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Study of biodegradation of xenobiotic polymers with change of microbial population

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Abstract

Microbial depolymerization processes of polyethylene glycol are studied. A mathematical model, developed originally for endogenous type depolymerization processes, is applied to exogenous type depolymerization processes. An inverse problem is solved numerically to determine a degradation rate. An initial value problem is solved numerically to simulate the transition of weight distribution.

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1 Introduction

Microbial depolymerization processes are categorized into exogenous type processes and endogenous type processes. In an exogenous depolymerization process, molecules reduce in size by truncation of monomer units from their terminals. Polyethylene (PE) is an example of a polymer subject to exogenous depolymerization processes. In PE biodegradation, there are two essential factors: the gradual weight loss of large molecules due to β-oxidation, which is an exogenous depolymerization process, and the direct consumption or absorption of small molecules by cells. A mathematical model based on those factors was proposed to study PE biodegradation [5, 16, 6].

Polymers subject to exogenous depolymerization processes include polyethylene glycol (PEG). PEG is one of the polyethers whose chemical structures are represented by the expression $HO(R\text{-}O)_nH$: for example, PEG, $R = CH_2CH_2$; PPG, $R = CH_3CHCH_2$; PTMG, $R = (CH_2)_4$ [1]. PEG is metabolized by liberating C_2 compounds exogenously [2, 3] (Figure 1). The mathematical techniques developed for PE biodegradation were extended to studies of the exogenous depolymerization processes of PEG [9]. Inverse problems were solved numerically to determine degradation rates based on the weight distribution of PEG with respect to molecular weight before and after cultivation of a microbial consortium E-1. Once a degradation rate was found, the transition

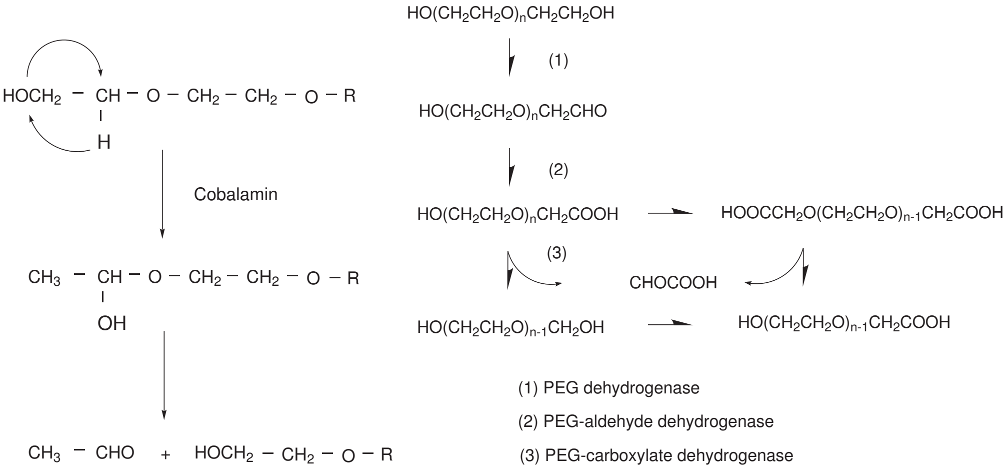

Figure 1: Metabolic pathways of PEG. Anaerobic metabolism (left) and aerobic metabolism (right).

of the weight distribution was simulated by solving an initial value problem. Dependence of degradation rate on time was also considered in modeling and simulation of depolymerization processes of PEG [11, 14, 13, 15].

Analysis of PEG biodegradation is continued. A model originally developed for endogenous depolymerization processes is applied to the exogenous depolymerization processes. Unlike exogenous type depolymerization processes in which monomer units are truncated from terminals, molecules are cleaved internally in endogenous type depolymerization processes. Derivation of the model is described, and an inverse problem is solved numerically to determine a degradation rate. An initial value problem is solved numerically to simulate transition of the weight distribution. Numerical techniques are illustrated and numerical results are introduced.

