Numerical Study of Microbial Depolymerization Process with the Newton-Raphson Method and the Newton's Method

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Abstract*—Computational techniques are proposed for a numerical solution of an inverse problem that arises in a study of a microbial depolymerization processes. The Newton-Raphson method in conjunction with the Newton's method is applied to a time factor that involves three parameters. The Newton-Raphson method reduces a system of three equations for three unknowns to a single variable equation, which is solved with the Newton's method. Those techniques were applied to a microbial depolymerization process of polyethylene glycol. Introduction of experimental results into analysis leads to simulation of a microbial depolymerization problem.*

Keywords*— Newton's method, Newton-Raphson method, biodegradation, polymer, mathematical model, numerical simulation.

I. INTRODUCTION

Petroleum-based polymers have been produced since the early part of the twentieth century. A large amount of those xenobiotic compounds have been accumulated on the surface of the earth, and they are now sources for carbon dioxide emission. Although those macromolecules had been nonexistent until they were invented, some of microorganisms are able to utilize the carbon sources. Mechanisms of microbial depolymerization processes must be clarified for appropriate assessment of the carbon cycle. Microbial depolymerization processes are categorized into exogenous type processes and endogenous type processes. Monomer units are liberated one by one from terminals of molecules in an exogenous type depolymerization process. Polymers degraded in exogenous type depolymerization processes include polyethylene (PE) and polyethylene glycol (PEG). Unlike exogenous type depolymerization processes, primary factor of an endogenous type depolymerization process is arbitrarily scission. Polymers degraded in endogenous type depolymerization processes include polyvinyl alcohol (PVA) and polylactic acid (PLA).

A PE biodegradation process involves two primary factors, gradual weight reduction due to the β-oxidation and direct absorption by cells. A PE molecule liberates a two carbon unit from its terminal 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. A mathematical model based on those factors was proposed for simulation of PE biodegradation processes [1 - 4]. Polyethylene glycol (PEG) is another polymer depolymerized in exogenous type depolymerization processes. The initial step of liberation from a PEG molecule is oxidation of a terminal unit to produce an aldehyde, which is further oxidized to a monocarboxylic acid. The oxidation is followed by the cleavage of the ether bond, and the molecule reduces by one glycol unit [27]. Numerical techniques developed for PE biodegradation were applied for simulation of an exogenous type depolymerization process of PEG [5]. Temporal factors of degradation rates were taken into consideration [6 - 8].

A mathematical model of endogenous type depolymerization processes was proposed for an enzymatic degradation process of PVA [9, 10]. The model was applied to an enzymatic hydrolysis of polylactic acid (PLA), and degradabilities of PVA and PLA were compared [11]. Temporal dependence of the degradation rate was taken into consideration for the depolymerization process of PLA [14]. The model proposed for endogenous type depolymerization processes was reformulated for exogenous type depolymerization processes of PEG [13] and PE [14]. Numerical techniques developed for PE biodegradation were applied to an exogenous depolymerization process of PEG [15]. Temporal dependence of degradability was taken into consideration for depolymerization processes of PEG [16 – 23, 25, 26].

The study on microbial depolymerization processes of PEG was continued. In previous studies, weight distributions of PEG before and after cultivation of microbial consortium E1 were introduced into analysis, and techniques to evaluate parameters for a time factor of degradation rate were proposed. In this study, those techniques were improved. The Newton-Raphson method reduces a system of three equations with three unknowns to a single equation of one variable equation which is

solved numerically by the Newton's method. Our techniques are illustrated with results obtained from application to weight distributions before and after cultivation of Microbial consortium E1 for two days, four days, and seven days

II. DESCRIPTION OF PROBLEMS IN ANALYSIS OF EXOGENOUS TYPE DEPOLYMERIZATION PROCESSES

Molecules of a single polymer all have the same chemical structure, while their molecular weight varies from one molecule to another. In order to model a microbial depolymerization process, let t and M be the time and the molecular weight, respectively, and let $w(t,M)$ be the weight distribution with respect to the molecular weight M at time t, that is, the total mass of polymer molecules for $A \le M \le B$ is the integral

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

Let $\sigma(t)$ be the microbial population at time t. The following system of equations was proposed in previous studies (*cf.* [25]) under the assumption that the liberated amount distributes exponentially [24].

