Numerical Study of Inverse Problems in Modeling and Simulation of Microbial Depolymerization Processes

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Abstract: A mathematical model proposed in previous studies was analyzed for simulation of an exogenous type microbial depolymerization process. Inverse problems for a molecular factor and a time factor of degradation rate were solved numerically with experimental outcomes before and after cultivation of microbial consortium E1 in a culture media in which polyethylene glycol was the sole carbon source. Values of three parameters were obtained with the Newton-Raphson method and the Gauss-Newton method.

Key–Words: Biodegradation, Polymer, Mathematical model, Inverse problem, Numerical simulation

1 Introduction

In microbial depolymerization processes, microorganisms utilizes polymer molecules as carbon sources. Those processes are generally categorized into two types; exogenous type processes and endogenous type processes. Monomers are liberated from terminals of molecules and absorbed into cells in an exogenous type depolymerization process. Polymers depolymerizable in exogenous type depolymerization processes include polyethylene (PE) and polyethylene glycol (PEG). Oxidation of an *n*-alkane starts with hydroxylation to produce a primary (or secondary) alcohol, which is oxidized further to an aldehyde (or ketone) and to an acid. Carboxylated *n*-alkanes are structurally analogous to fatty acids and sustain the β-oxidation for production of acetic acids. A PE molecule liberates a monomer unit in one cycle of β-oxidation, and reduces in size undergoing successive β-oxidation processes until it becomes small enough to be absorbed directly into cells. Thus primary factors of PE biodegradation are size reduction of large molecules due to β-oxidation, and direct consumption or absorption of small molecules by cells. A mathematical model was constructed from those principles for simulation of the PE biodegradation [3, 12, 4].

Besides PE, PEG is a polymer that undergoes an exogenous type depolymerization process. PEG is one of the polyethers whose chemical structures are expressed with the general structural formula $HO(R-O)_n H$ (PEG: $R = CH_2CH_2$). PEG molecules reduce in size liberating C_2 compounds (CH_2CH_2) . Mathematical techniques developed for PE biodegra-

dation were applied to exogenous type depolymerization processes of PEG [5]. Inverse problems were solved numerically for degradation rates based on the weight distribution with respect to the molecular weight before and after cultivation of microorganisms. Once a degradation rate was found, an initial value problem was solved numerically, and the transition of the weight distribution was simulated. Time dependence of degradation rates on time was also taken into account in modeling and simulation of depolymerization processes of PEG [7, 9, 10].

Unlike exogenous type depolymerization processes, molecules sustain breakdowns due to arbitrary scission in endogenous type depolymerization processes. Examples of polymers depolymerizable in endogenous type depolymerization processes include polyvinyl alcohol (PVA) and polylactic acid (PLA). PVA is depolymerized by oxidation followed by cleavage of a carbon-carbon chain. A mathematical model was proposed for an enzymatic depolymerization process of PVA . [14, 6]. The model was applied to enzymatic hydrolysis of PLA, and the degradability of PVA and PLA was compared [17]. Time dependence of degradation rate was taken into account in study of endogeous type depolymerization processes pf PLA [8]. A model originally proposed for endogenous type depolymerization processes was applied to an exogenous type depolymerization process of PEG [11].

In this study, exogenous depolymerization process of PEG is revisited. A microbial depolymerization of PEG was analyzed with a model proposed

in previous studies. Inverse problem for a molecular factor and a time factor of degradation rate were solved numerically with experimental data introduced into analysis. In previous studies, weight distributions before and after cultivation of microbial consortium E1 for one day, three days, five days, seven days, and nine days were analyzed [10]. In one of the studies, the Newton-Raphson method and the bisection method were applied to an inverse problem for a time factor with weight distribution before and after three days, seven days, and nine days [13]. In another study, the Newton-Raphson method and the Newton's method were applied to an inverse problem for a time factor with weight distribution before after two days, four days, and seven days [16]. In this study, the application of Newton-Raphson method to an inverse problem for a time factor is demonstrated with numerical result based on weight distributions before and after cultivation of microbial consortium E1 for three days, five days, and seven days. The application of Gauss-Newton method to an inverse problem for a time factor is also demonstrated with numerical result based on weight distributions before and after cultivation for one day, three days, five days, seven days, and nine days.