2 Modeling depolymerization processes

Polyvinyl alcohol (PVA) is degraded in a succession of two processes: oxidation of a couple of pendant hydroxyl groups, either by oxidase or dehydrogenase; followed by hydrolysis. A sequence of reactions leads to cleavage of a carbon-carbon chain at a carbonyl group and an adjacent methyne group [4]. Matsumura et al. proposed a different metabolism of PVA by oxidation of a hydroxyl group and aldolase reaction of a monoketone structure, which results in cleavage of a carbon-carbon chain between a methyne group adjacent to a carbonyl group and an adjacent hydroxymethyne group [8]. Irrespective of metabolic pathways, PVA is in general depolymerized by oxidation and the resultant cleavage of a carbon-carbon chain between two carbonyl groups, or between a carbonyl group and an adjacent hydroxymethyne group, which produces smaller molecules.

In order to model endogenous depolymerization processes of polymers such as PVA, let $w(t, M)$ be the weight distribution with respect to the molecular weight M at time t. Denote by $C(A, B)$ the class of all molecules with molecular weight between A and B. Then the total molecular weight in $C(A, B)$ present at time t is

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

For $K \leqslant M$, let $p(t, K, M)$ denote the time rate of transition from $w(t, M)$ to $w(t, K)$. Then the transition of the weight from $C(A, B)$ to $C(D, E)$ per unit time is

$$\iint_R p(t, K, M)\, dM\, dK\,,$$

where the integral is over the domain

$$R = \{(K, M) \mid K \leqslant M\,,\ D \leqslant K \leqslant E\,,\ A \leqslant M \leqslant B\}\,.$$

The total weight decrease in $C(A, B)$ per unit time is

$$\int_A^B \int_0^M p(t, K, M)\, dK\, dM\,, \tag{2}$$

while the total weight increase per unit time is

$$\int_A^B \int_M^\infty p(t,M,K)\,dK\,dM\,. \tag{3}$$

The rate of change of quantity (1) equals the difference between quantities (2) and (3),

$$\begin{aligned}\frac{d}{dt}\int_A^B w(t,M)\,dM &= -\int_A^B \int_0^M p(t,K,M)\,dK\,dM \\ &\quad + \int_A^B \int_M^\infty p(t,M,K)\,dK\,dM\,.\end{aligned}$$

The equation

$$\frac{d}{dt}\int_A^B w(t,M)\,dM = \int_A^B \frac{\partial}{\partial t} w(t,M)\,dM$$

leads to

$$\int_A^B \left\{ \frac{\partial}{\partial t} w(t,M) + \int_0^M p(t,K,M)\,dK - \int_M^\infty p(t,M,K)\,dK \right\} dM = 0\,.$$

Since this equation holds for an arbitrary interval $[A,B]$, the integrand

$$\frac{\partial}{\partial t} w(t,M) + \int_0^M p(t,K,M)\,dK - \int_M^\infty p(t,M,K)\,dK = 0\,,$$

and so $w = w(t,M)$ satisfies [17, 10, 18]

$$\frac{\partial w}{\partial t} = -\int_0^M p(t,K,M)\,dK + \int_M^\infty p(t,M,K)\,dK\,. \tag{4}$$

Let $\gamma(t,M)$ be the loss of amount from $w(t,M)$ per unit time and per unit weight. The amount of loss from $w(t,M)$ per unit time is $\gamma(t,M)w(t,M)$ which is expressed in terms of the integral of $p(t,K,M)$:

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

This amount is distributed over the interval $[0, M]$. 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 $p(t, K, M) = \gamma(t, M)q(K, M)w(t, M)$. Equation (4) leads to

$$\frac{\partial w}{\partial t} = -\gamma(t, M)w + \int_M^\infty \gamma(t, K)q(M, K)w(t, K)\, dK\,. \tag{5}$$

