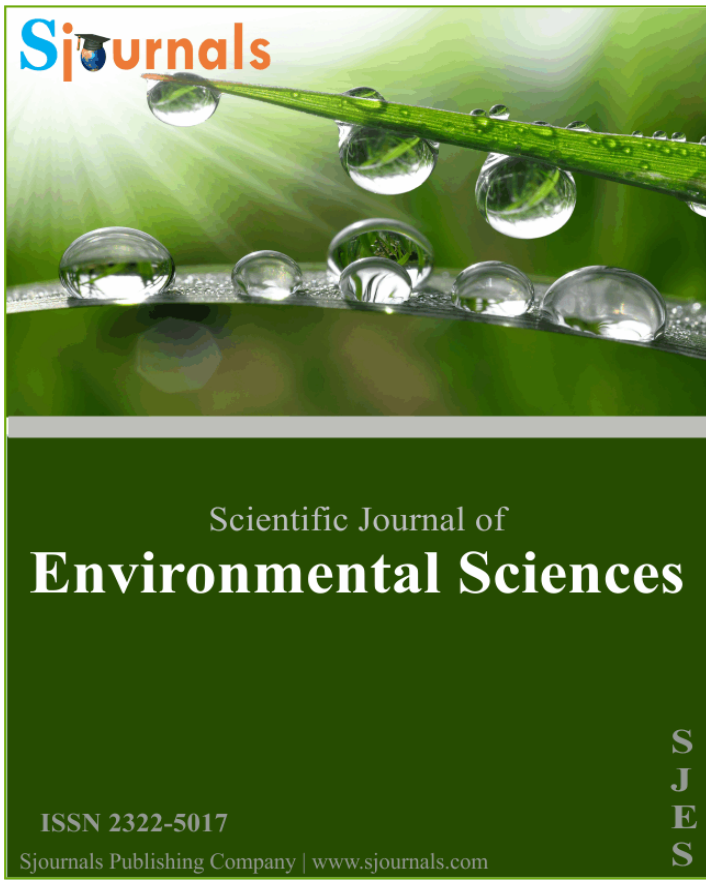

Scientific Journal of Environmental Sciences (2017) 6(9) 304-311
ISSN 2322-5017
doi: 10.14196/sjes.v6i9.2293

Contents lists available at Sjournals
Scientific Journal of **Environmental Sciences**
Journal homepage: www.Sjournals.com

Review article

Numerical techniques for inverse analysis in study of microbial depolymerization processes

Masaji Watanabe[a,*] **and Fusako Kawai**[b]
[a]*Graduate School of Environmental and Life Science, Okayama University, Japan.*
[b]*Center for Fiber and Textile Science, Kyoto Institute of Technology, Japan.*

*Corresponding author: watanabe@ems.okayama-u.ac.jp

ARTICLE INFO

Article history,
Received 17 August 2017
Accepted 13 September 2017
Available online 20 September 2017
iThenticate screening 19 August 2017
English editing 11 September 2017
Quality control 18 September 2017

Keywords,
Biodegradation
Polymer
Mathematical model
Numerical simulation
Inverse problem

ABSTRACT

A mathematical model for microbial depolymerization is described. An inverse problems for a molecular factor and a time factor of degradation rate are formulated. Numerical techniques for inverse analysis are illustrated, and numerical results are presented.

1. Introduction

The production of petroleum based polymers began in the early part of the twentieth century. Those products have been accumulated over the surface of the earth since then, and their significant portions now remain as sources for carbon dioxide emission. Those macromolecules had been nonexistent until they were invented; nevertheless studies have shown that some of those are utilizable by microorganisms. Now mechanisms of microbial depolymerization processes should be clarified.

