

An example of nonlinear toxic mass spreading

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Abstract. A one-dimensional, nonlinear problem of reproductive toxic mass spreading is studied in this paper. The nonlinearity is due to the difference of the reproduction rates in the toxic region and the nontoxic region. Multiple steady state solutions are found and their stability and instability are proved. Due to the instability, there may exist turning points (also called saddle-node bifurcation points), at which an infinitesimal perturbation of some parameters may cause a catastrophic change in the location of the steady state toxic front (the interface of the toxic region and the nontoxic region). For the time dependent case, the propagation of the toxic front is considered. An integral equation is derived to determine the propagation of the toxic front. Some numerical results are found for a specific example.

1. Introduction

Toxic mass spreading has been attracting attention of environmental engineers [4], ground water designers [10], and many others [6]. Needless to say, analysis of this kind of spreading is important in the quality control of ground water. In this paper we consider a particular model of toxic mass spreading. We make the following assumptions:

- (i) the spreading is solely due to diffusion,
- (ii) the toxic mass is highly reproductive if its concentration is higher than a critical value, and
- (iii) the problem is spatially one-dimensional.

Assumption (ii) implies a reproduction rate that depends nonlinearly on the local concentration and gives positive feedback. Assumption (iii) is to model the case of unidirectional diffusion, such as chemical diffusion in a slender trough (see Fig. 1).

One usually is interested in two aspects of the toxic mass spreading: stability and instability of steady state solutions, and propagation of the toxic front. The first problem is addressed in Section 3 and the second in Section 4.

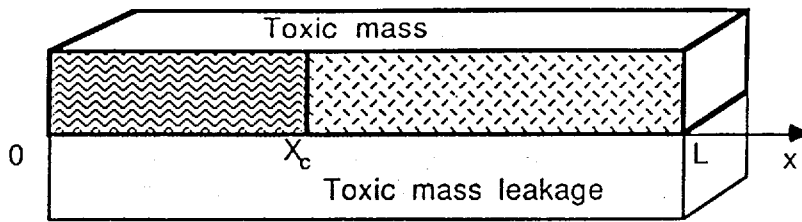


Fig. 1. Configuration of the toxic mass spreading.

Our study focuses on mathematical analysis of the above two problems and leads to qualitative conclusions.

The conservation of the toxic mass from the assumption (i) and (ii) yields a “heat” equation with positive feedback. It is the character of this feedback that makes our model nonlinear and different from others. In addition, it adds some fascinating features to the solutions of the problem, such as multiple steady state solutions and jump discontinuous dependence on the reproduction rate due to the instability. Mathematically, this jump discontinuity is referred to as a saddle-node bifurcation phenomenon. For reaction-diffusion systems, this type of bifurcation has attracted attention of scientists in different fields (see [1–3, 7–9] and the references therein). One part of this paper is devoted to a study of the discontinuous dependence of the stationary toxic front on the reaction rate.

Our study is new and different from the work of [1–3, 6, 8, 9] mainly in the following three aspects:

- (a) our problem has an interfacial free boundary,
- (b) we have proved a slope stability theorem for stationary solutions, and
- (c) we have computed propagation of the toxic front and have found “waiting” times for some specific situations in the time dependent case.

Let

$$I = I(x, t), \quad 0 \leq x \leq L, \quad 0 \leq t < \infty$$

be the concentration of the toxic mass. Suppose the toxic mass spreads from left to right. Then $I(x, t)$ is a monotonically decreasing function of x for all t . Let I_c be the critical concentration. That is, when $I(x, t) > I_c$, the reaction which produces toxic mass is greatly accelerated; when $I(x, t) < I_c$, that reaction is slowed appreciably. For simplicity I_c is taken as the standard toxicity level. Namely if $I(x, t) > I_c$, then the toxicity at the point x and time t is too strong to be acceptable. Hence the equation $I(x_c, t) = I_c$ determines the position x_c which separates toxic and nontoxic regions. This position is referred to as the *toxic front*. Clearly, x_c is a function of time.

Thus $x_c(t)$ represents the propagation of the toxic front. In the case of steady state, the toxic front is fixed at $x_c \equiv x_c = \text{constant}$.

In our model, we found that there may exist multiple steady state fronts, some of which are unstable. On the operating curve (the relation of x_c vs. the reproduction rate R), the solutions corresponding to the negative slope are unstable and all other solutions are stable (or neutrally stable). This result is referred to as the *slope stability theorem*.

The content of this paper is arranged in the following way. In Section 2, we formulate the mathematical problem. Steady state solutions and their stability are discussed in Section 3. An integral equation which governs the propagation of the toxic front is derived in Section 4. We find an approximate solution to this equation for a specific case. Concluding remarks are given in Section 5.