2 Description of Model for Exogenous Type Microbial Depolymerization Process

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, that is, the total weight of residual polymer for $A \leq M \leq B$ at time t is the integral

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

Let $v(t)$ be the total residual polymer at time t. The residual polymer $v(t)$ is given by

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

which can be approximated with the integral (1) for appropriate values of A and B. Let $p(t, K, M)$ be the total weight of molecules with molecular weight M to become molecules of molecular weight K at time t per unit time at time t. The principle of mass conservation leads to the equation (3) [15].

$$
\begin{aligned}
\frac{\partial w}{\partial t} = & -\int_0^M p(t, K, M) \, dK \\
& + \int_M^\infty \frac{M}{K} p(t, M, K) \, dK.
\end{aligned} \quad (3)
$$

Let $\gamma(t, M)$ be the weight lost from $w(t, M)$ per unit time and unit weight at time t. Let $q(K, M)$ be the weight transfer per unit weight from $w(t, M)$ to $w(t, K)$ for $0 \leq K \leq M$. Note that

$$\int_0^M q(K, M) \, dK = 1 \quad (4)$$

holds. The amount of loss from $w(t, M)$ per unit time is $\gamma(t, M) w(t, M)$, and

$$p(t, K, M) = \gamma(t, M) q(K, M) w(t, M) \quad (5)$$

holds. Note that the equation (4) leads to

$$\int_0^M p(t, K, M) \, dK = \gamma(t, M) w(t, M). \quad (6)$$

Time factors of degradability such as temperature, dissolved oxygen, and microbial population act evenly on molecules regardless of the molecular weight. The degradation rate $\gamma(t, M)$ is a product of a function of t, which is denoted by $\sigma(t)$, and a function of M, which is denoted by $\lambda(M)$, so that

$$\gamma(t, M) = \sigma(t) \lambda(M). \quad (7)$$

Liberation of monomers in an exogenous depolymerization process is memoryless, which means that an amount liberated from a molecule at one stage does not depend on the amount liberated at the previous stage, and amount J liberated from a molecule follows exponential distribution $\rho e^{-\rho J}$ [1]. In an exogenous depolymerization process, amount $M - K$ is truncated from a molecule with molecular weight M in transformation to a molecule with molecular weight K. Substitution $J = M - K$ and scaling according to condition (4) lead to the expression of $q(K, M)$ given by

$$q(K, M) = \frac{\rho}{1 - e^{-\rho M}} e^{-\rho(M-K)}. \quad (8)$$

The parameter ρ is referred to as the intensity of the exponential distribution. In order to determine the value of the parameter, liberation of monomer units in the exogenous depolymerization process is considered. In an exogenous type depolymerization process, molecules reduce in size through successive liberation of monomers. Let L be the molecular weight of monomer unit truncated from a terminal of a molecule in one cycle of depolymerization process, e.g. PE: $L = 28$ (CH_2CH_2), PEG: $L = 44$, (CH_2CH_2O). Expression of ρ in terms of L,

$$\rho = \frac{1}{L} \log 2. \quad (9)$$

was obtained in a previous study [15].

Substituting expressions (5) - (8) into equation (3), eqation (10) is obtained.

$$\frac{\partial w}{\partial t} = \sigma(t)\left[-\lambda(M)w + c(M)\int_M^\infty \lambda(K)\,d(K)\,w(t,K)\,dK\right], \quad (10)$$

where

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

The growth rate of microbial population depends on the residual polymer in the culture medium. Suppose that the microbial population is stationary for the total mass per individual h. The microbial population increases over a time interval in which $h < v(t)/\sigma(t)$ and decreases over an interval in which $h > v(t)/\sigma(t)$. The value of the expression

$$1 - h\frac{\sigma(t)}{v(t)}$$

is a margin of increment for the microbial population. The time rate of change of $\sigma(t)$ per individual is a constant multiple of this expression, and the microbial population $\sigma(t)$ satisfies

$$\frac{d\sigma}{dt} = k\left(1 - h\frac{\sigma}{v(t)}\right)\sigma, \quad (11)$$