There are two types of microbial depolymerization processes; exogenous type and endogenous type. Molecules reduce in size liberating monomers from their terminals in an exogenous type depolymerization process. Polymers depolymerized in exogenous type depolymerization processes include polyethylene (PE) and polyethylene glycol (PEG). A mathematical model was proposed for studies of PE biodegradation processes (Watanabe et al., 2004). Mathematical techniques developed in studies of PE biodegradation were applied to PEG biodegradation processes (Watanabe and Kawai, 2005). The dependence of degradability on time was incorporated in formulation of PEG depolymerization process\cite{Watanabe_Kawai_EMAC2009}. Unlike exogenous type depolymerization processes, molecules reduce in size undergoing arbitrary scission in endogenous type depolymerization processes. Polymers depolymerizable in exogenous type depolymerization processes include Polyvinyl alcohol (PVA) and polylactic acid (PLA) are examples of depolymerized in endogenous type depolymerization processes. A mathematical model was proposed in study of PVA enzymatic degradation (Watanabe and Kawai, 2003; Watanabe and Kawai, 2006). Mathematical techniques developed for the enzymatic degradation of PVA was applied to enzymatic hydrolysis of PLA, and degradability between PVA and PLA was compared (Watanabe et al., 2007). The dependence of degradability on time was incorporated in formulation of enzymatic hydrolysis of PLA (Watanabe and Kawai, 2008). A model formulated for endogenous type depolymerization processes was reformulated for exogenous type depolymerization processes of PEG (Watanabe and Kawai, 2011) and PE (Watanabe and Kawai, 2012a). Time dependence of degradability was incorporated in formulation of an exogenous type depolymerization process of PEG (Watanabe and Kawai, 2012b). In this study, analysis of microbial depolymerization is continued. In the following sections, a mathematical model was described, inverse problems for time factor and molecular factor of degradation rate are formulated, and numerical techniques are illustrated.

2. Description of exogenous type microbial depolymerization model

In order to formulate a microbial depolymerization process, let $w(t, M)$ be the weight distribution with respect to the molecular weight M at time t, such that the total weight of residual polymer for A≤M≤B at time t is:

$$\int_A^B w(t, M)\, dM . \qquad (1)$$

In particular, the total residual polymer at time t, $v(t)$ is given by:

$$v(t) = \int_0^\infty w(t, M)\, dM . \qquad (2)$$

The total residual polymer (2) can be approximated with the integral (1) for appropriate values of A and B.

The following system of equation for $w(t, M)$ and $\sigma(t)$ was proposed in previous studies (Watanabe and Kawai, 2016a; Watanabe and Kawai, 2016b; Watanabe and Kawai, 2015a; Watanabe and Kawai, 2015b).

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

$$\frac{d\sigma}{dt} = k\left(1 - h\frac{\sigma}{A(t)}\right)\sigma, \qquad (4)$$

Where

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

Here L is the molecular weight of monomer unit liberated from a molecule in one cycle of exogenous type depolymerization process, *e.g.* PE: L=28 (CH_2CH_2), PEG: L=44, (CH_2CH_2O). Function $\lambda(M)$ is the molecular factor of the degradation rate. Function $\sigma(t)$ is the time factor of the degradation rate that corresponds to the microbial population. Let $f_0(M)$ and σ_o be the initial weight distribution and the initial microbial population, respectively. System of equations (3), (4) from an initial value problem with the initial condition:

$$w(0, M) = f_0(M), \qquad (5)$$

$$\sigma(0) = \sigma_0 . \qquad (6)$$

3. Inverse problem for time factor of degradation rate in exogenous type depolymerization process

In order for the initial value problem (3), (4), (5), (6) to be solvable, the molecular factor λ(*M*) and time factor σ(*t*) must be prescribed. Consider the change of variables from *t* to τ defined by the integral:

$$\tau = \int_0^t \sigma(s)\, ds . \qquad (7)$$

Let

$$W(\tau, M) = w(t, M), \qquad S(\tau) = \sigma(t), \qquad V(\tau) = v(t).$$

For which the change of variables (\ref{eq07}) holds. Note that:

$$\frac{d\tau}{dt} = \sigma(t). \qquad (8)$$

According to the formula (8):

$$\frac{\partial W}{\partial \tau} = \frac{\partial w}{\partial t}\frac{\partial t}{\partial \tau} = \frac{1}{\sigma(t)}\frac{\partial w}{\partial t},$$

And the equation (3) leads to:

$$\frac{\partial W}{\partial \tau} = -\lambda(M)W + c(M)\int_M^\infty \lambda(K)d(K)W(\tau, K)\, dK \qquad (9)$$