Note that

$$\begin{aligned} \int_A^B \gamma(t, M)w(t, M)\, dM &= \int_A^B \int_0^M p(t, K, M)\, dK\, dM \\ &= \int_A^B \int_0^M \gamma(t, M)q(K, M)w(t, M)\, dK\, dM \\ &= \int_0^M q(K, M)\, dK \int_A^B \gamma(t, M)w(t, M)\, dM\,, \end{aligned}$$

and that

$$\int_0^M q(K, M)\, dK = 1\,. \tag{6}$$

Given an initial weight distribution in terms of a prescribed function $f(M)$, equation (5) and the initial condition

$$w(0, M) = f(M) \tag{7}$$

form an initial value problem, provided the degradation rate $\gamma(t, M)$ is given. Given an additional weight distribution at $t = T$ $(T > 0)$ in terms of a prescribed function $g(M)$,

$$w(0, M) = g(M), \tag{8}$$

equation (5) and the conditions (7) and (8) form an inverse problem to find the degradation rate $\gamma(t, M)$, for which the solution of the initial value problem (5) and (7) also satisfies the condition (8). Inputs of the inverse problem are an initial weight distribution $f(M)$ and a final weight distribution $g(M)$. As is seen in Section 4, experimental studies have made those inputs available.

3 Reduction to a model with time independent degradation rate

Time factors of degradability include temperature, dissolved oxygen, and microbial population. Experimental results introduced in Section 4 were obtained from incubation under constant temperature and aeration by a shaker, and the only factor that affects the degradation rate is the microbial population. The number of molecules depolymerized per unit time and unit volume is proportional to the product of the microbial concentration and the polymeric concentration in a solution. Note that the number of molecules with molecular weight M is inversely proportional to the molecular weight, and that the concentration of polymeric molecules with molecular weight M is also inversely proportional to the molecular weight. The total number of molecules with molecular weight M which are depolymerized per unit time is also a product of the microbial population and a function of M, and the degradation rate $\gamma(t,M)$ is a product of a function of t, $\sigma(t)$, and a function of M, $\lambda(M)$, so that equation (5) becomes

$$\frac{\partial w}{\partial t} = -\sigma(t)\lambda(M)w + \sigma(t)\int_M^\infty \lambda(M)q(M,K)w(t,K)\,dK\,. \tag{9}$$

Let $\tau = \int_0^t \sigma(s)\,ds$ and $W(\tau,M) = w(t,M)$. Then

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

and equation (9) becomes

$$\frac{\partial W}{\partial \tau} = -\lambda(M)W + \int_M^\infty \lambda(K)q(M,K)W(\tau,K)\,dK\,. \tag{10}$$

Equation (5) and the initial condition

$$W(0,M) = f(M) \tag{11}$$

form an initial value problem provided $\lambda(M)$ is known. Let $\mathcal{T} = \int_0^T \sigma(s)\,ds$. Then equation (10), together with the initial condition (11) and the condition

$$W(\mathcal{T}, M) = g(M), \tag{12}$$

form an inverse problem to find the degradation rate $\lambda(M)$ for which the solution of the initial value problem (10) and (11) also satisfies the condition (12). The initial value problem (5) and (7) corresponds to the initial value problem (10) and (11), and the inverse problem (5), (7) and (8) corresponds to the inverse problem (10), (11) and (12).

4 Computational results for an exogenous depolymerization process

Suppose that $q(K, M)$ is a product of a function of K, $c(K)$, and a function of M, $d(M)$, so that the equation (10) becomes

$$\frac{\partial W}{\partial \tau} = -\lambda(M)W + c(M)\int_M^\infty \lambda(K)d(K)W(\tau, K)\,dK\,. \tag{13}$$

In view of the condition (6),

$$\int_0^M q(K, M)\,dK = \int_0^M c(K)d(M)\,dK = d(M)\int_0^M c(K)\,dK = 1\,.$$

If the number of molecules is uniformly distributed over the interval $[0, M]$, then [17, 10, 18]

$$c(K) = 2K\,, \quad d(M) = \frac{1}{M^2}\,. \tag{14}$$

For these $c(K)$ and $d(M)$, equation (13) is the model proposed originally for enzymatic degradation of polyvinyl alcohol. If the molecular weight is uniformly distributed over the interval $[0, M]$, then [12]

$$c(K) = 1\,, \quad d(M) = \frac{1}{M}\,. \tag{15}$$

Differentiation of the both sides of equation (13) and substitution of the expression for the integral obtained from equation (13) lead to

$$\frac{\partial}{\partial M}\left\{\frac{\partial W}{\partial \tau}+\lambda(M)W\right\}=\frac{c'(M)}{c(M)}\left\{\frac{\partial W}{\partial \tau}+\lambda(M)W\right\} \\ -\lambda(M)c(M)d(M)W\,. \qquad (16)$$