for some positive constant k. System of equations (10), (11) is associated with the initial condition

$$w(0,M) = f_0(M), \quad (12)$$

$$\sigma(0) = \sigma_0, \quad (13)$$

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

3 Inverse Analysis for Molecular Factor and Time Factor of Degradation Rate

Consider the change of variable from t to τ defined by

$$\tau = \int_0^t \sigma(s)\,ds. \quad (14)$$

Note that

$$\frac{d\tau}{dt} = \sigma(t) \quad (15)$$

holds. Let

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

for which the relationship (14) holds. According to the equation (15),

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

and the equation

$$\frac{\partial W}{\partial \tau} = -\lambda(M)W + c(M)\int_M^\infty \lambda(K)\,d(K)\,W(\tau,K)\,dK \quad (16)$$

is obtained from the equation (10). Similarly, the equation (11) is converted to

$$\frac{dS}{d\tau} = k\left(1 - h\frac{S}{V(\tau)}\right). \quad (17)$$

Suppose that $F_1(M)$ and $F_2(M)$ are the weight distribution for $\tau = T_1$ and $\tau = T_2$, respectively ($0 \le T_1 < T_2$). Given $\lambda(M)$, equation (16) and the initial condition

$$W(\tau_1, M) = F_1(M) \quad (18)$$

form an initial value problem. Equation (16), the initial condition (17), and the terminal condition

$$W(\tau_2, M) = F_2(M) \quad (19)$$

form an inverse problem for the degradation rate $\lambda(M)$ for which the solution of the initial value problem (16), (18) also satisfies the condition (19). Techniques to solve the inverse problem were developed in previous studies [11]. In particular, the molecular factor $\lambda(M)$ was obtained for $T_1 = 0$, $T_2 = 4$, $F_1(M)$, and $F_2(M)$ were the weight distributions of PEG after cultivation of the microbial consortium E1 for one day and five days, respectively. Once $\lambda(M)$ was obtained, the initial value problem consisting of the equation (16) and the initial condition

$$W(0, M) = f_0(M) \quad (20)$$

was solved, and values of τ corresponding to values of t were obtained numerically by solving the equations $V(\tau) = v(t)$, where

$$V(\tau) = \int_A^B W(\tau, M)\,dM. \quad (21)$$

Table 1 shows that $t = 1.0$, $t = 3.0$, $t = 5.0$, $t = 7.0$, and $t = 9.0$ correspond to $\tau \approx 0.060$, $\tau \approx 0.553$, $\tau \approx 4.062$, $\tau \approx 7.932$, and $\tau \approx 7.080$, respectively, according to the change of variables (14). It also shows that $v(1)/v(0) \approx V(0.060)/V(0) \approx 0.980$, $v(3)/v(0) \approx V(0.553)/V(0) \approx 0.778$, $v(5)/v(0) \approx V(4.062)/V(0) \approx 0.097$, $v(7)/v(0) \approx V(7.932)/V(0) \approx 0.017$, and $v(9)/v(0) \approx V(7.0080)/V(0) \approx 0.023$.

4 Application of the Newton-Raphson Method in Inverse Analysis of Time Factor

The solution of equation (17) with the initial value σ_0 depends not only on τ but also on σ_0, k, and h. Denote by $S(\tau, \sigma_0, k, h)$ the solution of (17) which satisfies the initial condition $S(0, \sigma_0, k, h) = \sigma_0$. Let

$$u(\tau, \sigma_0, k, h) = \int_0^\tau \frac{1}{S(q, \sigma_0, k, h)}\, dq. \qquad (22)$$

In view of the expression (10), $t = u(\tau, \sigma_0, k, h)$. Suppose that t_1, t_2, and t_3 correspond to τ_1, τ_2, and τ_3 according to the change of variables (14), so that $t_i = u(\tau_i, \sigma_0, k, h)$ $(i = 1, 2, 3)$. Let $g_i(\sigma_0, k, h) = u(\tau_i, \sigma_0, k, h) - t_i$, and consider the system of equations

$$g_i(\sigma_0, k, h) = 0 \qquad (i = 1, 2, 3) \qquad (23)$$

for the unknowns σ_0, k, and h.