Similarly, the equation (4) leads to:

$$\frac{dS}{d\tau} = k\left(1 - h\frac{S}{B(\tau)}\right) \qquad (10)$$

Suppose that $F_1(M)$ and $F_2(M)$ are the weight distributions for $\tau = T_1$ and $\tau = T_2$, respectively ($0 \le T_1 \le T_2$). Given the molecular factor λ(*M*), equation (9) and the initial condition:

$$W(T_1, M) = F_1(M) \qquad (11)$$

From an initial value problem. Equation (9), the initial condition (11), and the condition:

$$W(T_2, M) = F_2(M) \qquad (12)$$

Form an inverse problem for the degradation rate λ(*M*) for which the solution of the initial value problem (9), (11) also satisfies the condition (12). Techniques for the inverse problem were developed in previous studies (Watanabe and Kawai, 2011). The molecular factor λ(*M*) was obtained by solving.

Table 1: Values of *t* and *τ* and residual PEG before and after cultivation of microbial consortium E1 for one day, three days, five days, seven days, and nine days. Equation $V(\tau)=v(t)$ was solved numerically, where $V(\tau)$ is given by the formula (13) ($A=10^{3.2}$, $B=10^{4.2}$), and the values of *τ* that correspond to *t*=1.0, 3.0, 5.0, 7.0 and 9.0 were obtained numerically.

Table 1

Values of *t* and *τ* and residual PEG before and after cultivation of microbial consortium E1.

t	***τ***	**Residual PEG (%)**
0.0	0.00000000000000000	100.00000000000000000
1.0	0.17448802940997643	97.95198159634348656
3.0	2.1204368266621220	77.76599322364261013
5.0	19.68732430723412108	9.68345996176650736
7.0	34.58514617286267168	1.65477164993089931
9.0	31.65791489135981251	2.34153807149406745

The inverse problem, in which conditions (11) and (12) were weight distributions after cultivation of microbial consortium E1 for one day and three days. Once the molecular factor λ(*M*) is obtained, equation (9) was solved with the initial condition:

$$W(0,M) = f_0(M)$$

Where $f_0(M)$ was the initial weight distribution and

$$V(\tau) = \int_0^\infty W(\tau, M)\, dM$$

was obtained and the integral was approximated by:

$$\int_A^B W(\tau, M)\, dM$$

For appropriate values of A and B. It is shown in a previous study (Watanabe and Kawai, 2015a), $V(\tau)$ is well approximated with an exponential function. Here, assumption

$$V(\tau) = V(0)e^{-\mu\tau} \qquad (13)$$

is made. The following value of μ was obtained from application of the least square approximation:

$$\mu = 0.11859158097011033.$$

This value of μ was used in inverse analysis for the time factor.

Microbial consortium E1 was cultivated in culture media in which PEG was the sole carbon source, and the weight distributions $f_0(M)$, $f_1(M)$, $f_2(M)$, $f_3(M)$, $f_4(M)$ and $f_5(M)$, before and after one day, three days, five days seven days and nine days were obtained. The correspondence between values of t and τ are summarized in Table 1.

4. Application of the Newton-Raphson method and Gauss-Newton method to inverse problem for time factor

The solution of equation (10) with the initial value σ_0 depends not only on τ but also on σ_0, k, and h. Let $S(\tau, \sigma_0, k, h)$ be the solution of (10) which satisfies the initial condition $S(o, \sigma_0, k, h)=\sigma_0$.

Let

$$u(\tau, \sigma_0, k, h) = \int_0^\tau \frac{dq}{S(q, \sigma_0, k, h)}. \qquad (14)$$

In view of the expression (8), $t=u(\tau, \sigma_0, k, h)$. Suppose that $t_1, t_2,\ldots,t_m$ correspond to $t_1, t_2,\ldots,t_m$ according to the change of variables (7), so that $t_i = u(\tau_i, \sigma_0, k, h)$. Let $g_i(\sigma_0, k, h)= u(\tau_i, \sigma_0, k, h)-t_i$. Appropriate values of the parameters σ_0, k and h satisfy the system of equations:

$$g_i(\sigma_0, k, h) = 0 \quad (i = 1, 2, \ldots, m). \qquad (15)$$

Numerical techniques for the system (15) were developed in previous studies (Watanabe and Kawai, 2016a; Watanabe and Kawai, 2016b; Watanabe and Kawai, 2015a). The Newton-Raphson method was applied to the system (15) for m=3, and t_1=3, t_2=5 and t_3=7 and corresponding values of τ shown in Table 1. The following values of parameters were obtained.