Numerical techniques were developed for the inverse problem to find the degradation rate $\lambda(M)$ for which the solution of the initial value problem (16) and (11) also satisfies the condition (12) in case $c(M)$ and $d(M)$ are given by (14). Those techniques can be extended to cover the general case. Figure 2(a) shows the weight distribution of PEG before and after incubation of a microbial consortium E1 for seven days. The weight distributions shown in Figure 2(a) were set as initial and final conditions for the inverse problem. The weight distribution before cultivation was set as the initial condition (11), and the weight distribution after the cultivation for three days was set as the final condition (12) to solve the inverse problem numerically for the functions $c(K)$ and $d(M)$ given by expressions (15). Figure 2(b) shows the graph of the degradation rate $\lambda(M)$.

The initial value problem was solved numerically to simulate the transition of weight distribution of PEG for seven days (Figure 2(c)). Figure 3(a) shows the experimental result and a numerical result for the weight distribution of PEG after cultivation for three, five, and seven days.

5 Discussion

The mathematical model originally proposed for the endogenous depolymerization processes is applied to exogenous depolymerization processes of PEG. The dependence of degradation rate on time is shown in numerical results. The results shown in Figures 2(c) and 3(a) were obtained with a time independent or time averaged degradation rate. Figure 3(a) shows that

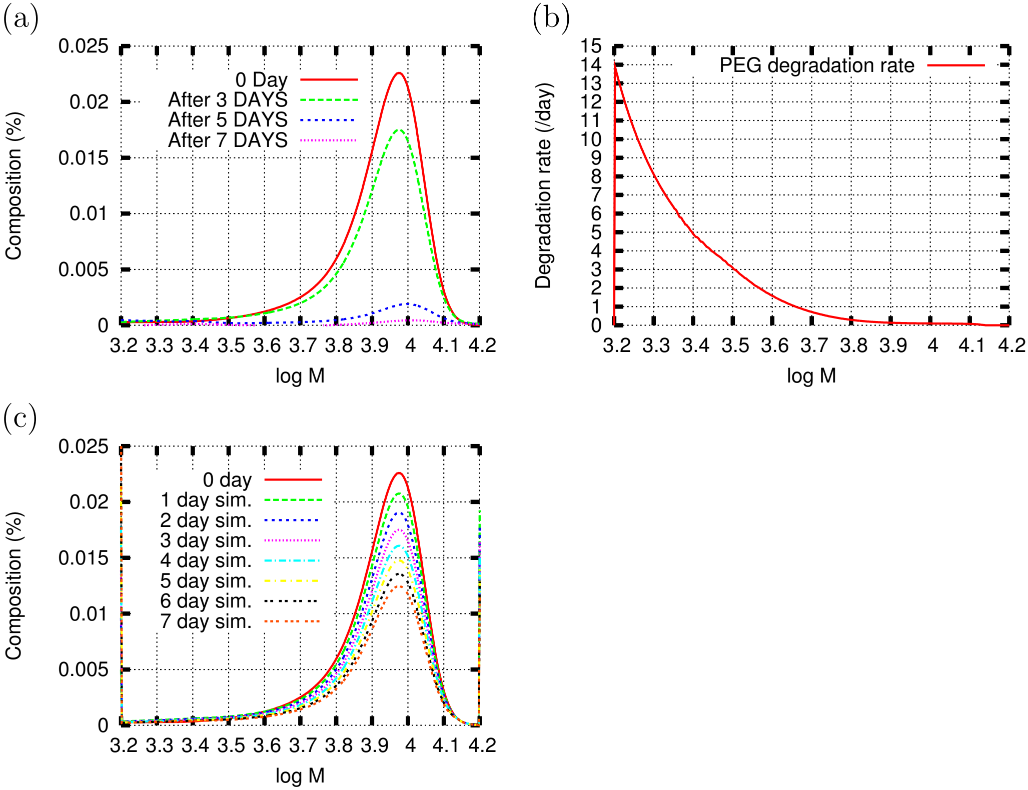

Figure 2: (a) Weight distribution of peg before and after cultivation of microbial consortium E1[13, 15]. (b) Degradation rate of peg based on the weight distributions before and after cultivation for three days (Figure 2(a)). (c) Transition of weight distribution for seven days based on the degradation rate shown in Figure 2(b).

