

8/8/'98

# A distributed bioremediation problem with modal switching

**Thomas I. Seidman**

Department of Mathematics and Statistics

University of Maryland Baltimore County

Baltimore, MD 21228, USA

e-mail: <seidman@math.umbc.edu>

## 1. Introduction

We consider the use of bacteria for removal of some undesirable pollutant (or conversion to an innocuous form: cometabolism) — i.e., bioremediation. For some further exposition of the nature and significance of bioremediation as a practical application we refer the reader, e.g., to [2], [6] or the talk [4] of the present conference. Our present concerns, however, will be purely mathematical — an analysis dominated by the dynamical discontinuities implied by the characteristic feature of this model: at any moment  $t$  the bacteria at a given point  $x$  may be either in an *active* or a *dormant* mode.

The state of the system is thus a *hybrid*: partly continuous, partly discrete. The concentrations,  $\beta$ ,  $\pi$ , of bacteria and pollutant are continuous-valued components of the state, as is the concentration  $\alpha$  of some ‘critical nutrient’. On the other hand, there is a state component  $\chi$ , taking discrete values  $\{0, 1\}$ , which indicates the mode: 0 for ‘dormant’, 1 for ‘active’.

An idealized version of the modal transitions (compare [1]) is given by the *switching rules*:

- If the bacteria are active ( $\chi = 1$ ) and the concentration  $\alpha$  drops below some minimum  $\alpha_*$  (with  $\alpha_* > 0$ ), then they become dormant.

- If the bacteria are dormant ( $\chi = 0$ ), they will be re-activated when  $\alpha$  rises above  $\alpha^*$  (with  $\alpha^* > \alpha_*$ ).

It is clear that  $\chi$  can take either value (depending on the preceding history) when  $\alpha_* < \alpha < \alpha^*$ , so  $\chi$  is not simply a function of  $\alpha$  and must be introduced as an additional (discrete) state component, along with the more traditional continuous components  $\alpha, \beta, \pi$ .

We note that the rules above define the ‘elementary hysteron operator’ ( $W : \alpha(\cdot) \mapsto \chi$ ) as treated, e.g., by Krasnosel’skiĭ and Pokrovskiĭ [3]; see also [8]. It should be noted that  $W[\cdot]$  is generally well-behaved and isotone as a map from, e.g., Lipschitzian inputs to piecewise constant outputs — but is inherently multi-valued in certain anomalous cases (e.g., if  $\chi = 0$  and  $\alpha$  rises to  $\alpha^*$  but not above; cf., e.g., [7]) which will not affect our present analysis..

We consider a fixed interval  $[0, T]$  in time. The one-dimensional spatial region  $[0, \ell]$  initially contains some pollutant (distribution  $\pi_0$ ) and also some bacteria ( $\beta_0$ ), which are present but dormant. We are assuming that the bacteria are fixed in position and, for simplicity, will assume that the activity of the biomass is controlled by availability of a single critical nutrient (concentration  $\alpha$ , initially 0). This nutrient is supplied (as a control, at rate  $u(\cdot)$ ) first to re-activate the bacteria and then keeping them active to reduce the pollutant. Our principal technical concern will be the existence and characterization of solutions for specified  $u(\cdot)$  with the existence of optimal controls following easily from that for, e.g., the problem of minimizing  $\mathcal{J} = [\text{cost of nutrient}] - [\text{value of pollutant removal}]$ .

We assume that the nutrient is soluble in, e.g., an underwater groundflow of given velocity  $v = v(t) > 0$ , so we are injecting nutrient into this flow at  $x = 0$ , the left boundary. The pollutant may or may not also be carried by the flow (with mobility  $0 \leq \mu \leq 1$ ). Thus, we have the system:

$$\begin{aligned}
 (1.1) \quad \alpha_t + v\alpha_x &= D\alpha_{xx} - \varphi\chi\beta \\
 &\begin{cases} -D\alpha_x + v\alpha = u & \text{at } x = 0 \\ D\alpha_x = 0 & \text{at } x = \ell \end{cases} \\
 \beta_t &= \Gamma(\alpha, \beta)\chi \\
 \pi_t + \mu v\pi_x &= \hat{D}\pi_{xx} - \psi\chi\beta \\
 &\begin{cases} -\hat{D}\pi_x + \mu v\pi = \hat{\pi} & \text{at } x = 0 \\ \hat{D}\pi_x = 0 & \text{at } x = \ell \end{cases}
 \end{aligned}$$