$$\sigma_0 = 0.0676386887599191577, \quad k = 1.2293702927811472, \quad h = 3.8880353779411290. \qquad (16)$$

Figures 1 and 2 show numerical results. The Gauss-Newton method was applied to the system of equations (15) for m=4 and t_1=1, t_2=3, t_3=5 and t_4=7 and corresponding values of τ shown in Table 1. The following values of parameters were obtained.

$$\sigma_0 = 0.0848937646372523169, \quad k = 1.1623684037791651, \quad h = 3.8726526801320893. \qquad (17)$$

Figures 3 and 4 show numerical results. The Gauss-Newton method was applied to the system of equations (15) also for m=5 and t_1=1, t_2=3, t_3=5, t_4=7 and t_5=9 and corresponding values of τ shown in Table 1. The following values of parameters were obtained.

$$\sigma_0 = 0.18753766061747670, \quad k = 0.76815144641353228, \quad h = 4.0053480510926853. \qquad (18)$$

Figure 5 and 6 show numerical results.

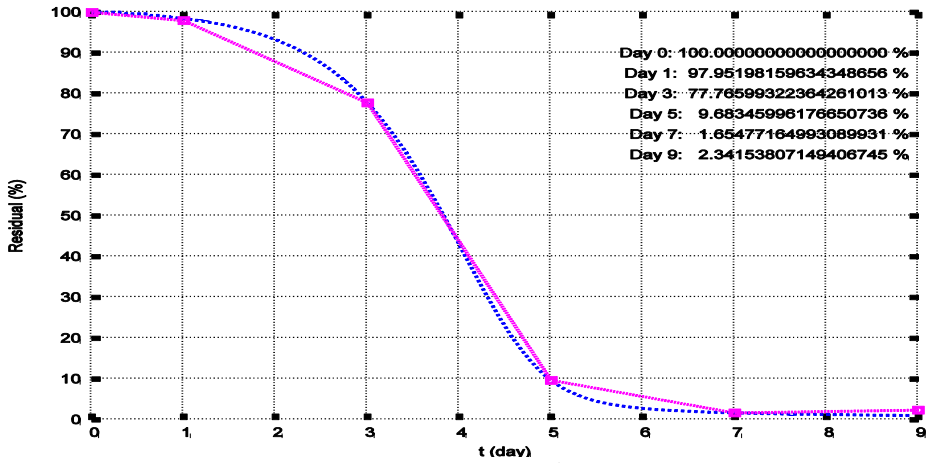

Fig. 1. Transition of residual PEG. The curve ($u(\tau, \sigma_0, k, h)$, $V(\tau)/V(0)$x100.0) for the values of σ_0, k and h (16) is shown. The figure also shows the residual PEG before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.

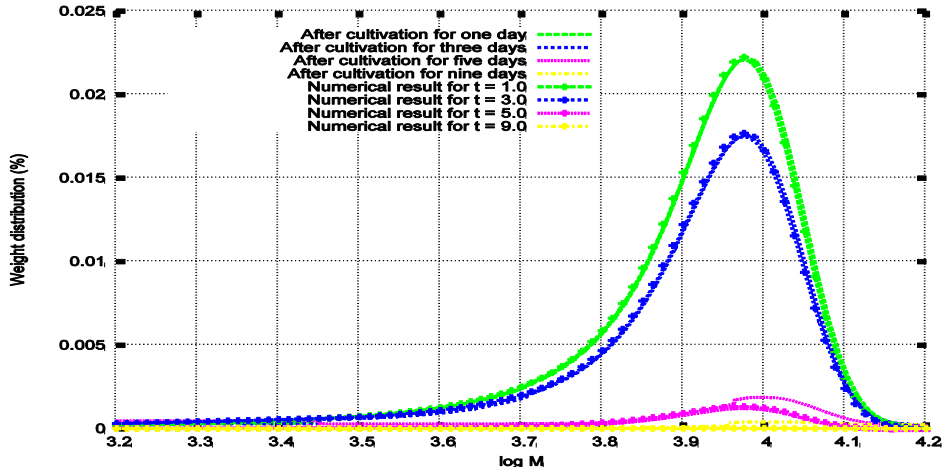

Fig. 2. Transition of weight distribution. The figure shows profiles of a numerical solution of the initial value problem (3), (4), (5), (6) for the values of σ_0, k and h (16). The figure also shows weight distributions before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.