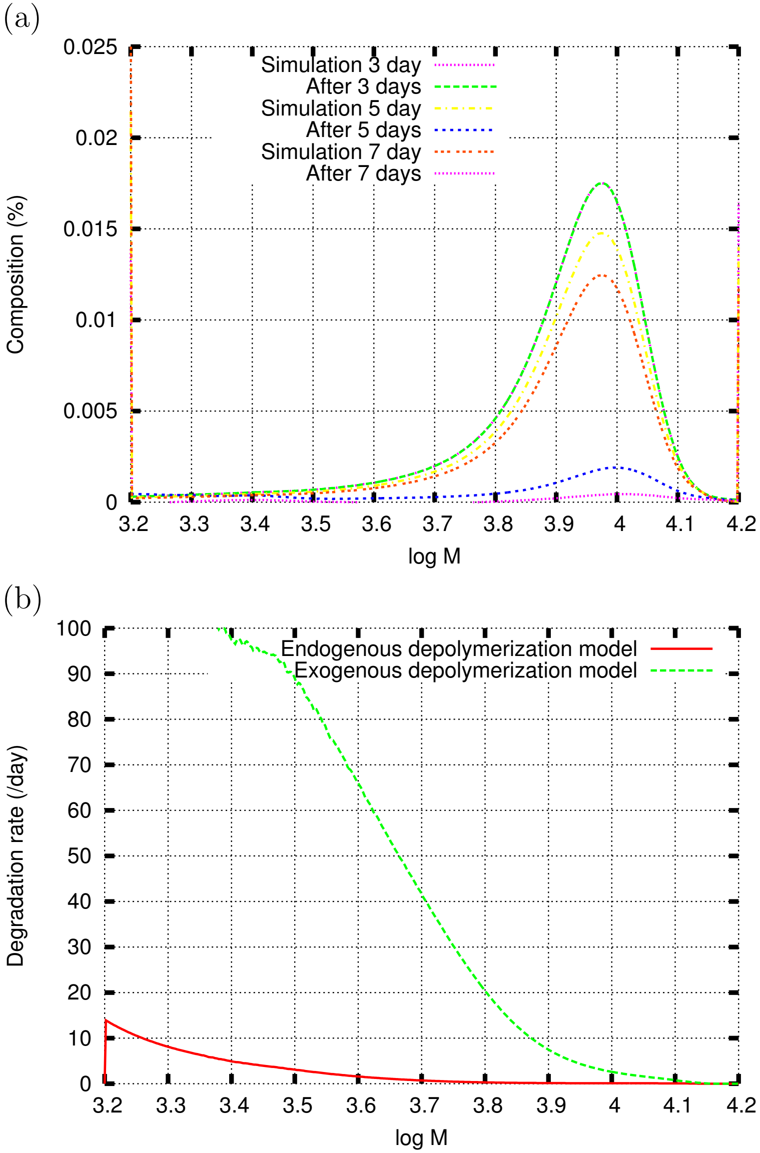

Figure 3: (a) Experimental results and numerical results for the weight distribution after cultivation for three, five, and seven days. (b) Degradation rates based on exogenous depolymerization model and endogenous depolymerization model.

the degradation rate over the first three days of cultivation is smaller than over the next two days, which was suggested in the previous studies. The dependence of degradation rate on time is due to the change of microbial population. Figure 3(b) shows the degradation rate from Figure 2(b) and the degradation rate obtained by the exogenous depolymerization model [13, 15].

Numerical results show that the model originally proposed for endogenous depolymerization processes is widely applicable not only to the endogenous depolymerization processes, but also to the exogenous depolymerization processes, and that depolymerization processes of mixed type can be analyzed with the model.