Here, the coefficients  $\varphi, \psi > 0$  represent the respective rates at which (when active) the bacteria consume nutrient and pollutant; we take these as dependent only on  $\alpha$  except that  $\psi$  becomes 0 at  $\pi = 0$ . The bacterial growth rate  $\Gamma$  may be taken simply as  $\gamma(\alpha)\beta$  or, e.g., as Monod kinetics, limiting  $\beta$ . We assume that  $D, \hat{D} \geq 0$ , that  $0 < \underline{v} \leq v \leq \bar{v}$ , and that  $0 < \underline{\beta} \leq \beta_0 \leq \bar{\beta}$  at  $t = 0$ . Etc. Note that  $\hat{\pi}(\cdot) \geq 0$  is a known input and that  $u(\cdot) \geq 0$  is our control function (although in taking  $v$  as time-dependent we anticipate some possibility that this too might be controlled).

In this paper we concentrate on the extreme case of negligible diffusion but first note that the other extreme would be ‘perfect mixing’ (e.g., for small  $\ell$ ), giving a lumped parameter model:

$$(1.2) \quad \dot{\alpha} = -\varphi\chi\beta - \lambda\alpha + u, \quad \dot{\beta} = \Gamma\chi, \quad \dot{\pi} = -\psi\chi\beta$$

where the term ‘ $-\lambda\alpha$ ’ corresponds to flowthrough of nutrient, the control  $u$  now appears in the equation, and we have taken  $\mu = 0, \hat{\pi} = 0$ . This problem has already been treated in [5], showing: existence of solutions for any non-decreasing  $U(t) = \int_0^t u$ ; computational approximation; existence (with some characterization) of optimal controls, e.g., minimizing  $\mathcal{J} = [U(T) + b\pi(T)]$ .

## 2. Formulation, Solutions

Taking  $D, \hat{D} = 0$  in (1.1) to consider pure convection, the system becomes:

$$(2.1) \quad \begin{aligned} \alpha_t + v\alpha_x &= -\varphi\chi\beta \\ \beta_t &= \Gamma(\alpha, \beta)\chi \\ \pi_t + \mu v\pi_x &= -\psi\chi\beta \end{aligned}$$

with  $v\alpha = u$  at  $x = 0$  and (if  $\mu > 0$ )  $\mu v\pi = \hat{\pi}$  — as well as initial data for  $\alpha, \beta, \pi$ . To this we adjoin the switching rules:  $\chi = W[\alpha]$ , independently for each  $x \in [0, \ell]$ , with  $\chi \equiv 0$  at  $t = 0$ . As noted, this constitutes the significant mathematical novelty of this model — which does not fall within the types treated in [8] but which may be viewed as the free boundary problem of determining the region  $\mathcal{R} = \{(t, x) : \chi(t, x) = 1\}$  in which the bacteria are active.

Our first observation is that the final equation in (2.1) decouples, along with (2.2), so the dynamics — in this case, the determination of  $\mathcal{R}$  for a fixed

control function  $u$  — will be given entirely by the first two equations of (2.1) together with the switching rules, although the equation for  $\pi$  is, of course, relevant for the optimization of, e.g.,

$$(2.2) \quad \mathcal{J} = \int_0^T u(t) dt - b \int_{\mathcal{R}} \psi \beta dx dt.$$

In considering the dynamics it is convenient to use the coordinate system  $[\tau, x]$  where

$$(2.3) \quad \tau = \tau(t, x) := \int_0^t \frac{ds}{v(s)} - x.$$

This is only relevant for  $\tau > 0$  since  $\chi = 0$  (so nothing happens) before that. Since  $\tau$  increases with  $t$  at each  $x$ , the switching rules can equivalently be expressed in terms of the  $\tau$ -history of  $\alpha$ . Using (2.3), the relevant portion of (2.1) becomes

$$(2.4) \quad \begin{aligned} v\alpha_x &= -\varphi\chi\beta \quad (v\alpha = u \text{ at } x = 0) \\ v\beta_\tau &= \Gamma(\alpha, \beta)\chi. \end{aligned}$$

Assuming  $\chi \equiv 1$  on  $(0, x)$  for some fixed  $\tau$ , this gives

$$(2.5) \quad \alpha(\tau, x) = \left[ u - \int_0^x \varphi \beta \right] / v$$

whence  $\alpha$  is a nonincreasing function of  $x$  (with  $\alpha \leq u/v$ ). Given a bound on  $u$ , we have  $\alpha$  uniformly bounded (so  $\varphi(\alpha)$  is bounded above and below by compactness) and then have  $\beta$  bounded above and below (away from 0, using that  $\beta_0 \geq \underline{\beta} > 0$ ). We also immediately obtain uniform Lipschitz continuity of  $\alpha$  with respect to  $x$  and of  $\beta$  with respect to  $\tau$ .