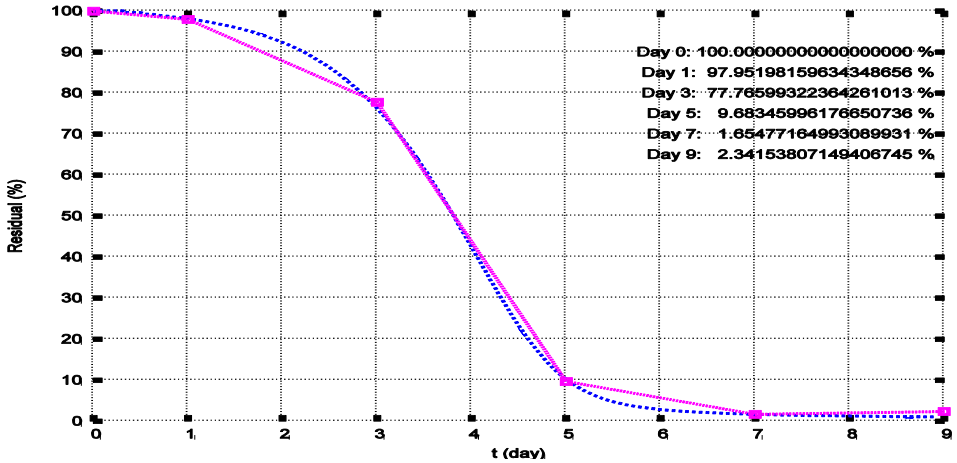

Fig. 3. Transition of residual PEG. The curve ($u(\tau, \sigma_0, k, h)$, $V(\tau)/V(0)$x100.0) for the values of σ_0, k and h (17) is shown. The figure also shows the residual PEG before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.

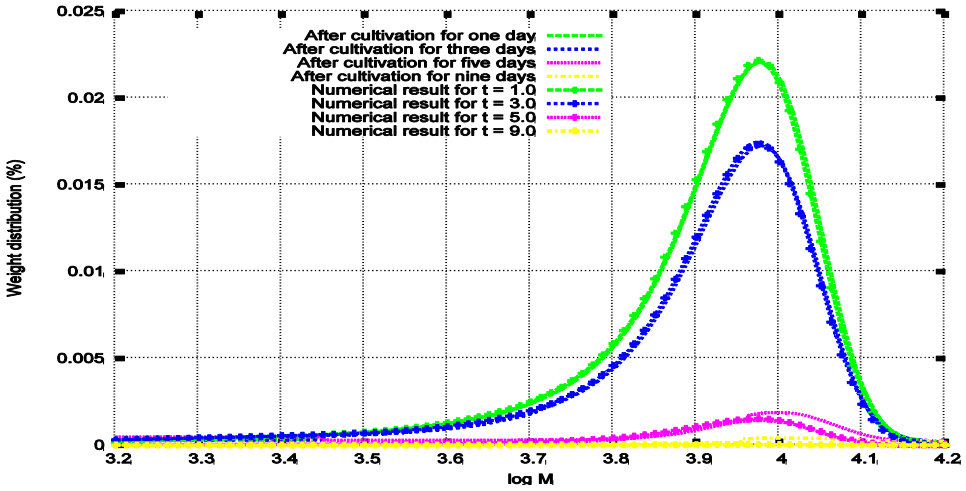

Fig. 4. Transition of weight distribution. The figure shows profiles of a numerical solution of the initial value problem (3), (4), (5), (6) for the values of σ_0, k and h (17). The figure also shows weight distributions before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.