2. Mathematical formulation

Consider a one-dimensional toxic mass spreading in a slender trough (Fig. 1). The toxic mass is reproductive if its concentration $I[\text{kg} \cdot \text{m}^{-3}]$ exceeds the critical value I_c . Then the conservation of mass gives

$$C \frac{\partial I}{\partial t} - \frac{\partial}{\partial x} \left(k(x) \frac{\partial I}{\partial x} \right) + u_0 + u_1 I = RS(x)f(x; x_c),$$

$$0 < x < L, \quad 0 < t < \infty. \tag{2.1}$$

Here C is the nondimensional saturation capacity which is equal to one for most chemicals. $-(\partial/\partial x)(k(x)(\partial I/\partial x))$ is the longitudinal diffusion. The diffusion coefficient $k[\text{m}^2 \cdot \text{sec}^{-1}]$ is a positive function. The term $u_0 + u_1 I (u_0 > 0, u_1 > 0)$ represents the mass loss due to bottom leakage, external pumping, or surface radiation. The right hand side, $RS(x)f(x; x_c)$, represents the reproduction of the toxic mass due to chemical or biochemical reaction. In this expression, $S(x)$ is positive and determined by topography of the problem, $f(x; x_c)$ is the control factor of the reproduction, and $R[\text{kg} \cdot \text{m}^{-3} \cdot \text{sec}^{-1}]$ is the reproduction rate.

In most circumstances, $S(x)$ and $k(x)$ are twice differentiable and non-increasing, and the control factor $f(x; x_c)$ has a discontinuity of the first kind at $x = x_c$. The position x_c of the toxic front is determined by the toxic front condition $I(x_c, t) = I_c$. In our problem we assume

$$f(x, x_c) = \begin{cases} f_s(x) > 0 & \text{if } 0 \leq x < x_c, \\ f_w(x) \geq 0 & \text{if } x_c < x \leq L \end{cases} \tag{2.2}$$

where both $f_s(x)$ and $f_w(x)$ are continuous and nonincreasing. $f_s(x_c) > f_w(x_c)$ when $0 < x_c < L$. It is the discontinuity at $x = x_c$ that introduces nonlinearity and positive feedback to our problem. The assumption implies that the reproduction rate is much stronger when $I > I_c$ than when $I < I_c$. This is plausible because in many chemical processes, such as titration, an infinitesimal increase of the concentration of a tested chemical near its critical value results in an apparent jump of reaction rate. This is usually seen as a sudden color change of chemical solution in a test tube. Such a catastrophic phenomenon is also common in biological systems.

It is assumed that both ends of the trough are completely blocked. So we have the boundary conditions

$$\left. \frac{\partial I}{\partial x} \right|_{x=0,L} = 0. \quad (2.3)$$

Then, the equations (2.1), (2.3) and the toxic front condition

$$I(x, t)|_{x=x_c} = I_c \quad (2.4)$$

are the governing equations for our problem. The objective of this paper is to solve the following two problems. First, for a given trough and chemical, what choices of constants u_0 , u_1 and R will force x_c to be fixed at a desired point between 0 and L . This question can be answered by finding steady state solutions of the problem (2.1) and (2.3–4). The details are shown in Section 3. Secondly, for a given trough and chemical as well as an initial distribution of the concentration of the chemical, how does the toxic front $x_c(t)$ propagate? To answer this question, we need to solve an initial boundary value problem (2.1), (2.3–4) and

$$I(x, t = 0) = g(x), \quad 0 \leq x \leq L. \quad (2.5)$$

An approximate solution to this problem is found in section 4.

3. Steady state solutions and their stability

For the steady state problem $x_c(t)$ is a constant which is denoted as x_c . I is a function of x only, denoted as $I_c(x)$. We need to solve the problem

$$-\frac{d}{dx} \left(k(x) \frac{dI_c}{dx} \right) + u_0 + u_1 I_c = RS(x)f(x; x_c), \quad 0 < x < L, \quad (3.1)$$

$$\left. \frac{\partial I_e}{\partial x} \right|_{x=0,L} = 0, \tag{3.2}$$

$$I_e|_{x=x_c} = I_c. \tag{3.3}$$

The technique of eigenfunction expansion is employed here. Let eigenpairs of

$$-\frac{d}{dx} \left(k(x) \frac{d\varphi}{dx} \right) = \lambda\varphi, \quad 0 < x < L, \tag{3.4}$$

$$\left. \frac{d\varphi}{dx} \right|_{x=0,L} = 0 \tag{3.5}$$

be $\{\lambda_n, \varphi_n\}_{n=0}^\infty$ with

$$\int_0^L \varphi_m(x)\varphi_n(x) dx = \delta_{mn},$$

where δ_{mn} is the Kronecker delta. By standard Sturm–Liouville theory [5], one has

$$0 = \lambda_0 < \lambda_1 < \lambda_2 < \lambda_3 < \dots,$$

and

$$\lim_{n \rightarrow \infty} \lambda_n = \infty.$$

Moreover $\{\varphi_n(x)\}$ forms an orthonormal basis of $L^2([0, L], \mathbb{R})$. If $I_c \in L^2([0, L], \mathbb{R})$, then

$$I_c(x) = \sum_{n=0}^\infty I_n \varphi_n(x), \quad \text{a.e.} \tag{3.6}$$

where the I_n are simply the Fourier coefficients of $I_c(x)$.