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A Description of numerical techniques for the inverse problem and the initial value problem

In depolymerization processes, weight is shifted from larger molecular weight classes to smaller molecular weight classes. The initial weight distribution $f(M)$ defined on the interval $[0, \infty)$ has compact support, and the weight distribution function $W(\tau, M)$ also has a compact support. The inverse problem is formulated to determine the unknown degradation rate $\lambda(M)$ for which the solution of the initial value problem (16) and (11) also satisfies the final condition (12). Equation (16) is reduced to an ordinary differential equation. Let $\mu = b - M$. Then the inverse problem consisting of (16), (11) and (12) is converted to

$$\frac{\partial}{\partial \mu}\left(\frac{\partial v}{\partial \tau} + \kappa(\mu) v\right) = -\frac{c'(b-\mu)}{c(b-\mu)}\left(\frac{\partial v}{\partial \tau} + \kappa(\mu) v\right)$$

$$+ \kappa(\mu)c(b-\mu)d(b-\mu)v\,, \tag{17}$$

$$v(0,\mu) = \phi(\mu), \tag{18}$$

$$v(\mathcal{T},\mu) = \psi(\mu), \tag{19}$$

where $v(\tau,\mu) = W(\tau, b-\mu)$, $\kappa(\mu) = \lambda(b-\mu)$, $\phi(\mu) = f(b-\mu)$, and $\psi(\mu) = g(b-\mu)$.

Let

$$u = \frac{\partial v}{\partial \tau} + \kappa(\mu)v\,. \tag{20}$$

Then equation (17) becomes

$$\frac{\partial u}{\partial \mu} = r(\mu, u, \tau), \tag{21}$$

where

$$r(\mu, u, \tau) = -\frac{c'(b-\mu)}{c(b-\mu)}u + \kappa(\mu)c(b-\mu)d(b-\mu)v\,, \tag{22}$$

in which v is given in terms of u according to the equation (20). Then, for a fixed but arbitrary $\tau \in [0, \mathcal{T}]$, equation (21) is an ordinary differential equation whose solution is a function of the variable μ, and it should be associated with an initial condition in terms of a prescribed function $h(\tau)$

$$u(\mu_0, \tau) = h(\tau). \tag{23}$$

Suppose that $v(\mu,\tau)$ satisfies the problem (17), (18) and (19) with a prescribed degradation rate $\kappa(\mu)$. Define $u = u(\mu,\tau)$ and $r(\mu,u,\tau)$ by equations (20) and (22) with $v = v(\mu,\tau)$, respectively. Then, for a fixed but arbitrary $\tau \in [0,\mathcal{T}]$, $u = u(\mu,\tau)$ satisfies equation (21). For $c(K)$ and $d(M)$ given by the expressions (15), used for the numerical results in Section 4, equation (22) becomes

$$r(\mu, u, \tau) = \frac{\kappa(\mu)}{b-\mu}v\,.$$

For the problem to determine the degradation rate, given a nonnegative continuous function $u = u(\mu,\tau)$, the function $r(\mu,u,\tau)$ can be specified as follows. The value of $\kappa(\mu)$ is a positive value of a parameter η, for which the unique solution $\nu(\tau,\mu,u,\eta)$ of the initial value problem (24) and (25) also satisfies the final condition (26)

$$\frac{\partial \nu}{\partial \tau} + \eta\nu = u(\mu,\tau), \tag{24}$$

$$\nu(0,\mu,u,\eta) = \phi(\mu), \tag{25}$$

$$\nu(\mathcal{T},\mu,u,\eta) = \psi(\mu). \tag{26}$$

We show that such a value is necessarily unique whenever it exists, and set $\kappa_u(\mu)$ equal to that unique value. Then $r(\mu,u,t)$ is given by substituting $\nu = \nu(\tau,\mu,u,\kappa_u(\mu))$ in equation (22).