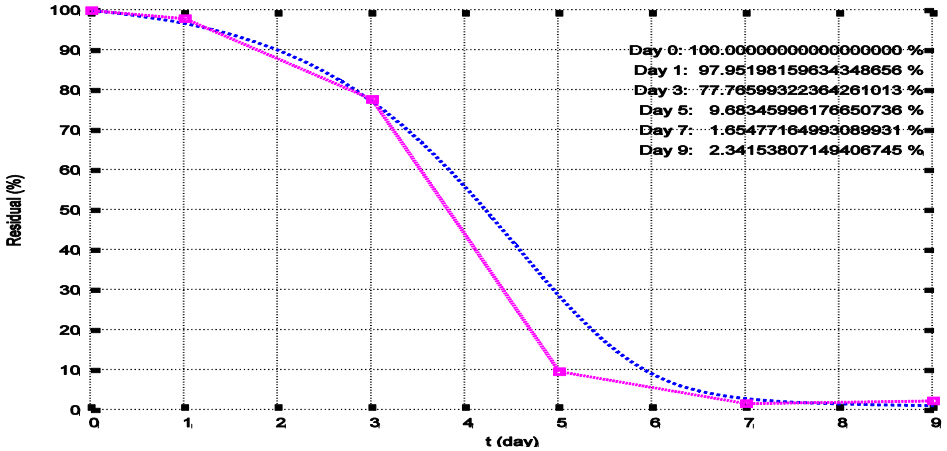

Fig. 5. Transition of residual PEG. The curve $u(\tau, \sigma_0, k, h)$, $V(\tau)/V(0)$x100.0 for the values of σ_0, k and h (18) is shown. The figure also shows the residual PEG before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.

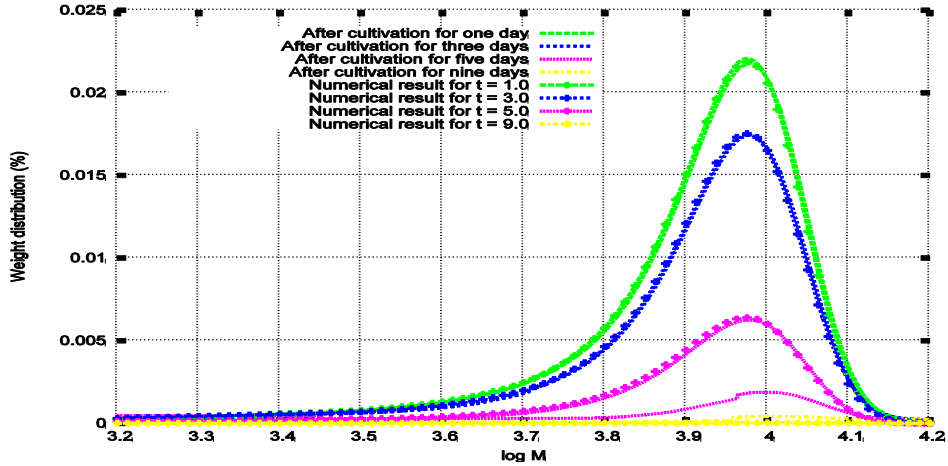

Fig. 6. Transition of weight distribution. The figure shows profiles of a numerical solution of the initial value problem (3), (4), (5), (6) for the values of σ_0, k and h (18). The figure also shows weight distributions before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.

5. Conclusion

In previous studies, the Newton-Raphson method was applied to the system consisting of the first two equations of system (15) for m=3 and functions σ_0=ø(h)$ and k=ψ(h) were obtained numerically. The bisection method (Watanabe and Kawai, 2015a) and the Newton's method (Watanabe and Kawai, 2016b) were applied to the equation g_3(ø(h), ψ(h), h)=0. In this study, application of the Newton-Raphson method and the Gauss-Newton method to the system of equations (15) was demonstrated where V(τ) was an exponential function. Figures 1, 2, 3, and 4 show acceptable agreement between the numerical result and the experimental result for t=3, t=5 and t=7. The numerical results shown in Figures 1 and 2 appear almost identical with the numerical results obtained from application of the Gauss-Newton method for m=4 (Figures 3 and 4), which shows that the assumption that V(τ) is an exponential function is appropriate. Figures 5 and 6 show large mismatches between the numerical result obtained from application of the Gauss-Newton method (m=5) and the experimental result for t=5. Those mismatches were caused by loss of monotonicity of data sets, which violates the assumption that the residual PEG is an exponential function.