$$\frac{\partial w}{\partial t} = \sigma(t)\left[-\lambda(M)w + c(M)\int_M^\infty \lambda(K)d(K)w(t,K)\,dK\right], \tag{2}$$

$$\frac{d\sigma}{dt} = k\left(1-h\frac{\sigma}{v(t)}\right)\sigma, \tag{3}$$

where

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

Function $v(t)$ is the residual in the culture medium at time t, that is,

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

which is approximated as the integral (1) for appropriate values of A and B. The microbial consortium E1 is incubated in a culture medium where PEG 6000 was the sole carbon source. The weight distributions are obtained before and after cultivation for two days, four days, and seven days. Table 1 shows approximate values of the residual PEG $v(0)$, $v(2)$, $v(4)$, and $v(7)$ for $A = 10^{3.2}$, $B = 10^{4.2}$. The system of equations (2), (3) is associated with the initial condition

$$w(0,M) = f_0(M), \qquad \sigma(0) = \sigma_0, \tag{4}$$

Where $f_0(M)$ and σ_0 are the initial weight distribution and the initial microbial population, respectively. The system of the equations (2), (3) and the initial condition (4) form an initial value problem. Given the initial weight distribution $f_0(M)$, the initial value problem (2), (3), (4) is solvable provided the molecular factor $\lambda(M)$ and the initial microbial population σ_0, and the values of the parameters k and h are given. In what follows, techniques for determination of those unknowns are described. Suppose that weight distributions at $t = t_0$, $t = t_1$, $t = t_2$, and $t = t_3$ are expressed with prescribed functions $f_0(M)$, $f_1(M)$, $f_2(M)$, and $f_3(M)$, respectively. Here $t_0 = 0$ and $f_0(M)$ is the initial weight distribution. A problem posed in previous studies is to determine the values of the parameters σ_0, k and h, which satisfy

$$w(t_1,M) = f_1(M),\quad w(t_2,M) = f_2(M),\quad w(t_3,M) = f_3(M). \tag{5}$$

Equation (2) involves $\sigma(t)$ while equation (3) involves $v(t)$, the integral of $w(t,M)$ with respect to M. In order to remove the mutual dependence, consider the change of independent variables from t to τ by

$$\tau = \int_0^t \sigma(s)ds. \tag{6}$$

Note that

$$\frac{d\tau}{dt} = \sigma(t) \tag{7}$$

holds. Let

$$W(\tau, M) = w(t, M), \quad S(\tau) = \sigma(t).$$

In view of the expression (7), equations (2) and (3) are converted to

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

$$\frac{dS}{d\tau} = 1 - h\frac{S}{v(t)}, \tag{9}$$

Respectively. Note that the equation (8) now involves only one of the unknown variables W, which makes the inverse problem for the molecular factor $\lambda(M)$ solvable, while the equation (2) involves two unknown variables w and σ.

Given the molecular factor of the degradation rate $\lambda(M)$ and a weight distribution $F_1(M)$ for $\tau = T_1$, equation (8) and the initial condition

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

form an initial value problem. Given an additional weight distribution $F_2(M)$ for $\tau = T_2$, equation (8), the initial condition (10), and the additional condition

$$W(T_1, M) = F_1(M) \tag{11}$$

form an inverse problem for $\lambda(M)$, for which the solution of the initial value problem (8), (10) also satisfies the condition (11). Techniques to solve the inverse problem were developed in the previous studies. In particular, the molecular factor $\lambda(M)$ was evaluated for $T_1 = 0$ and $T_2 = 2$, for which $F_1(M)$ and $F_2(M)$ were the weight distributions of PEG after cultivation of the microbial consortium E1 for two days and four days, respectively. Once $\lambda(M)$ was obtained, the initial value problem consisting of the equation (8) and the initial condition