In application of the Newton-Raphson method, a sequence of approximate solutions $\boldsymbol{x}_0$, $\boldsymbol{x}_1$, ... is generated with the recurrence formula

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n - J_n^{-1} \boldsymbol{g}_n \qquad (n = 0, 1, \ldots), \quad (24)$$

where

$$\boldsymbol{x}_n = \begin{bmatrix} \sigma_{0,n} \\ k_n \\ h_n \end{bmatrix}, \quad \boldsymbol{g}_n = \begin{bmatrix} g_{1,n} \\ g_{2,n} \\ g_{3,n} \end{bmatrix},$$

$$J_n = \begin{bmatrix} \xi_{1,n} & \eta_{1,n} & \zeta_{1,n} \\ \xi_{2,n} & \eta_{2,n} & \zeta_{2,n} \\ \xi_{3,n} & \eta_{3,n} & \zeta_{3,n} \end{bmatrix},$$

$$\xi_{i,n} = \left. \frac{\partial g_i}{\partial \sigma_0} \right|_{\sigma_0 = \sigma_{0,n},\, k = k_n,\, h = h_n}, \qquad (25)$$

$$\eta_{i,n} = \left. \frac{\partial g_i}{\partial k} \right|_{\sigma_0 = \sigma_{0,n},\, k = k_n,\, h = h_n}, \qquad (26)$$

$$\zeta_{i,n} = \left. \frac{\partial g_i}{\partial h} \right|_{\sigma_0 = \sigma_{0,n},\, k = k_n,\, h = h_n}, \qquad (27)$$

$$g_{i,n} = g_i(\sigma_{0,n}, k_n, h_n). \qquad (28)$$

Note that

$$\frac{\partial g_i}{\partial \sigma_0} = \left. \frac{\partial u}{\partial \sigma_0} \right|_{\tau = \tau_i},$$

$$\frac{\partial g_i}{\partial k} = \left. \frac{\partial u}{\partial k} \right|_{\tau = \tau_i}, \qquad (29)$$

$$\frac{\partial g_i}{\partial h} = \left. \frac{\partial u}{\partial h} \right|_{\tau = \tau_i}.$$

Partial derivative $\partial u/\partial \sigma_0$ is the solution of the initial value problem

$$\frac{d}{d\tau}\left(\frac{\partial u}{\partial \sigma_0}\right) = -\frac{1}{[S(\tau)]^2}\left(\frac{\partial S}{\partial \sigma_0}\right),$$

$$\left. \frac{\partial u}{\partial \sigma_0} \right|_{\tau = 0} = 0, \qquad (30)$$

while partial derivative $\partial S/\partial \sigma_0$ is the solution of the initial value problem

$$\frac{d}{d\tau}\left(\frac{\partial S}{\partial \sigma_0}\right) = -\frac{kh}{V(\tau)}\left(\frac{\partial S}{\partial \sigma_0}\right),$$

$$\left. \frac{\partial S}{\partial \sigma_0} \right|_{\tau = 0} = 1. \qquad (31)$$

Similarly, partial derivative $\partial u/\partial k$ is the solution of the initial value problem

$$\frac{d}{d\tau}\left(\frac{\partial u}{\partial k}\right) = -\frac{1}{[S(\tau)]^2}\left(\frac{\partial S}{\partial k}\right),$$

$$\left. \frac{\partial u}{\partial k} \right|_{\tau = 0} = 0. \qquad (32)$$

and $\partial S/\partial k$ is the solution of the initial value problem

$$\frac{d}{d\tau}\left(\frac{\partial S}{\partial k}\right) = 1 - \frac{h}{V(\tau)}S(\tau) - \frac{kh}{V(\tau)}\left(\frac{\partial S}{\partial k}\right),$$

$$\left. \frac{\partial S}{\partial k} \right|_{\tau = 0} = 0. \qquad (33)$$

Partial derivative $\partial u/\partial h$ is the solution of the initial value problem

$$\frac{d}{d\tau}\left(\frac{\partial u}{\partial h}\right) = -\frac{1}{[S(\tau)]^2}\left(\frac{\partial S}{\partial h}\right),$$