Multiplying (3.1) by $\varphi_n(x)$ and integrating the resulting equation, we obtain

$$I_n(x_c) = \frac{1}{\lambda_n + u_1} \left[-u_0 \delta_{0n} + R \int_0^L S(x) f(x; x_c) \varphi_n(x) dx \right],$$

$$n = 0, 1, 2, \dots \tag{3.7}$$

The expansion coefficients I_n in (3.7) make $I_c(x)$ given by (3.6) satisfy (3.1). Since $\{\varphi_n(x)\}$ are the eigenfunctions of (3.4–5), $I_c(x)$ expanded in the form of (3.6) satisfies (3.2). To satisfy the toxic front condition (3.3) we need to choose proper x_c . By (3.6–7), (3.3) becomes

$$\sum_{n=0}^{\infty} \frac{1}{\lambda_n + u_1} \left[-u_0 \delta_{0n} + R \int_0^L S(x) f(x; x_c) \varphi_n(x) dx \right] \varphi_n(x_c) = I_c. \tag{3.8}$$

For simplicity, (3.8) can, after subtraction of I_c from both sides, be denoted as

$$G(x_c, R) = 0. \tag{3.9}$$

This is the nonlinear equation for x_c and is called *the bifurcation equation*. It usually has multiple solutions for given u_0 , u_1 and R . But physically meaningful solutions are those with $0 \leq x_c \leq L$. Next we work out an example and show how x_c depends on R , u_0 and u_1 .

EXAMPLE: $k(x) = 1$, $S(x) = 1$, $u_0 = 0$, $f_s(x) = \alpha_1 x^3 + \beta_1 x^2 + \gamma_1 x + \delta_1$, $f_u(x) = \alpha_2 x^3 + \beta_2 x^2 + \gamma_2 x + \delta_2$, and $L = 1$.

In this case, the steady state problem (2.1) and (2.3–4) can be solved analytically. The bifurcation equation (3.8) becomes

$$\begin{aligned} & R \{ \cosh \lambda(1 + x_c) (u_1 \gamma_1 + 6\alpha_1) + \cosh (\lambda x_c) \cosh \lambda(1 + x_c) \\ & \quad \times [3(\alpha_2 - \alpha_1) u_1 x_c^2 + 2(\beta_2 - \beta_1) u_1 x_c + u_1(\gamma_2 - \gamma_1) + 6(\alpha_2 - \alpha_1)] \\ & \quad - \lambda \sinh (\lambda x_c) \cosh \lambda(1 + x_c) [(\alpha_2 - \alpha_1) u_1 x_c^3 + (\beta_2 - \beta_1) u_1 x_c^2 \\ & \quad + (u_1(\gamma_2 - \gamma_1) + 6(\alpha_2 - \alpha_1)) x_c + u_1(\delta_2 - \delta_1) + 2(\beta_2 - \beta_1)] \\ & \quad - \cosh (\lambda x_c) (3\alpha_2 u_1 + 2\beta_2 u_1 + \gamma_2 u_1 + 6\alpha_2) \\ & \quad + \lambda \sinh \lambda [\alpha_2 u_1 x_c^3 + \beta_2 u_1 x_c^2 + (\gamma_2 u_1 + 6\alpha_2) x_c + (u_1 \delta_2 + 2\beta_2)] \} \\ & = \lambda u_1^2 I_c \sinh \lambda \end{aligned} \tag{3.10}$$

where $\lambda = \sqrt{u_1}$, and $0 < x_c < 1$.

Based upon the bifurcation equation (3.10), x_c is usually a multiple valued function of R for other given parameters. We computed this function for the