$$W(0_1, M) = f_0(M) \tag{12}$$

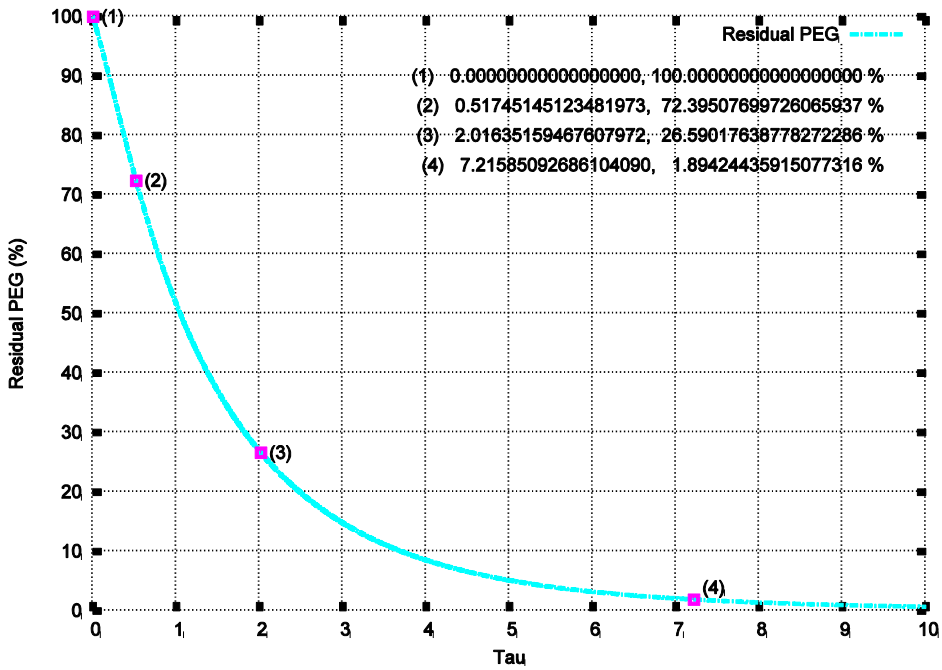

FIGURE 1: Transition of residual PEG for $0 \le \tau \le 10$ based on the solution of the initial value problem (8), (12). The initial value problem (8), (12) was solved numerically, and curve $(\tau, y(\tau))$ was generated $\left(y(\tau) = \frac{V(\tau)}{V(0)} \times 100 \right)$,

$V(\tau) = \int_A^B W(\tau, M)\, dM$, $A = 10^{3.2}$ and $B = 10^{4.2}$.

TABLE 1

Values of t and τ, and residual PEG before and after cultivation of microbial consortium E1 for two days, four days, and seven days ($A = 10^{3.2}$ and $B = 10^{4.2}$). The table shows the values of t, approximate values of τ, and approximate values of the residual PEG (%) based on the conditions (5).

t	τ	Residual PEG
0.00000	0.00000	100.00000
2.00000	0.51745	72.39508
4.00000	2.01635	26.59018
7.00000	7.21585	1.89424

was solved, and the residual PEG $V(\tau)$ as a function of τ,

$$V(\tau) = \int_A^B W(\tau, M)\, dM \tag{13}$$

was obtained ($A = 10^{3.2}$ and $B = 10^{4.2}$). Figure 1 shows the curve $(\tau, V(\tau))$ for $0 \le \tau \le 10$. Values of τ corresponding to values of t were obtained by solving the equations $V(\tau) = v(t)$ for $t = 0$, 2, 4, and 7 (Table 1). Table 1 shows that $t = 2.0$, $t = 4.0$, and $t = 7.0$ correspond to $\tau \approx 0.51745$, $\tau \approx 2.01635$, and $\tau \approx 7.21585$, respectively.

III. NUMERICAL TECHNIQUES FOR EVALUATION OF PARAMETERS OF TIME FACTOR

The solution S of equation (9) with the initial value σ_0 depends not only on τ but also on σ_0, k and h. Denote by $S = S(\tau, \sigma_0, k, h)$ the solution of (9) which satisfies the initial condition $S(0, \sigma_0, k, h) = \sigma_0$. Let

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

In view of the expression (7), $t=u(\tau,\sigma_0,k,h)$. Suppose that t_1, t_2, and t_3 correspond to τ_1, τ_2, and τ_3 according to the change of variables (6), that is,

$$t_i=u(\tau_i,\sigma_0,k,h) \qquad (i=1,2,3). \tag{14}$$

Let $g_i(\sigma_0,k,h)=u(\tau_i,\sigma_0,k,h)-t_i$, and consider the system of equations for the unknowns σ_0, k and h obtained from the conditions (14),

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

In order to solve the system of equations (15), consider the first two equations

$$g_1(\sigma_0,k,h)=0, \qquad g_2(\sigma_0,k,h)=0 \tag{16}$$

for a fixed non-negative value of h. System of equations (15) can be solved for σ_0 and k numerically by the Newton-Raphson method to generate functions $\phi(h)$ and $\psi(h)$ such that a solution of the system is given by $\sigma_0=\phi(h)$, $k=\psi(h)$, that is, a sequence of approximate solutions $(\sigma_{0,0},k_0),(\sigma_{0,1},k_1),(\sigma_{0,2},k_2),\ldots$ is generated by the recurrence formula

$$\begin{aligned}
\sigma_{0,m+1}&=\sigma_{0,m}-\left(\frac{\partial g_1}{\partial\sigma_0}\frac{\partial g_2}{\partial k}-\frac{\partial g_2}{\partial\sigma_0}\frac{\partial g_1}{\partial k}\right)^{-1}\left(\frac{\partial g_2}{\partial k}g_1-\frac{\partial g_1}{\partial k}g_2\right),\\
k_{m+1}&=k_m-\left(\frac{\partial g_1}{\partial\sigma_0}\frac{\partial g_2}{\partial k}-\frac{\partial g_2}{\partial\sigma_0}\frac{\partial g_1}{\partial k}\right)^{-1}\left(-\frac{\partial g_2}{\partial\sigma_0}g_1+\frac{\partial g_1}{\partial\sigma_0}g_2\right), \qquad m=0,1,2,\ldots,
\end{aligned} \tag{17}$$