$$\left. \frac{\partial u}{\partial h} \right|_{\tau = 0} = 0. \qquad (34)$$

and $\partial S/\partial h$ is the solution of the initial value problem

$$\frac{d}{d\tau}\left(\frac{\partial S}{\partial h}\right) = -\frac{k}{V(\tau)}\left(S(\tau) + \frac{\partial S}{\partial k}\right),$$

$$\left. \frac{\partial S}{\partial h} \right|_{\tau = 0} = 0. \qquad (35)$$

Initial value problem (31) is solved for $\partial S/\partial \sigma_0$, and then the initial value problem (30) is solved for $\partial u/\partial \sigma_0$. Initial value problem (33) is solved for $\partial S/\partial k$, and then the initial value problem (32) is solved for $\partial u/\partial k$. Initial value problem (35) is solved

for $\partial S/\partial h$, and then the initial value problem (34) is solved for $\partial u/\partial h$.

Values 3, 5, and 7 were set for t_1, t_2, and t_3, and the corresponding values of τ_1, τ_2, and τ_3 were set according to table 1. The system of equations (23) was solved numerically with techniques described previously. Table 2 shows the results obtained from application of the Newton-Raphson method. Figure 1 shows the curve $(u(\tau, \sigma_0, k, h), V(\tau))$ for the value of the parameters obtained from application of the Newton-Raphson method.

5 Application of the Gauss-Newton Method in Inverse Analysis of Time Factor

Suppose that t_1, t_2, ..., t_m correspond to τ_1, τ_2, ..., τ_m according to the change of variables (14), so that $t_i = u(\tau_i, \sigma_0, k, h)$ $(i = 1, 2, ..., m)$. Let $g_i(\sigma_0, k, h) = u(\tau_i, \sigma_0, k, h) - t_i$, and consider the nonlinear least squares problem for parameter values to minimize the square sum

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

Suppose that $\xi_{i,n}$, $\eta_{i,n}$, $\zeta_{i,n}$, and $g_{i,n}$ $(i = 1, 2, ..., m)$ are given by the formulas (24), (25), (26), and (27), respectively, and the partial derivatives of g_i are evaluated with the formulas (28) - (34). In application of the Gauss-Newton method to the nonlinear least squares problem [2], a sequence of approximate solutions $\boldsymbol{x}_0$, $\boldsymbol{x}_1$, ... is generated with the recurrence formula

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n - \left(J_n^T J_n \right)^{-1} J_n^T \boldsymbol{g}_n , \qquad (36)$$

where

$$\boldsymbol{x}_n = \begin{bmatrix} \sigma_{0,n} \\ k_n \\ h_n \end{bmatrix} , \qquad \boldsymbol{g}_n = \begin{bmatrix} g_{1,n} \\ g_{2,n} \\ \vdots \\ g_{m,n} \end{bmatrix} ,$$

$$J_n = \begin{bmatrix} \xi_{1,n} & \eta_{1,n} & \zeta_{1,n} \\ \xi_{2,n} & \eta_{2,n} & \zeta_{2,n} \\ \vdots & \vdots & \vdots \\ \xi_{m,n} & \eta_{m,n} & \zeta_{m,n} \end{bmatrix} .$$

Values 1, 3, 5, 7, and 9 were set for t_1, t_2, t_3, t_4, and t_5, and the corresponding values of τ_1, τ_2, τ_3, and τ_4 were set according to table 1. Tables 3 and 4 show the results obtained from application of the Gauss-Newton method for $m = 4$ and

$m = 5$, respectively. Figures 2 and 3 show the curve $(u(\tau, \sigma_0, k, h), V(\tau))$ for the value of the parameters obtained from application of the Gauss-Newton method for $m = 4$ and $m = 5$, respectively.