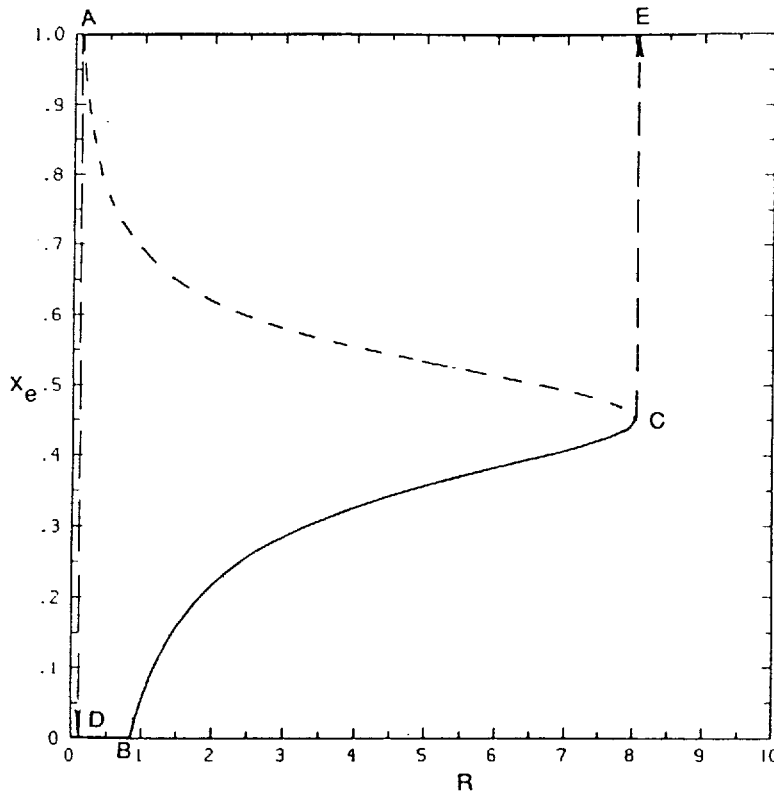


Fig. 2. Operating curve for the example of steady state problem: x_e is the position of the interface and R is the reproduction rate. Parameter values are: $\alpha_1 = 0$, $\beta_1 = 0$, $\gamma_1 = 0$, $\delta_1 = 40$, $\alpha_2 = -20$, $\beta_2 = -10$, $\gamma_2 = -10$, $\delta_2 = 40$, and $u_1 = 2.5$.

following two groups of specific parameters:

(i) $\alpha_1 = 0$, $\beta_1 = 0$, $\gamma_1 = 0$, $\delta_1 = 40$, $\alpha_2 = -20$, $\beta_2 = -10$,

$\gamma_2 = -10$, $\delta_2 = 40$, $u_1 = 2.5$, and $I_c = 10$;

(ii) $\alpha_1 = -10$, $\beta_1 = -5$, $\gamma_1 = -5$, $\delta_1 = 30$, $\alpha_2 = 0$, $\beta_2 = 0$,

$\gamma_2 = 0$, $\delta_2 = 10$, $u_1 = 1.46$, and $I_c = 10$.

The corresponding curves of the functions $x_e = x_e(R)$ for the two groups of parameters above are shown in Fig. 2 and Fig. 3. These curves in the R, x_e plane are referred to as the *operating curves*.

Notice that at $(x_e = 1^-, R = R_A)$ an increase of R will keep the whole trough toxic. Thus the line segment $\{(R, x_e) | R \geq R_A \text{ and } x_e = 1\}$ is a part of the operating curve. Similarly, at $(x_e = 0^+, R = R_B)$ a decrease of R will keep the whole trough nontoxic. Thus, $\{(R, x_e) | R \leq R_B \text{ and } x_e = 0\}$ is also

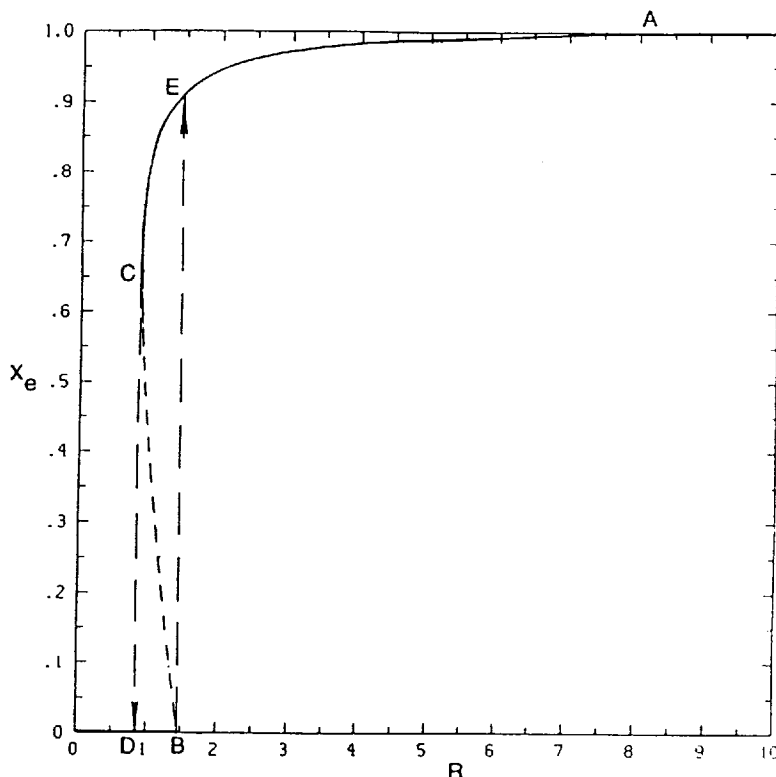


Fig. 3. Operating curve for the example of steady state problem: x_e is the position of the interface and R is the reproduction rate. Parameter values are: $\alpha_1 = -10$, $\beta_1 = -5$, $\gamma_1 = -5$, $\delta_1 = 30$, $\alpha_2 = 0$, $\beta_2 = 0$, $\delta_2 = 10$, and $u_1 = 1.46$.

a part of the operating curve. Mathematically, the above conclusion can be justified as follows.