where the functions g_1 and g_2 and their partial derivatives are evaluated at $\sigma_0=\sigma_{0,n}$ and $k=k_n$. Note that

$$\frac{\partial g_i}{\partial\sigma_0}=\left.\frac{\partial u}{\partial\sigma_0}\right|_{\tau=\tau_i}, \quad \frac{\partial g_i}{\partial k}=\left.\frac{\partial u}{\partial k}\right|_{\tau=\tau_i}, \quad \frac{\partial g_i}{\partial h}=\left.\frac{\partial u}{\partial h}\right|_{\tau=\tau_i}, \tag{18}$$

while the partial derivatives $\partial u/\partial\sigma_0$, $\partial u/\partial k$, and $\partial u/\partial h$ are the solutions of the initial value problems

$$\frac{d}{d\tau}\left(\frac{\partial u}{\partial\sigma_0}\right)=-\frac{1}{[S(\tau)]^2}\frac{\partial S}{\partial\sigma_0}, \qquad \left.\frac{\partial u}{\partial\sigma_0}\right|_{\tau=0}=0, \tag{19}$$

$$\frac{d}{d\tau}\left(\frac{\partial u}{\partial k}\right)=-\frac{1}{[S(\tau)]^2}\frac{\partial S}{\partial k}, \qquad \left.\frac{\partial u}{\partial k}\right|_{\tau=0}=0, \tag{20}$$

$$\frac{d}{d\tau}\left(\frac{\partial u}{\partial h}\right)=-\frac{1}{[S(\tau)]^2}\frac{\partial S}{\partial h}, \qquad \left.\frac{\partial u}{\partial h}\right|_{\tau=0}=0. \tag{21}$$

Partial derivatives $\partial S/\partial\sigma_0$, $\partial S/\partial k$, and $\partial S/\partial h$ are the solutions of the initial value problems

$$\frac{d}{d\tau}\left(\frac{\partial S}{\partial\sigma_0}\right)=-\frac{kh}{V(\tau)}\left(\frac{\partial S}{\partial\sigma_0}\right), \qquad \left.\frac{\partial S}{\partial\sigma_0}\right|_{\tau=0}=1, \tag{22}$$

$$\frac{d}{d\tau}\left(\frac{\partial S}{\partial k}\right)=1-\frac{hS(\tau)}{V(\tau)}-\frac{kh}{V(\tau)}\left(\frac{\partial S}{\partial k}\right), \qquad \left.\frac{\partial S}{\partial k}\right|_{\tau=0}=0, \tag{23}$$

$$\frac{d}{d\tau}\left(\frac{\partial S}{\partial h}\right)=-\frac{k}{V(\tau)}\left(S(\tau)+h\frac{\partial S}{\partial h}\right), \qquad \left.\frac{\partial S}{\partial h}\right|_{\tau=0}=0. \tag{24}$$

Those initial value problems are solved for the partial derivatives which appear in the recurrence formulas (17) [26].

Note that the system (16) leads to

$$\begin{aligned}\phi'(h)&=\left(\frac{\partial g_1}{\partial\sigma_0}\frac{\partial g_2}{\partial k}-\frac{\partial g_2}{\partial\sigma_0}\frac{\partial g_1}{\partial k}\right)^{-1}\left(\frac{\partial g_2}{\partial k}\frac{\partial g_1}{\partial h}-\frac{\partial g_1}{\partial h}\frac{\partial g_2}{\partial k}\right),\\ \psi'(h)&=\left(\frac{\partial g_1}{\partial\sigma_0}\frac{\partial g_2}{\partial k}-\frac{\partial g_2}{\partial\sigma_0}\frac{\partial g_1}{\partial k}\right)^{-1}\left(\frac{\partial g_2}{\partial\sigma_0}\frac{\partial g_1}{\partial h}-\frac{\partial g_1}{\partial\sigma_0}\frac{\partial g_2}{\partial h}\right),\end{aligned} \tag{25}$$

for $\sigma_0=\phi(h)$ and $k=\psi(h)$. Let

$$Z(h)=g_3(\phi(h),\psi(h),h). \tag{26}$$

Once the solution $\sigma_0=\phi(h),\ k=\psi(h)$ of the system (16) is obtained, the Newton's method can be applied to

$$Z(h)=0, \tag{27}$$

that is, a sequence of approximate solutions $h_0, h_1, h_2, \ldots$ can be generated by

$$h_{n+1}=h_n-\frac{Z(h_n)}{Z'(h_n)}, \qquad n=0,\ 1,\ 2,\ \ldots. \tag{28}$$

Note that

$$Z'(h)=\frac{\partial g_3}{\partial\sigma_0}\phi'+\frac{\partial g_3}{\partial k}\psi'+\frac{\partial g_3}{\partial h}$$

for $\sigma_0=\phi(h)$ and $k=\psi(h)$. Derivatives ϕ' and ψ' are given by the expressions (25), while the partial derivatives of g_1, g_2, and g_3 with respect to σ_0, k and h are given by expressions (18) - (24).