6 Conclusion

In previous studies, the Newton-Raphson method was applied to the system consisting of the first two equations of system (23), and functions $\sigma_0 = \phi(h)$ and $k = \psi(h)$ were obtained numerically. The bisection method [13] and the Newton's method [16] were applied to the equation $g_3(\phi(h), \psi(h), h) = 0$. In this study, application of the Newton-Raphson method to the equation (23) was demonstrated. Table 2 shows that it took eleven iterations for residuals between two consecutive approximations to reduce to 10^{-12}. Application of the Gauss-Newton method to the nonlinear least squares problem was also demonstrated. Table 3 shows that it took seventeen iterations for the residual between two consecutive approximations to reduce to 10^{-12} for $m = 4$. Table 4 shows that it took twenty nine iterations for the residual between two consecutive approximations to reduce to 10^{-12} for $m = 4$.

Figure 1 shows an acceptable agreement between the numerical result obtained with the Newton-Raphson method and the experimental result for $t = 3.0$, $t = 5.0$, and $t = 7.0$. The numerical result shown in Figure 1 seems almost identical with the numerical result obtained with the Gauss-Newton method for $m = 4$ (Figure 2). However, while the numerical result shown in Figure 1 matches the experimental result closer than the one shown in Figure 2 does for $t = 3.0$, the latter matches the experimental result closer than the former does for $t = 1.0$. Figure 3 shows large mismatch between the numerical result obtained with the Gauss-Newton method ($m = 5$) for $t = 5.0$.

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 (21) ($A = 10^{3.2}$, $B = 10^{4.2}$), and the values of τ that correspond to $t = 1.0, 3.0, 5.0, 7.0$, and 9.0 were obtained numerically.

t	τ	Residual PEG (%)
0.0	0.0000000000000000	100.00000000000000000
1.0	0.06047187563063424	97.95198159634348656
3.0	0.55262989011516628	77.76599322364261013
5.0	4.06234786958022198	9.68345996176650736
7.0	7.93233059730225154	1.65477164993089931
9.0	7.07970651673239981	2.34153807149406745

Table 2: Change of parameter values and iteration counts for $\sigma_{0,0} = 0.01$, $k_0 = 1.0$, and $h_0 = 20.0$ in application of the Newton-Raphson method (24).

n	$\sigma_{0,n}$	k_n	h_n	$\|\boldsymbol{x}_n - \boldsymbol{x}_{n-1}\|$
1	0.0206190050374885	1.0569374889037175	14.2935242054778477	5.70676971197607234
2	0.0258948028875955	1.0556100159478528	13.9348881321916647	0.3586773331136723
3	0.0258864474608785	1.0556129743416875	13.9316782982441367	0.0032098461857155
4	0.0258874557283682	1.0556121877644171	13.9316796483408663	0.0000018595882104
5	0.0258873343993537	1.0556122823964127	13.9316794581136527	0.0000002446678097
6	0.0258873490016520	1.0556122710071971	13.9316794810081230	0.0000000294465298
7	0.0258873472442556	1.0556122723779036	13.9316794782528142	0.0000000035438687
8	0.0258873474557585	1.0556122722129566	13.9316794785844653	0.0000000004265366
9	0.0258873474303045	1.0556122722328056	13.9316794785446110	0.0000000000512860
10	0.0258873474333677	1.0556122722304133	13.9316794785493983	0.0000000000061664
11	0.0258873474330002	1.0556122722306820	13.9316794785488032	0.0000000000007492

Table 3: Change of parameter values and iteration counts for $\sigma_{0,0} = 0.01$, $k = 1.0$, and $h = 20.0$ in application of the Gauss-Newton method (36) for $m = 4$.

n	$\sigma_{0,n}$	k_n	h_n	$\|\boldsymbol{x}_n - \boldsymbol{x}_{n-1}\|$
1	0.0231411611889465	1.0089676400743921	14.2793379891037127	5.7206841331782909
2	0.0319096555956675	0.9882370245947713	13.7165469107693490	0.5632410165862217
4	0.0321456493525573	0.9908265643744594	13.7197124845133196	0.0008490000374433
6	0.0321529614675779	0.9907949218247025	13.7195745147797066	0.0000328264021488
8	0.0321532196695331	0.9907938009225293	13.7195696373668969	0.0000011601003378
10	0.0321532287936919	0.9907937613098488	13.7195694650100606	0.0000000409956529
12	0.0321532291161225	0.9907937599100173	13.7195694589192758	0.0000000014485198
14	0.0321532291275163	0.9907937598605535	13.7195694587043295	0.0000000000514120
16	0.0321532291279201	0.9907937598587845	13.7195694586964674	0.0000000000015920
17	0.0321532291279376	0.9907937598587064	13.7195694586961352	0.0000000000003417