Existence and uniqueness of the solution to the following linear boundary value problem

$$-\frac{d}{dx} \left(k(x) \frac{dI_e}{dx} \right) + u_0 + u_1 I_e = RS(x) \begin{cases} f_s(x) \\ f_w(x), \end{cases}$$

$$\left. \frac{dI_e}{dx} \right|_{x=0,L} = 0$$

is elementary and well known [5]. Let $I_e(x; R)$ represent the solution I_e of the above linear problem, with the argument R included as an independent variable of I_e is to emphasize that the reaction rate is R . By comparison theorem of boundary value problems for ordinary differential equations, we have $I_e(x; R_1) \leq I_e(x; R_2)$ if $R_1 \leq R_2$. Therefore, if $I_e(x; R_B)$ is a nontoxic solution, then $I_e(x; R)$ is also a nontoxic solution provided that $R \leq R_B$.

Hence, $\{(R, x_e) | R \geq R_A \text{ and } x_e = 1\}$ and $\{(R, x_e) | R \leq R_B \text{ and } x_e = 0\}$ are parts of the operating curves.

On the operating curves, the end points of the unstable sections (denoted by broken lines) are turning points (or called saddle-node bifurcation points). Due to the instability, an infinitesimal change of the reaction rate R may cause a large jump in the position of the toxic front x_e . For instance, a small increase of R at point C in Fig. 2 will result in the jump of the position of the toxic front from C to E . All the jump possibilities for the given two groups of data are shown in Figs. 2-3.

Next, we consider the stability of the equilibrium state (R, x_e) by using a method similar to that used in [7]. Let $\eta(x, t)$ and $\zeta(t)$ be small perturbations of $I_e(x)$ and x_e respectively. That is, in (2.1) and (2.3), let

$$I(x, t) = I_e(x) + \eta(x, t), \tag{3.11}$$

$$x_e(t) = x_e + \zeta(t). \tag{3.12}$$

Substituting (3.11-12) into (2.1), we obtain

$$C \frac{\partial \eta}{\partial t} - \frac{\partial}{\partial x} \left(k(x) \frac{\partial \eta}{\partial x} \right) + u_1 \eta = RS(x) (f(x; x_e + \zeta) - f(x; x_e)). \tag{3.13}$$

Let

$$\eta = \eta_1(x) e^{-\lambda t}, \tag{3.14}$$

$$\zeta = \zeta_1 e^{-\lambda t}. \tag{3.15}$$

Then (3.13) becomes

$$-\lambda C \eta_1 - \frac{d}{dx} \left(k(x) \frac{d\eta_1}{dx} \right) + u_1 \eta_1(x) = RS(x) (f(x; x_e + \zeta) - f(x; x_e)) e^{\lambda t}, \tag{3.16}$$

and $\eta_1(x)$ can be expressed by eigenfunction expansion as follows:

$$\eta_1(x) = \sum_{n=0}^{\infty} H_n \varphi_n(x).$$

Then multiplying both sides of (3.16) by $\varphi_n(x)$, integrating the resulting equation with respect to x from 0 to L , and finally linearizing the right hand side with respect to ζ , we obtain

$$H_n = \frac{RS(x_e)\zeta_1 \Delta f \varphi_n(x_e)}{\lambda_n + u_1 - \lambda C},$$

where

$$\Delta f = f_s(x_e) - f_w(x_e) > 0 \quad \text{when } 0 < x_e < L.$$

Thus

$$\begin{aligned} \eta_1(x) &= \sum_{n=0}^{\infty} H_n \varphi_n(x) \\ &= RS(x_e)\zeta_1 \Delta f \sum_{n=0}^{\infty} \frac{\varphi_n(x_e)\varphi_n(x)}{\lambda_n + u_1 - \lambda C}. \end{aligned} \quad (3.17)$$

Now let us use the condition of the toxic front.

$$\begin{aligned} I_c &= I_c(x_e) \\ &= I_c(x_e + \zeta) + \eta(x_e + \zeta, t) \\ &= I_c(x_e) + I'_c(x_e)\zeta + \eta(x_e, t) + \text{higher order terms} \\ &= I_c + I'_c(x_e)\zeta + \eta(x_e, t) + \text{higher order terms,} \end{aligned}$$

where $I'_c(x_e)$ is a short notation for $(dI_c/dx)|_{x=x_e}$. Omitting the higher order terms we have

$$\zeta(t) = -\eta(x_e, t)/I'_c(x_e).$$

Hence

$$\zeta_1 = -\eta_1(x_e)/I'_c(x_e). \quad (3.18)$$

Next we compute the slope of the operating curve. If $x_e = \bar{x}_e$ is not a critical point of $G(x_e, R)$ in (3.8.9) (i.e., $\partial G/\partial x_e \neq 0$ at $x_e = \bar{x}_e$), then the implicit function theorem implies that x_e is a differentiable function of R in

a neighborhood of \bar{x}_e determined by (3.9). By (3.8–9),

$$\begin{aligned} \frac{\partial G}{\partial R} &= \sum_{n=0}^{\infty} \left(\frac{1}{\lambda_n + u_1} \int_0^L S(x) f(x; x_e) \varphi_n(x) dx \right) \varphi_n(x_e) \\ &= \frac{1}{R} \left(I_c + \frac{u_0}{u_1} \right). \end{aligned} \tag{3.19}$$