IV. NUMERICAL RESULTS FROM ANALYSIS OF INVERSE PROBLEM FOR TIME FACTOR

Let $V(\tau)$ be the residual PEG obtained from a numerical solution of the initial value problem (8), (12), that is, $V(\tau)$ is the function defined by the expression (13) for $A=10^{3.2}$ and $B=10^{4.2}$. The system of equations (15) was solved numerically for σ_0, k and h with the techniques described in the previous section. Table 2 shows the results from application of the Newton-Raphson method to system (16) and the Newton's method to equation (27). Figure 2 shows the transition of the residual PEG obtained from a numerical solution of the initial value problem (8), (9), (12) with $S(0,\sigma_0,k,h)=\sigma_0$. Figure 2 also shows the transition of residual PEG obtained from a numerical solution of the initial value problem (2), (3), (4) for the values of the parameters σ_0, k and h in the last row of table (2). The initial value problem (2), (3), (4) was solved numerically using values of parameters σ_0, k and h in the last row of table (2). Figure 3 shows the transition of the residual PEG obtained from a numerical solution of (2), (3), (4).

TABLE 2

Change of parameter values and iteration counts of the Newton-Raphson method and the Newton's method. The table shows that $|h_{n+1}-h_n|\le 10^{-12}$ for $n=5$ in the sequence generated by the Newton's method (28). It also shows that $\sqrt{(\sigma_{0,m+1}-\sigma_{0,m})^2+(k_{m+1}-k_m)^2}\le 10^{-12}$ for $m=16$ at each step of the Newton's method. Entries in the columns $\sigma_{0,n}$ and k_n are the last values of the Newton-Raphson iterations at the n th step of the Newton's method. The initial value of each application of the Newton-Raphson method was fixed ($\sigma_{0,0}=0.2, k_0=0.5$).

n	h_{n+1}	Count	$\sigma_{0,n}$	k_n	$g_3(\sigma_{0,n},k_n,h_n)$
0	12.91011526876690	16	0.14381126167661	0.54194442446577	−0.20163026883843
1	12.75353240846410	16	0.14343204594116	0.54498679389487	0.01215719681922
2	12.75316315092790	16	0.14345256753083	0.54482207592820	0.00002849758473
3	12.75316339202850	16	0.14345261590947	0.54482168762418	−0.00000001860676
4	12.75316339186900	16	0.14345261587788	0.54482168787771	0.00000000001231
5	12.75316339186950	16	0.14345261587790	0.54482168787755	−0.00000000000004