Acknowledgments

The authors thank Ms. Y. Shimizu for her technical support. This work was supported by JSPS KAKENHI Grant Number 24540127.

References

Watanabe, M., Kawai, F., 2003. Numerical simulation for enzymatic degradation of poly (Vinyl alcohol). Polymer Degrad. Stabil., 81, 393-399.

Watanabe, M., Kawai, F., 2005. Numerical simulation of microbial depolymerization process of exogenous type. In Rob May and Roberts, A.J., editors, Proceedings of 12th Computational Techniques and Applications Conference, CTAC-2004, Melbourne, Australia in September 2004. ANZIAM J., 46(E), C1188-C1204.

Watanabe, M., Kawai, F., 2006. Mathematical modelling and computational analysis of enzymatic degradation of xenobiotic polymers. Appl. Math. Model., 30, 1497-1514.

Watanabe, M., Kawai, F., 2008. Modeling and analysis of biodegradation of xenobiotic polymers based on experimental results. In Mercer, G.N., Roberts, A.J., editors, Proceedings of the 8th Biennial Engineering Mathematics and Applications Conference, EMAC-2007. ANZIAM J., 49, C457-C474.

Watanabe, M., Kawai, F., 2010. Effects of microbial population in degradation process of xenobiotic polymers. In Howlett, P., Nelson, M., Roberts, A.J., editors, Proceedings of the 9th Biennial Engineering Mathematics and Applications Conference, EMAC-2009. ANZIAM J., 51, C682-C696.

Watanabe, M., Kawai, F., 2011. Study of biodegradation of xenobiotic polymers with change of microbial population. In McLean, W., Roberts, A.J., editors, Proceedings of the 15th Biennial Computational Techniques and Applications Conference, CTAC-2010. ANZIAM J., 52, C410-C429.

Watanabe, M., Kawai, F., 2012a. Modeling biodegradation of polyethylene with memoryless behavior of metabolic consumption. J. Bioremed. Biodegrad., 3(146).

Watanabe, M., Kawai, F., 2012b. Study on microbial depolymerization processes of xenobiotic polymers with mathematical modelling and numerical simulation. In Nelson, M., Coupland, M., Sidhu, H., Hamilton, T., Roberts, A.J., editors, Proceedings of the 10th Biennial Engineering Mathematics and Applications Conference, EMAC-2011. ANZIAM J., 53, C203-C217.

Watanabe, M., Kawai, F., 2015a. Numerical techniques for inverse problems from modeling of microbial depolymerization processes. Proceedings of Intelisys. Int. J. Appl. Eng. Res., 11(8), 5461-5468.

Watanabe, M., Kawai, F., 2015b. Solutions of inverse problems for biodegradation of xenobiotic polymers. AIP Conf. Proc., 1707, Conference date: 18-21 August, Location: Yogyakarta, Indonesia.

Watanabe, M., Kawai, F., 2016a. Numerical study of inverse problems in modeling and simulation of microbial depolymerization processes. Proceedings of 9th International Conference on Environmental and Geological Science and Engineering (EG'16). Int. J. Chem. Chem. Eng. Syst., 1, 45-55.

Watanabe, M., Kawai, F., 2016b. Numerical study of microbial depolymerization process with the Newton-Raphson method and the Newton's method. Int. J. Eng. Res. Sci., 2, 119-130.

Watanabe, M., Kawai, F., Shibata, M., Yokoyama, S., Sudate, Y., Hayashi, S., 2004. Analytical and computational techniques for exogenous depolymerization of xenobiotic polymers. Math. Biosci., 192, 19-37.

Watanabe, M., Kawai, F., Tsuboi, S., Nakatsu, S., Ohara, H., 2007. Study on enzymatic hydrolysis of polylactic acid by endogenous depolymerization model. Macromolecular Theory and Simulations, 16, 619-626.

How to cite this article: Watanabe, M., Kawai, F., 2017. Numerical techniques for inverse analysis in study of microbial depolymerization processes. Scientific Journal of Environmental Sciences, 6(9), 304-311.