Also by (3.8–9),

$$\frac{\partial G}{\partial x_e} = RS(x_e) \Delta f \sum_{n=0}^{\infty} \frac{\varphi_n^2(x_e)}{\lambda_n + u_1} + I'_e(x_e). \tag{3.19, a}$$

The $I'_e(x_e)$ on the right hand side of the above equation can be computed from (3.17–18).

$$I'_e(x_e) = -RS(x_e) \Delta f \sum_{n=0}^{\infty} \frac{\varphi_n^2(x_e)}{\lambda_n + u_1 - \lambda C}. \tag{3.20}$$

Hence

$$\frac{\partial G}{\partial x_e} = -RS(x_e) \Delta f \sum_{n=0}^{\infty} \frac{C \lambda \varphi_n^2(x_e)}{(\lambda_n + u_1)(\lambda_n + u_1 - \lambda C)}. \tag{3.21}$$

By (3.19) and (3.21), in a neighborhood of \bar{x}_e we have

$$\begin{aligned} \frac{dR}{dx_e} &= - \frac{\partial G}{\partial x_e} \Big/ \frac{\partial G}{\partial R} \\ &= \frac{R^2 u_1 S(x_e) \Delta f \sum_{n=0}^{\infty} \frac{C \lambda \varphi_n^2(x_e)}{(\lambda_n + u_1)(\lambda_n + u_1 - \lambda C)}}{u_1 I_c + u_0} \\ &\equiv \Gamma(\lambda). \end{aligned} \tag{3.22}$$

Now we consider the graph of the function $\Gamma(\lambda)$. From standard results on Sturm–Liouville problems [5],

$$\lambda_n = O(n^2) \text{ as } n \rightarrow \infty,$$

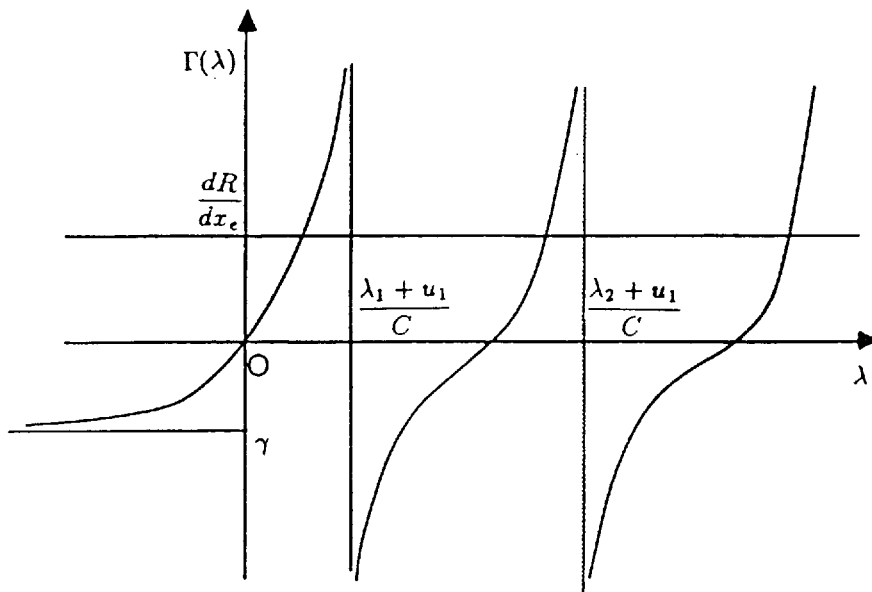


Fig. 4. The graph of the function $\Gamma(\lambda)$ defined by (3.22).

and $\{\varphi_n(x)\}_{n=0}^\infty$ is uniformly bounded. Hence

$$\sum_{n=0}^\infty \frac{\varphi_n^2(x_e)}{\lambda_n + u_1} \quad \text{and} \quad \sum_{n=0}^\infty \frac{\varphi_n^2(x_e)}{\lambda_n + u_1 - \lambda C}$$

are both convergent. Also we have the limit

$$\begin{aligned} \Gamma(\lambda) &= \frac{R^2 u_1 S(x_e) \Delta f}{u_1 I_c + u_0} \sum_{n=0}^\infty \left(-\frac{\varphi_n^2(x_e)}{\lambda_n + u_1} + \frac{\varphi_n^2(x_e)}{\lambda_n + u_1 - \lambda C} \right) \\ &\rightarrow -\frac{R^2 u_1 S(x_e) \Delta f}{u_1 I_c + u_0} \sum_{n=0}^\infty \frac{\varphi_n^2(x_e)}{\lambda_n + u_1} \equiv \gamma < 0 \text{ as } \lambda \rightarrow -\infty. \end{aligned} \quad (3.23)$$

The graph of the function $\Gamma(\lambda)$ is shown in Fig. 4.

From Fig. 4, we see that if $dR/dx_e > 0$ (or $= 0$), then (3.22) has only positive (or nonnegative respectively) roots. Thus the corresponding steady state solutions are stable (or neutrally state respectively). If $\gamma < dR/dx_e < 0$, then (3.22) has exactly one negative root, which corresponds to an unstable mode. Thus the corresponding steady state solutions are unstable.