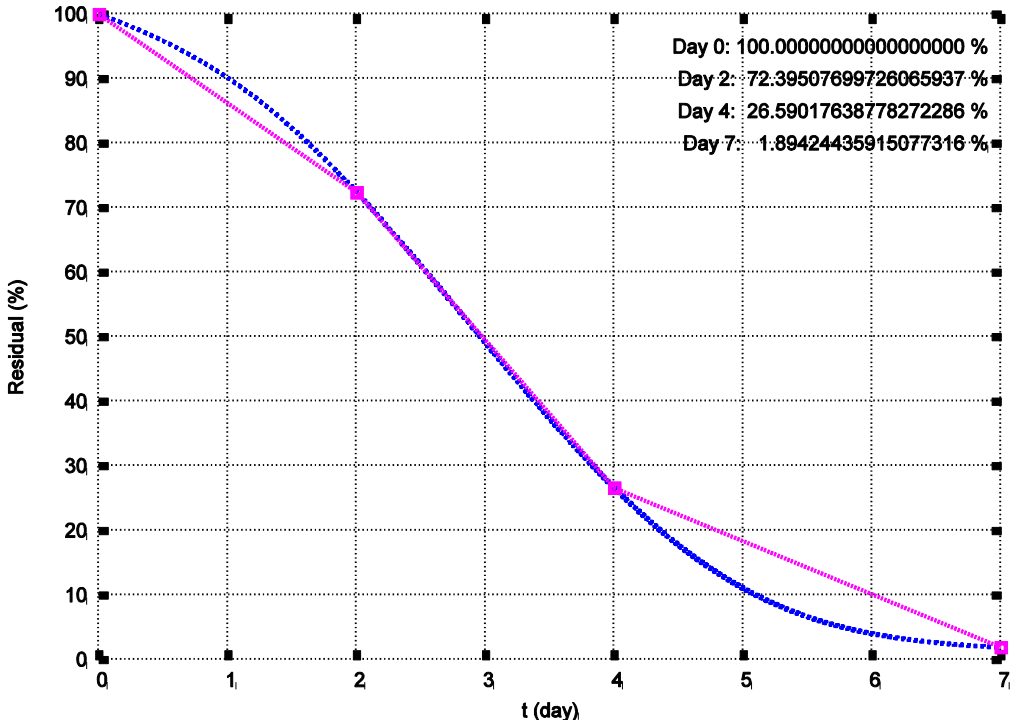

FIGURE 2: Transition of residual PEG for seven days based on the initial value problem (8), (9), (12). The curve $(u(\tau,\sigma_0,k,h),y(\tau))$ is shown $\left(y(\tau)=\frac{V(\tau)}{V(0)}\times 100\right)$. Function $u(\tau,\sigma_0,k,h)$ was generated from a numerical solution of the initial value problem (8), (9), (12) with the initial condition $S(0,\sigma_0,k,h)=\sigma_0$ for the values of the parameters σ_0, k and h in the last raw of table 2.

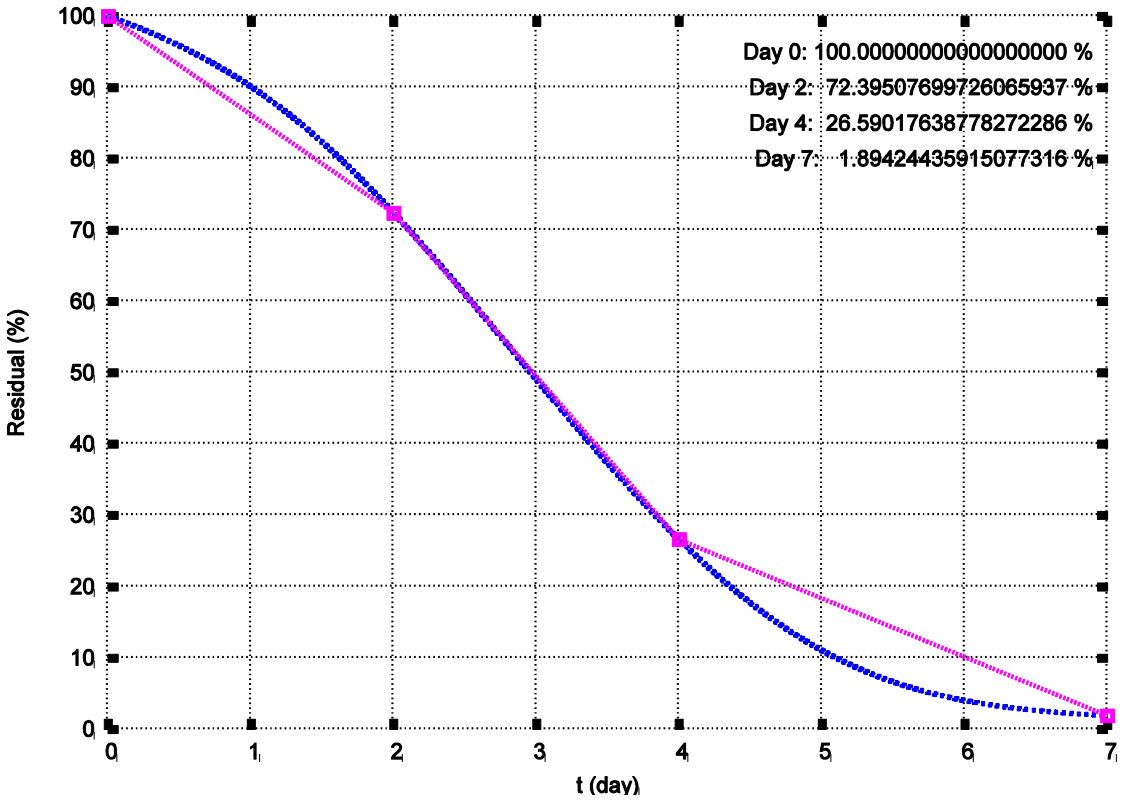

FIGURE 3: Transition of residual PEG for seven days based on the initial value problem (2), (3), (4). The curve $(t, z(t))$ is shown $\left(z(t)=\frac{v(t)}{v(0)}\times 100\right)$. Function $v(t)$ was generated from a numerical solution of the initial value problem (2), (3), (4) for the values of the parameters σ_0, k and h in the last raw of table 2.