For a fixed but arbitrary positive η, the solution $\nu(\tau,\mu,u,\eta)$ of the initial value problem (24) and (25) is

$$\nu(\tau,\mu,u,\eta) = e^{-\eta\tau}\left[\phi(\mu) + \int_0^\tau e^{\eta s} u(\mu,s)\,ds\right]. \tag{27}$$

The equation

$$\Phi_u(\mu,\eta) = 0 \tag{28}$$

holds for $\eta = \kappa_u(\mu)$, where the function $\Phi_u(\mu,\eta)$ is

$$\Phi_u(\mu,\eta) = \nu(\mathcal{T},\mu,u,\eta) - \psi(\mu) = e^{-\eta\mathcal{T}}\left[\phi(\mu) + \int_0^{\mathcal{T}} e^{\eta s} u(\mu,s)\,ds\right] - \psi(\mu). \tag{29}$$

Note that

$$\Phi_u(\mu,0) = \phi(\mu) + \int_0^{\mathcal{T}} u(\mu,s)\,ds - \psi(\mu),$$

and that

$$\lim_{\eta\to\infty} \Phi_u(\mu,\eta) = -\psi(\mu) < 0$$

under the condition $\psi(\mu) > 0$. It follows that a sufficient condition for the equation (28) to have a positive solution is

$$\Phi_u(\mu,0) = \phi(\mu) + \int_0^{\mathcal{T}} u(\mu,s)\,ds - \psi(\mu) > 0\,. \tag{30}$$

The partial derivative of $\Phi_u(\mu,\eta)$ with respect to η is

$$\frac{\partial \Phi_u}{\partial \eta}(\mu,\eta) = \frac{\partial \nu}{\partial \eta}(\mathcal{T},\mu,u,\eta) = -e^{-\eta T}\left[\mathcal{T}\phi(\mu) + \int_0^{\mathcal{T}} (\mathcal{T}-s)e^{\eta s}u(\mu,s)\,ds\right], \tag{31}$$

and is always negative, a positive solution of equation (28) is unique, and (30) is a necessary and sufficient condition for the unique positive solution of the equation (28) to exist.

In order to solve the inverse problem numerically, the interval $[0,\mathcal{T}]$ is divided into K intervals of equal length, and $K+1$ equally spaced points

$$\tau_i = i\Delta\tau \quad (i = 0,1,2,\ldots,K),$$

where $\Delta\tau = \mathcal{T}/K$. Given a nonnegative function $u(\mu,\tau)$, we denote our approximate value of $u(\mu,\tau_i)$ by $u_i \equiv u_i(\mu)$. Then the initial value problem (21) and (23) becomes an initial value problem for the unknown variables $u_0, u_1, \ldots, u_K$:

$$\frac{du_i}{d\mu} = r_i(\mu, u_0, u_1, \ldots u_K), \qquad u_i(\mu_0) = h(\tau_i).$$

Let $\nu(\tau,\mu,u,\eta)$ be the solution of the initial value problem (24) and (25). An approximate value $\nu_i = \nu_i(\mu, u_0, u_1, \ldots, u_M, \eta)$ at $\tau = \tau_i$ is obtained by application of a numerical integration rule to the integral in equation (27), and an approximate value of the function $\Phi_u(\mu,\eta)$ obtained by setting $\Phi_u(\mu,\eta) \approx \nu_K - \psi(\mu)$. For the numerical results shown in Section 4, Simpson's rule was applied to the integral in equation (27) to obtain the expression

$$\begin{aligned}\Phi_u(\mu,\eta) &= -\psi(\mu) + e^{-\eta\mathcal{T}}\Big\{\phi(\mu) \\ &\qquad + \frac{\Delta\tau}{3}\sum_{j=1}^{K}\left(e^{\eta\tau_{2j-2}}u_{2j-2} + 4e^{\eta\tau_{2j-1}}u_{2j-1} + e^{\eta\tau_{2j}}u_{2j}\right)\Big\}.\end{aligned}$$

Similarly, an approximate value of the partial derivative of $\Phi_u(\mu,\eta)$ with respect to η is also obtained by application of a numerical integration rule to the integral in the expression (31), and an application of Simpson's rule results in

$$\begin{aligned}\frac{\partial \Phi_u}{\partial \eta}(\mu,\eta) = -e^{-\eta\mathcal{T}}\Bigg(\mathcal{T}\phi(\mu) + \frac{\Delta\tau}{3}\sum_{j=1}^{K}\Big\{(\mathcal{T}-\tau_{2j-2})e^{\eta\tau_{2j-2}}u_{2j-2}\\ + (\mathcal{T}-\tau_{2j-1})e^{\eta\tau_{2j-1}}u_{2j-1} + (\mathcal{T}-\tau_{2j})e^{\eta\tau_{2j}}u_{2j}\Big\}\Bigg).\end{aligned}$$