But a question arises at this stage. If $dR/dx_e < \gamma < 0$, then (3.22) has only non-negative roots. This implies that the corresponding solutions with negative slope are not unstable. Is it possible? The rest of the proof of the slope stability theorem is to show that this can never happen. Namely, we show that at any point (R, x_e) on the operation curve, $dR/dx_e > \gamma$.

Since $I_e(x)$ is a strictly decreasing function, we have $I'_e(x_e) < 0$. Hence (3.19, a) implies

$$\frac{\partial G}{\partial x_e} < RS(x_e)\Delta f \sum_{n=0}^{\infty} \frac{\phi_n^2(x)}{\lambda_n + u_1}.$$

By (3.19), $(\partial G/\partial R) > 0$ as long as $I_c + u_0/u_1 > 0$. Therefore

$$\begin{aligned} \frac{dR}{dx_e} &= - \frac{\partial G}{\partial x_e} / \frac{\partial G}{\partial R} \\ &> - \frac{RS(x_e)\Delta f \sum_{n=0}^{\infty} \frac{\phi_n^2(x_e)}{\lambda_n + u_1}}{\frac{1}{R} \left(I_c + \frac{u_0}{u_1} \right)} \\ &= \gamma. \end{aligned} \tag{3.24}$$

This completes the proof of the slope stability theorem.

THEOREM: *The steady state solution of (2.1) and (2.3–4) is linearly stable (unstable) if $dR/dx_e > 0$ (< 0 respectively), and is neutrally stable if $dR/dx_e = 0$.*

4. Propagation of toxic front

The objective of this section is to find the function $x_c = x_c(t)$. Namely we want to describe the propagation of the interface between the toxic region and nontoxic region. To realize this objective we need to solve the initial boundary value problem (2.1), (2.3–5).

In (2.1) and (2.3–5), let

$$I(x, t) = \sum_{n=0}^{\infty} i_n(t)\phi_n(x) \tag{4.1}$$

where $\{\phi_n(x)\}_{n=0}^{\infty}$ are orthonormal eigenfunctions of (3.4–5). Substituting (4.1) into (2.1), we have

$$C \frac{di_n}{dt} + \lambda_n i_n(t) + u_0 \delta_{0n} + u_1 i_n(t) = \int_0^L RS(x)f(x; x_c)\phi_n(x) dx.$$

From (2.5) we obtain the initial condition

$$i_n(0) = \int_0^L g(x) \varphi_n(x) dx,$$

for the first order ordinary differential equation above. This initial value problem for the ordinary differential equation can be solved formally to obtain

$$\begin{aligned} i_n(t) = & i_n(0) + \frac{1}{C} \int_0^t \exp \left[\frac{\lambda_n + u_1}{C} (\tau - t) \right] \\ & \times \left[\int_0^L RS(x) f(x; x_c(\tau)) \varphi_n(x) dx - u_0 \delta_{0n} \right] d\tau, \quad n = 0, 1, 2, \dots \end{aligned} \quad (4.2)$$

By the condition (2.4), we have

$$\begin{aligned} \sum_{n=0}^{\infty} \left\{ i_n(0) + \frac{1}{C} \int_0^t \exp \left[\frac{\lambda_n + u_1}{C} (\tau - t) \right] \right. \\ \left. \times \left[\int_0^L RS(x) f(x; x_c(\tau)) \varphi_n(x) dx - u_0 \delta_{0n} \right] d\tau \right\} \\ \times \varphi_n(x_c(t)) = I_c. \end{aligned} \quad (4.3)$$

It is this nonlinear integral equation that determines $x_c(t)$. This integral equation is too complicated to be solved in general. Nevertheless, for specific cases, it can be solved numerically. To illustrate the solution procedure, we consider the following example.

EXAMPLE: $k(x) = 1$, $S(x) = 1$, $f_s(x) = 1$, $f_w(x) = x$, $L = 1$, $g(x) = H(1 - x)$ where H is a positive constant. From (3.4-5),

$$\lambda_0 = 0, \quad \lambda_1 = \pi^2, \quad \lambda_2 = (2\pi)^2, \dots;$$

$$\varphi_0(x) = 1, \quad \varphi_1(x) = \sqrt{2} \cos(\pi x), \quad \varphi_2(x) = \sqrt{2} \cos(2\pi x), \dots$$

Let us take two mode approximation, i.e., let

$$I(x, t) = i_0(t) + \sqrt{2} i_1(t) \cos(\pi x).$$

Then $i_0(t)$, $i_1(t)$ and $x_c(t)$ yield the following equations:

$$i_0(t) + \sqrt{2} i_1(t) \cos(\pi x_c) = I_c, \tag{4.4}$$

$$C \frac{di_0}{dt} + u_1 i_0 = -u_0 + R[\alpha + (1 - \alpha)x_c], \tag{4.5}$$

$$C \frac{di_1}{dt} + (\pi^2 + u_1)i_1 = \frac{\sqrt{2}R}{\pi} (1 - \alpha) \sin(\pi x_c). \tag{4.6}$$