Figure 1 shows that the residual PEG $V(\tau)$ may well be approximated by an exponential function. Suppose that $V(\tau)$ is a solution of

$$\frac{dV}{d\tau}=-\mu V, \tag{29}$$

so that $V(\tau)=V(0)e^{-\mu\tau}$. Suppose that the value of μ is determined by the conditions

$$V(\tau_1)=V_1, \qquad V(\tau_1)=V_2, \tag{30}$$

where V_1 and V_2 are the residual PEG at $\tau=\tau_1$ and $\tau=\tau_2$, respectively, so that

$$\mu=-\frac{\log V_2-\log V_1}{\tau_2-\tau_1}.$$

Figure 4 shows the curve $\left(\tau, e^{-\mu\tau}\times 100\right)$. The figure also shows the curve $(\tau, y(\tau))$ (Figure 1). Parameters σ_0, k and h were evaluated for $V(\tau)=V_0e^{-\mu\tau}$ with the techniques described in the previous section, where V_0 is the residual PEG before cultivation, that is,

$$V_0=\int_A^B w(0,M)dM \qquad \left(A=10^{3.2},\ \ B=10^{4.2}\right).$$

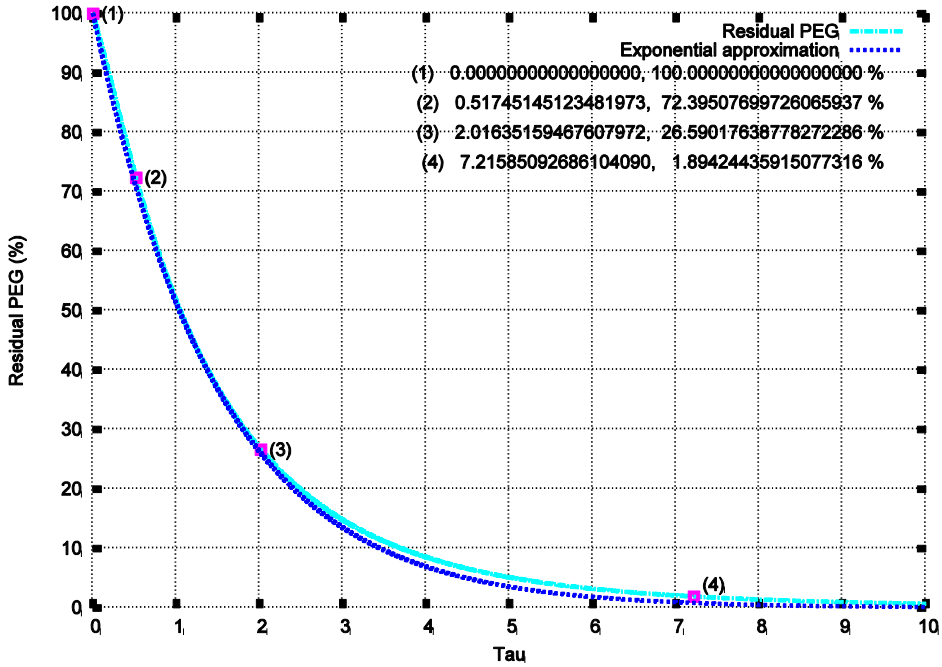

FIGURE 4: Curve $\left(\tau, e^{-\mu\tau}\times 100\right)$**. Curve** $(\tau, y(\tau))$ **is also shown** $\left(y(\tau)=\frac{V(\tau)}{V(0)}\times 100\right)$**,** $V(\tau)=\int_A^B W(\tau,M)\,dM$**,** $A=10^{3.2}$ **and** $B=10^{4.2}$**.**

TABLE 3

Change of parameter values and iteration counts of the Newton-Raphson method and the Newton's method for $V(\tau)=V_0e^{-\mu\tau}$**. The table shows that** $|h_{n+1}-h_n|\le 10^{-12}$ **for** $n=5$ **in the sequence generated by the Newton's method (28). It also shows that** $\sqrt{(\sigma_{0,m+1}-\sigma_{0,m})^2+(k_{m+1}-k_m)^2}\le 10^{-12}$ **for** $m=16$ **at each step of the Newton's method. . Entries in the columns** $\sigma_{0,n}$ **and** k_n **are the last values of the Newton-Raphson iterations at the** n **th step of the Newton's method. The initial value of each application of the Newton-Raphson method was fixed** $(\sigma_{0,0}=0.2, k_0=0.5)$**.**

n	h_{n+1}	Count	$\sigma_{0,n}$	k_n	$g_3(\sigma_{0,n},k_n,h_n)$
0	8.58671318397139	16	0.14379681030420	0.54208111099523	0.18837377402843
1	8.51606276891822	16	0.14398144583988	0.54059785942797	0.00856257414694
2	8.51591999712240	16	0.14399064713205	0.54052396031086	0.00001721986678
3	8.51592005463291	16	0.14399066572345	0.54052381099793	−0.00000000693634
4	8.51592005460980	16	0.14399066571597	0.54052381105807	0.00000000000279
5	8.51592005460968	16	0.14399066571597	0.54052381105804	0.00000000000001

Figure 5 shows the transition of the residual PEG obtained from a numerical solution of the initial value problem (8), (9), (12) with $S(0,\sigma_0,k,h)=\sigma_0$ and $V(\tau)=V_0e^{-\mu\tau}$ for the values of the parameters σ_0, k and h in the last raw of table 3.