Once those values are given, an approximate value $\tilde{\kappa}$ of the solution of equation (28), $\kappa_u(\mu)$, is obtained by Newton's method, and then an approximate value $r_i(\mu, u_0, u_1, \dots, u_K)$ of the function $r(\mu, u, \tau)$ at $\tau = \tau_i$ is

$$r_i(\mu, u_0, u_1, \dots, u_K) = -\frac{c'(b-\mu)}{c(b-\mu)}u_i + \tilde{\kappa}(\mu)c(b-\mu)d(b-\mu)\nu_i\,,$$

where $\nu_i = \nu_i(u_0, u_1, \dots, u_K, \mu, \tilde{\kappa})$, according to definition (22). In particular, application of the trapezoidal rule and Simpson's rule leads to

$$\begin{aligned}I_0 &= \frac{\Delta\tau}{2}u_0\,, \quad \nu_0 = \phi(\mu) + I_0\,,\\ I_{2j-1} &= I_{2j-2} + \frac{\Delta\tau}{2}\left(e^{\eta\tau_{2j-2}}u_{2j-2} + e^{\eta\tau_{2j-1}}u_{2j-1}\right),\\ \nu_{2j-1} &= e^{-\eta\tau_{2j-1}}\left(\phi(\mu) + I_{2j-1}\right),\\ I_{2j} &= I_{2j-2} + \frac{\Delta\tau}{3}\left(e^{\eta\tau_{2j-2}}u_{2j-2} + 4e^{\eta\tau_{2j-1}}u_{2j-1} + e^{\eta\tau_{2j}}u_{2j}\right),\\ \nu_{2j} &= e^{-\eta\tau_{2j}}\left(\phi(\mu) + I_{2j}\right), \quad j = 1, 2, \dots, K\,.\end{aligned}$$

The initial value problem (21) and (23) was solved numerically for $\mathcal{T} = 3$ and $K = 1000$ with the Adams–Bashforth–Moulton predictor and corrector in PECE mode, in conjunction with a Runge–Kutta method to generate approximate solutions for the first three steps [7]. Here, P, E, and C stand for an application of the predictor, an evaluation of a function, and an application of the corrector, respectively. The step length

$$\Delta\mu = \frac{b-a}{4000}\,,$$

where $a = 10^{3.2}$ and $b = 10^{4.2}$. The initial condition was set by $\mu_0 = 0$ and $h(\tau) = 0$ for all $\tau \in [0, \mathcal{T}]$.

Once the degradation rate $\lambda(M)$ is found, the weight distribution $W(\tau, M)$ is obtained numerically by solving the initial value problem (13) and (11) directly by applying a numerical integration rule to the integral in equation (13). In particular [17], the application of the trapezoidal rule over each interval $[M_{i-1}, M_i]$, $i = 1, 2, \ldots, N$, for the integral on the right-hand side of the equation (13) leads to the system

$$\frac{dW_i}{d\tau} = -\lambda_i W_i + c(M_i)\Delta M F_i\,, \quad i = 0, 1, 2, \ldots, N\,, \tag{32}$$

where

$$\Delta M = \frac{b-a}{N}\,, \quad M_i = a + i\Delta M\,, \quad \lambda_i = \lambda(M_i),$$
$$F_i = \frac{1}{2}d(M_i)\lambda_i W_i + \sum_{j=i+1}^{N-1} d(M_j)\lambda_j W_j + \frac{1}{2}d(M_N)\lambda_N W_N\,.$$

The unknown $W_i = W_i(\tau)$ denotes an approximate value of $W(\tau, M_i)$. The system (32) is associated with the initial condition

$$W_i(0) = f_i = f(M_i), \quad i = 0, 1, 2, \ldots, N\,. \tag{33}$$

The Adams–Bashforth–Moulton predictor and corrector in PECE mode, in conjunction with a Runge–Kutta method with the steplength 0.01, was applied for 300 steps to solve the initial value problem (32) and (33) numerically for $N = 4000$.

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