Initial conditions for $i_0(t)$ and $i_1(t)$ are computed as follows

$$i_0(0) = \int_0^1 g(x)\varphi_0(x) dx = \frac{H}{2}, \tag{4.7}$$

$$i_1(0) = \int_0^1 g(x)\varphi_1(x) dx = \frac{2\sqrt{2}H}{\pi^2}. \tag{4.8}$$

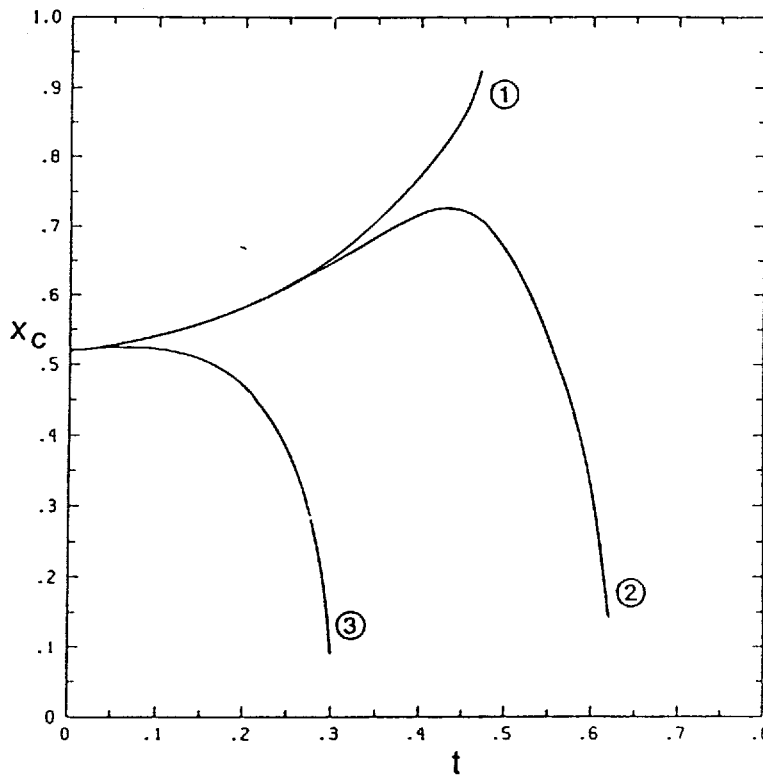


Fig. 5. Propagation of the toxic front: An approximate solution x_c vs. t obtained from section 4 (see equations (4.4–8)).

For the given parameters, the numerical solution for $x_c(t)$ of (4.4–8) is shown in Fig. 5. The three curves in Fig. 5 corresponds to of the same values of u_0 , I_c , R , H and α , namely, $u_0 = 0.35$, $I_c = 1.0$, $R = 0.2$, $H = 2.1$, $\alpha = 0.5$, but to three different values of u_1 . The curves ①, ② and ③ correspond to values $u_1 = 0.24$, 0.245 and 0.45 respectively. When $u_1 = 0.24$, the leakage rate is not high enough to balance the reproduction rate. The toxic front $x_c(t)$ advances due to the diffusion (see curve ① in Fig. 5). When $u_1 = 0.245$, the leakage rate is high enough to overcome the effects of the reproduction rate. The toxic front advances initially, but eventually the toxic front retreats. Therefore there is a finite “waiting” time interval from the beginning to the time when the toxic front retreats. For practical applications it is important to know the “waiting” time because it corresponds to the time interval which passes before the toxic front retreats. In the case ① the “waiting” time is defined as infinity. The “waiting” time is 0.43 for the case ②, and zero for the case ③. The larger the leakage rate, the shorter the “waiting” time. One can see this by comparing the curve ③ with the curve ② in Fig. 5. The above numerical results have been obtained from the two-mode approximation. The accuracy of these results remain to be justified. It would be interesting to solve the initial boundary value problem (2.1), (2.3–5) exactly by finite difference method or other numerical techniques and to compare the results with ours in this paper.

5. Concluding remarks

We have studied a nonlinear problem of toxic mass spreading. The non-linearity is introduced into the system by a positive feedback due to the reproduction of the toxic mass. Multiple steady state solutions are found. There exist two or more turning points. At these points, an infinitesimal perturbation of a parameter, such as an infinitesimal increase or decrease of the reproduction rate R , may cause a big jump of the interface of the toxic and nontoxic regions. Such a theoretically predicted catastrophic change of the stage of a chemical or biochemical system agrees with many experimental observations. Further research on the steady state problem is to study the global stability of the stationary solutions.

For the time dependent case, we have derived an integral equation for the toxic front. An approximate solution for a specific example has been obtained. But to solve the integral equation in the general case seems to be very difficult. An application of our computational procedure is to calculate the admissible maximum reaction rate at which the toxic front retreats.

The one-dimensional model may not be a satisfactory description for many practical applications. Nevertheless it provides some most interesting qualitative features. It remains to be seen whether these features appear in high dimensional situations.

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