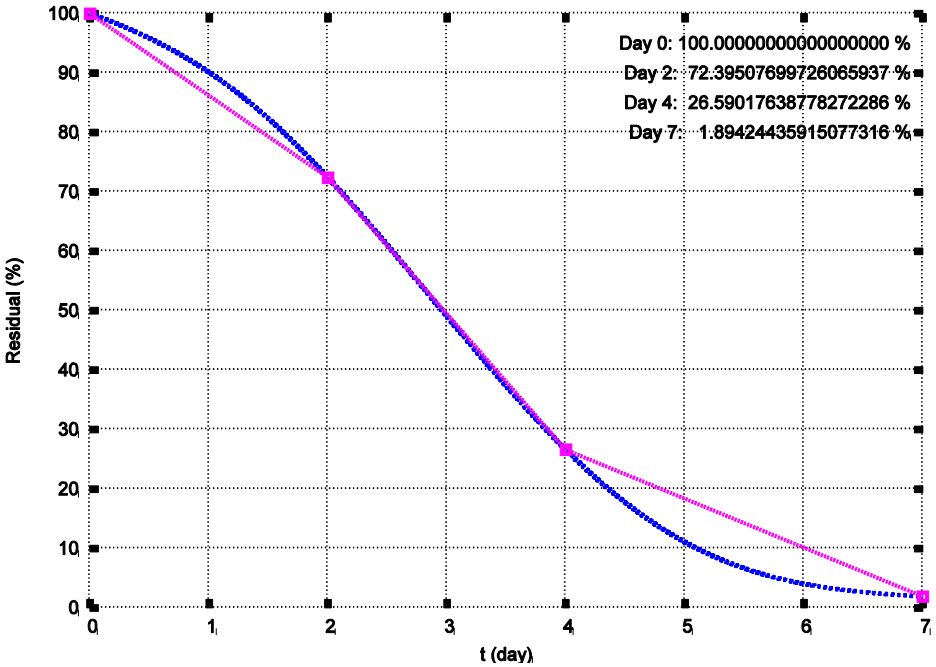

FIGURE 5: Transition of residual PEG for seven days based on the initial value problem (8), (9), (12). The curve $(u(\tau,\sigma_0,k,h),y(\tau))$ is shown $\left(y(\tau)=\frac{V(\tau)}{V(0)}\times 100,\quad V(\tau)=V_0e^{-\mu\tau}\right)$. Function $u(\tau,\sigma_0,k,h)$ was generated from a numerical solution of the initial value problem (8), (9), (12) with the initial condition $S(0,\sigma_0,k,h)=\sigma_0$ for the values of the parameters σ_0, k and h in the last raw of table 3.

V. CONCLUSION

Application of the Newton-Raphson method to the system (16) was demonstrated in a previous study, while the bisection method was applied to the equation (27) [26]. The techniques were tested by application to model problem in which $V(\tau)$ was a constant function. The techniques were also applied to an exponential function $V(\tau)=e^{-a\tau+b}$ where the least square approximation was applied to $V(\tau)$ based on weight distributions before and after cultivation of microbial consortium E1 for one day, three days, five days, and nine days, and the values of the parameters $\sigma_0\approx 0.14345$, $k\approx 1.5690$ and $h\approx 9.3784$ were obtained [26].

In this study, the application of the Newton's method to the equation (27) was illustrated. The techniques were applied to the residual PEG $V(\tau)$ based on the weight distributions before and after cultivation of microbial consortium E1 for two days, four days, and seven days. The values of the parameters $\sigma_0\approx 0.14345$, $k\approx 0.54482$ and $h\approx 12.75316$ (Table 2) were obtained. Values of σ_0 between numerical results in the previous study and this study are almost identical. However there are notable differences in values of k and h.

Equations (16) and (27) were also solved for the solution of the equation (29) with the initial value V_0, and the values of the parameters $\sigma_0\approx 0.14399$, $k\approx 0.54052$ and $h\approx 8.51592$ (Table 3) were obtained. Difference in values of σ_0 and k between shown in Table 2 and 3 is negligible. However there is a notable difference between the values of h shown in Tables 2 and 3. Nevertheless, transitions of residual PEG shown in Figures 3 and 5 are indistinguishable, and equation (8) may well be replaced with equation (29). In practical applications, there are cases where amounts of residual polymer is available at discrete points in time instead of weight distributions. Techniques developed in this study will be applicable to those cases.

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