As  $\varphi\beta$  is bounded away from 0, it is possible to define a pair of functions  $X^*(\tau)$ ,  $X_*(\tau)$  by solving  $\alpha = \alpha^*, \alpha_*$ , respectively, in (2.5):

$$(2.6) \quad \int_0^{X^*} \varphi \beta dx = u - \alpha^*, \quad \int_0^{X_*} \varphi \beta dx = u - \alpha_*.$$

Imposing a further admissibility requirement on the control  $u(\cdot)$ : that it satisfy a specified Lipschitz condition (with respect to  $t$  and so also  $\tau$ ), it then follows from (2.5) that  $\alpha$  is Lipschitz continuous jointly in  $(\tau, x)$  (although this will also require some analysis of the geometry of  $\mathcal{R}$ ) whence, by the Implicit Function Theorem,  $X^*, X_*$  are Lipschitz continuous in  $\tau$ ; we also

note that  $X_* - X^* \geq \text{const.} > 0$ . Causally in  $\tau$ , we now construct a new function  $\hat{X}$  as the output of a variant of the hysteretic ‘play operator’ of [3], taking the double input:  $[X_*, X^*]$ : imagine an inertial mass point (so it stays stationary where possible) which is ‘pushed’ up by the graph of  $X^*$  and down by the graph of  $X_*$  as needed to maintain  $X^* \leq \hat{X} \leq X_*$ . We note that this operator:  $[X^*, X_*] \mapsto \hat{X}$  is nonexpansive with respect to any weighted sup norm on  $C[0, T]$  with nonincreasing weight.

An analysis of our switching rules shows that, since  $\alpha$  is nonincreasing in  $x$ , the set-valued function  $\mathcal{R}(x) := \{\tau : \chi(\tau, x) = 1\}$  must also be non-increasing. The construction by way of (2.6) is now the heart of our characterization of  $\mathcal{R}$ , since it is easily seen that this  $\hat{X}$  provides the suitable boundary:

$$(2.7) \quad \mathcal{R} = \{(\tau, x) : x \leq \hat{X}(\tau)\}.$$

Noting that there is no difficulty in obtaining  $[\alpha, \beta]$  from (2.4) if  $\chi$  is given, we can consider the map:

$$\hat{X} \text{ (giving) } \chi \xrightarrow{(2.4)} [\alpha, \beta] \xrightarrow{(2.6)} [X^*, X_*] \mapsto \hat{X}.$$

The nonexpansivity of the play operator, as above, ensures that this map can be made contractive by the usual trick of selecting a suitable exponentially weighted norm for  $C[0, T]$ . Thus, there is a unique solution which, as we easily verify, depends continuously on  $u(\cdot) \in C[0, T]$ . As our admissibility assumption on  $u(\cdot)$  gives compactness, we then easily obtain existence of an optimal control for (2.2) by considering a minimizing sequence.

## References

- [1] E. Dawes, Growth and Survival of Bacteria, pp. 67–93 in *Bacteria in Nature*, vol. 2 (J. Poindexter and E.R. Leadbetter, editors), Plenum Publishers, New York, 1988.
- [2] National Research Council, *In situ Bioremediation: When does it work?*, National Academy Press, 1993.
- [3] M.A. Krasnosel’skiĭ and A.V. Pokrovskiĭ, *Systems with Hysteresis*, Nauka, Moscow, 1983 [*English transl.* Springer-Verlag, Berlin, 1989].

- [4] S.M. Lenhart, *Optimal control for PDE/ODE systems modeling bioreactors*, this conference.
- [5] S.M. Lenhart, T.I. Seidman, and J. Yong, *Optimal control of a hybrid bioreactor*, to appear.
- [6] R.D. Norris, et.al., *Handbook of Bioremediation*, Lewis Publishers, Boca Raton, 1994.
- [7] T.I. Seidman, *Switching systems, I*, Control and Cybernetics **19**, pp. 63–92 (1990).
- [8] A. Visintin, *Differential Models of Hysteresis*, Springer-Verlag, Berlin, 1994.