Table 4: Change of parameter values and iteration counts for $\sigma_{0,0} = 0.01$, $k = 1.0$, and $h = 20.0$ in application of the Gauss-Newton method (36) for $m = 5$.

| n	$\sigma_{0,n}$	k_n	h_n	$\|\boldsymbol{x}_n - \boldsymbol{x}_{n-1}\|$
1	0.0324187183171035	0.6822158382705551	15.4820874349381086	4.5291305255999399
2	0.0535619490611851	0.6534127090424661	11.9796142908157606	3.5026553900944801
4	0.0669639474045269	0.6251648808076438	11.6135998875715725	0.1147224553082999
6	0.0672170009756080	0.6240785258262013	11.6244685210194270	0.0072055993139356
8	0.0672172467493588	0.6240826968204979	11.6261177160891780	0.0009502346551702
10	0.0672168368709506	0.6240853627367611	11.6263374589919284	0.0001259623290875
12	0.0672167764475136	0.6240857454007310	11.6263666205200327	0.0000167078763031
14	0.0672167683493325	0.6240857965595676	11.6263704890296466	0.0000022163178083
16	0.0672167672739550	0.6240858033513482	11.6263710021988587	0.0000002939991594
18	0.0672167671312870	0.6240858042523756	11.6263710702717091	0.0000000389988860
20	0.0672167671123656	0.6240858043718742	11.6263710793013892	0.0000000051735729
22	0.0672167671098546	0.6240858043877328	11.6263710804996769	0.0000000006858154
24	0.0672167671095218	0.6240858043898341	11.6263710806581901	0.0000000000913485
26	0.0672167671094773	0.6240858043901154	11.6263710806792506	0.0000000000124427
