M)\, x + \beta(M+L)\, \frac{M}{M+L} y\,. \qquad (1)$$

Here $x = w(t, M)$, the total weight of M-molecules at time t, and $y = w(t, M+L)$, the total weight of $M+L$-molecules at time t.

Equation (1) is adequate for depolymerization processes over a period in which the microbial population is stationary. However, the change of microbial population should be taken into account for a period in which it is developing or diminishing. Time factors of depolymerization processes such as microbial population, dissolved oxygen, or temperature affect molecules regardless of sizes because depolymerization processes are restricted to terminals. Then the degradation rate is a product of a time factor, which we denote by $\sigma(t)$, and a molecular factor, which we denote by $\lambda(M)$. Then equation (1) becomes

$$\frac{dx}{dt} = -\sigma(t)\,\lambda(M)\, x + \sigma(t)\,\lambda(M+L)\, \frac{M}{M+L} y\,. \qquad (2)$$

Given an initial weight distribution $f(M)$, equation (2) is associated with the initial condition

$$w(0, M) = f(M)\,. \qquad (3)$$

Time averaged model

Let

$$\tau = \int_0^t \sigma(s)\, ds\,. \tag{4}$$

Let $W(\tau, M) = w(t, M)$, $X = W(\tau, M)$, $Y = W(\tau, M + L)$. Then equation (2) becomes

$$\frac{dX}{d\tau} = -\lambda(M)\, X + \lambda(M + L)\, \frac{M}{M + L} Y\,. \tag{5}$$

Given the initial weight distribution $f(M)$, equation (5) and the initial condition

$$W(0, M) = f(M) \tag{6}$$

form an initial value problem. Given an additional condition

$$W(\mathcal{T}, M) = g(M)\,, \tag{7}$$

equation (5) and the conditions (6) and (7) form an inverse problem to determine the degradation rate $\lambda(M)$ for which the solution of the initial value problem (5), (6) also satisfies the condition (7). When the solution $W(\tau, M)$ of the initial value problem (5), (6) satisfies the condition (7), the solution $w(t, M)$ of the initial value problem (2), (3) satisfies

$$w(T, M) = g(M)\,, \quad \mathcal{T} = \int_0^T \sigma(s)\, ds\,. \tag{8}$$

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.

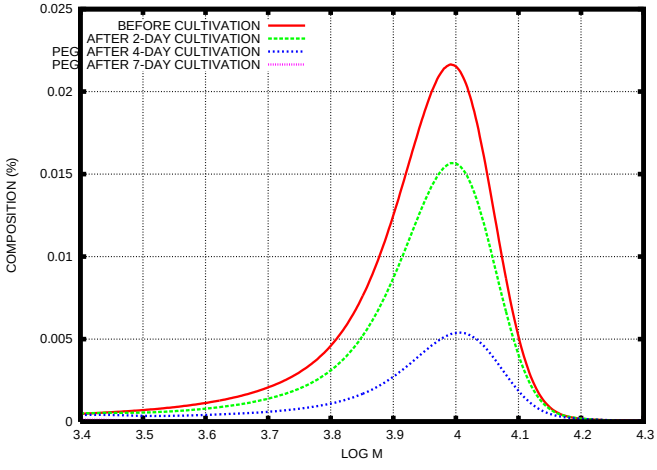

Figure 1: Weight distribution of PEG6000 before and after cultivation of a microbial consortium E1.

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References

[1] F. Kawai, M. Watanabe, M. Shibata, S. Yokoyama, Y. Sudate, and S. Hayashi. Comparative study on biodegradability of polyethylene wax by bacteria and fungi. *Polymer Degradation and Stability*, 86:105–114, 2004. doi: 10.1016/j.polymdegradstab.2004.03.015.

[2] M. Watanabe and F. Kawai. Numerical simulation of microbial depolymerization process of exogenous type. In Rob May and A. J. Robert, editors, *Proc. of 12th Computational Techniques and Applications Conference, CTAC-2004, Melbourne, Australia in September 2004, ANZIAM J. 46 E*, pages C1188–C1204, 2005. (http://anziamj.austms.org.au/V46/CTAC2004/Wata).

[3] M. Watanabe and F. Kawai. Mathematical analysis of microbial depolymerization processes of xenobiotic polymers. In Geoffry N. Mercer and A. J. Roberts, editors, *Proceedings of the 14th Biennial Computational Techniques and Application Conference, CTAC2008*, volume 50 of *ANZIAM J.*, pages C930–C946, 2009. (http://anziamj.austma.org.au/ojs/index.php/ANZIAMJ/article/view/1465).

[4] M. Watanabe, F. Kawai, M. Shibata, S. Yokoyama, Y. Sudate, and S. Hayashi. Analytical and computational techniques for exogenous depolymerization of xenobiotic polymers. *Mathematical Biosciences*, 192:19–37, 2004. doi: 10.1016/j.mbs.2004.06.006.