28	0.0672167671094710	0.6240858043901573	11.6263710806822935	0.0000000000014674
29	0.0672167671094707	0.6240858043901598	11.6263710806827980	0.0000000000005045
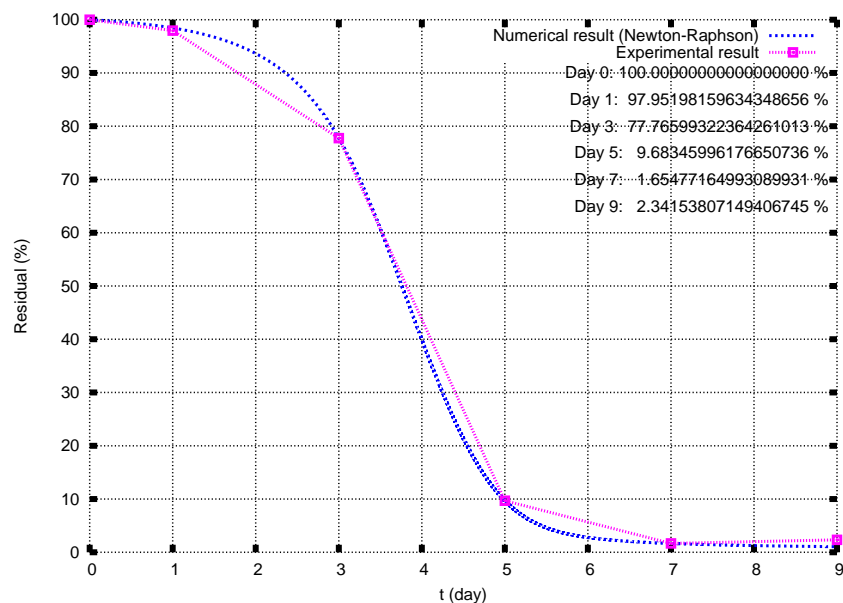
Figure 1: Transition of residual PEG. The curve $(u(\tau, \sigma_0, k, h), (V(\tau)/V(0)) \times 100)$ for the values of σ_0, k, and h (Table 2, $n = 11$) obtained from application of the Newton-Raphson method (24) is shown. The figure also shows the residual PEG before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.
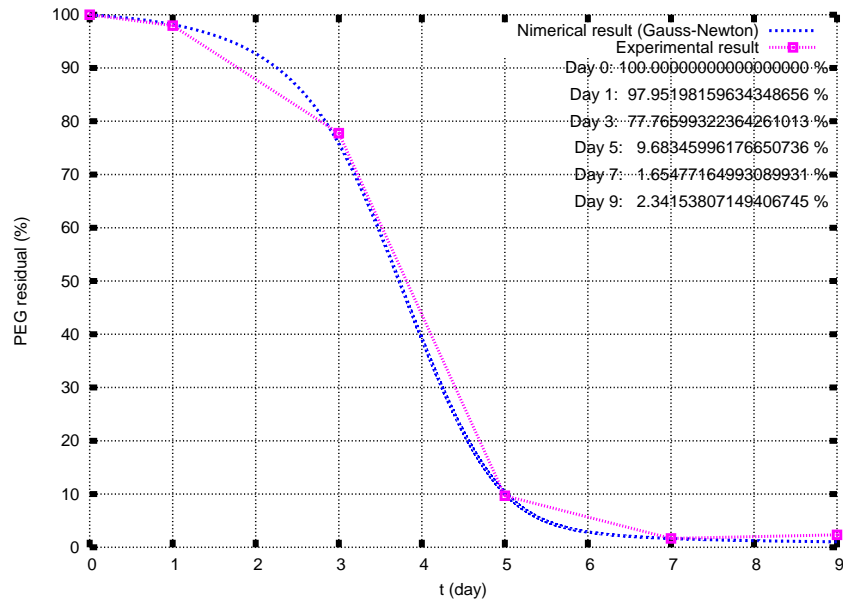
Figure 2: Transition of residual PEG. The curve $(u(\tau, \sigma_0, k, h), (V(\tau)/V(0)) \times 100)$ for the values of σ_0, k, and h (Table 3, $n = 17$) obtained from application of the Gauss-Newton method (36) ($m = 4$) is shown. The figure also shows the residual PEG before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.
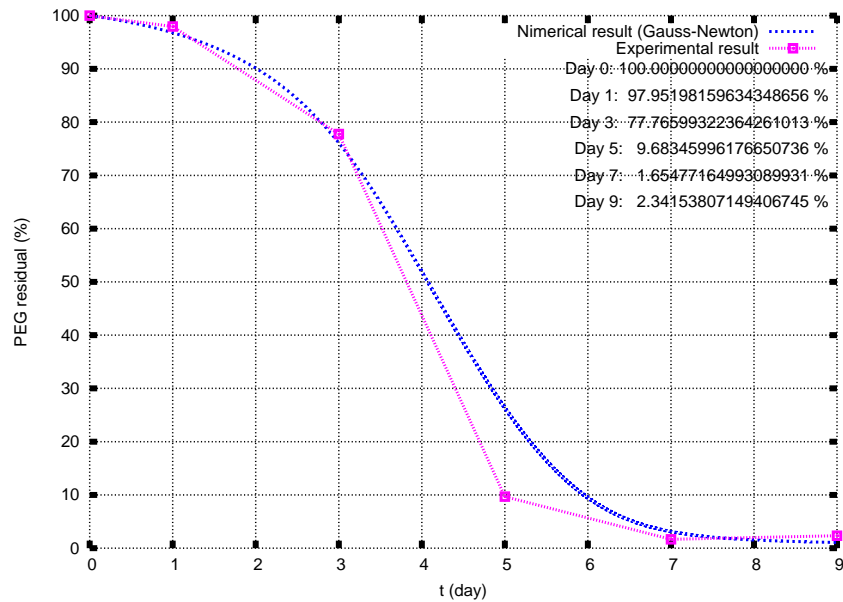

Figure 3: Transition of residual PEG. The curve $(u(\tau, \sigma_0, k, h), (V(\tau)/V(0)) \times 100)$ for the values of σ_0, k, and h (Table 4, $n = 29$) obtained from application of the Gauss-Newton method (36) ($m = 5$) is shown. The figure also shows the residual PEG before and after cultivation of the microbial consortium E1 for one day, three days, five days, seven days and nine days.

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