To the Graduate Council:

I am submitting herewith a dissertation written by **Sanjay Chawla** entitiled **"Applications of Optimal Control of Distributed Parameter Systems."** I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mathematics.

Suzanne Lenhart

Suzanne Lenhart, Major Professor

We have read this dissertation

and recommend its acceptance:

Philip W. Schaefer

Accepted for Council:

Associate Vice Chancellor
and Dean of The Graduate School

Applications of

Optimal Control Theory

to

Distributed Parameter Systems

A Dissertation

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Dedication

This dissertation is dedicated to

my parents

Mr. Inderjit Chawla

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and

Mrs. Kamla Chawla

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Abstract

The subject of this dissertation is the application of optimal control theory to distributed parameter systems. The dissertation is divided into three parts.

In part I, the general techniques of optimal control theory are discussed and highlighted with a help a of a simple but instructive example.

In Part II, a two dimensional parabolic system with competitive interactions is modeled as a two person zero sum game. The saddle point of the game is established and characterized. The controls are the kernels of the interaction terms.

Part III is devoted to the application of optimal control theory to a problem motivated from in situ bioremediation. In this remediation technology the indigenous sub-surface bacteria are stimulated by injecting compounds. The bacteria uses the injected compounds to break down chemical contaminants into less harmful substances. The way the compounds are injected is a crucial component of the technology. Optimal control theory is used to characterize an optimal injection function. The state system is a hybrid system consisting of both partial and oridinary differential equations.

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Part I

Introduction

Optimal control of distributed parameter systems or optimal control of systems governed by partial differential equations came of age with the ground breaking text of J.L. Lions [5]. Before then, optimal control theory was largely confined to situations where the "system to be controlled" was modeled by a system of ordinary differential equations. The cornerstones of deterministic finite dimensional (i.e. when the state system is governed by ordinary differential equations) optimal control theory are the *Pontryagin Maximum Principle* and the *Bellman dynamic programming principle* [2]. Much of the contemporary research in optimal control theory has been guided by the desire to extend the applicability of the above mentioned "principles" to distributed parameter systems (also called infinite dimensional systems) [8]. Our approach uses the ideas of Pontryagin's Maximum Principle and derives a characterization of the optimal control directly for a nonlinear system modelling a particular application. Instead of deriving extremely general necessary conditions for the existence of the optimal control (these necessary conditions are referred to as maximum principles in control theory jargon), we place more emphasis on the characterization of the optimal control via an *optimality system*. Our approach is more suitable for particular applications and submits to numerical implementation. For the PDEs with non-local interaction terms and PDE/ODE systems treated in this dissertation, there are no results on "maximum principles."

The generic optimal control problem is amenable to the following set up [5]:

1. A control u belongs to some set $\mathcal{U}_{ad}$, the set of admissible controls.

2. The state $y(u)$ of the system to be controlled, depending on u, is given by the

solution of the equation,

$$\Lambda y(u) = f(u)$$

where Λ is a known operator. The operator Λ could include a system of partial differential operators, ordinary differential operators, integral operators, or a "hybrid" system consisting of both PDE's and ODE's.

3. The "objective functional" $J(u)$, the quantity to be maximized or minimized, is defined in terms of $y(u)$ or u or both.

The objective is to find $u^* \in \mathcal{U}_{ad}$ such that

$$J(u^*) = \inf J(u), \qquad u \in \mathcal{U}_{ad}.$$

To give a flavour of the type of arguments that are to follow, we will put restrictions on the operator Λ and the cost functional $J(u)$ and carry out some heuristic analysis to characterize the optimal control. What follows has been extracted from [6].

We begin by recalling a few well known results from convex analysis.

Proposition 0.1 *Let*

$$v \to J(v)$$

be a real valued functional on $\mathcal{U}_{ad} \subset U$ *such that:*

$$U \textit{ is a Hilbert Space on } \mathbf{R}, \tag{0.1}$$

$$\mathcal{U}_{ad} \textit{ is a closed convex set in } U, \tag{0.2}$$

$$J \textit{ is strictly convex and continuous on } U_{ad}, \tag{0.3}$$

$$J(v) \to +\infty \quad \textit{if } \|v\| \to \infty. \tag{0.4}$$

Then there exists a unique $u \in \mathcal{U}_{ad}$ *such that*

$$J(u) \leq J(v) \textit{ for all } v \in \mathcal{U}_{ad}.$$

For a proof, see Ekeland and Temam[1, Prop 1.2, pg. 25] □

For a more precise characterization of the infimum, we define:

For $u, v \in \mathcal{U}_{ad}$, let

$$\lim_{h \to 0} \frac{J(u+hv) - J(u)}{h}$$

exist and be denoted by $J'(u; v)$. Then if there exists a $\bar{u} \in \mathcal{U}_{ad}$ such that

$$J'(u; v) = (v, \bar{u}) \qquad \textit{for all} \qquad v \in \mathcal{U}_{ad}$$

then $\bar{u}$ is called the *Gateaux derivative,* of J at u and is denoted by $J'(u)$. Note that (,) is the inner product on the Hilbert space U.

Proposition 0.2 *If* J *satisfies the conditions in Prop. 0.1 and has a continuous Gateaux derivative then the following our equivalent:*

$$\begin{aligned} &1) & J(u^*) &= \inf\nolimits_{u \in \mathcal{U}_{ad}} J(u) \\ &2) & (J'(u^*), v - u^*) &\geq 0 \qquad \forall v \in \mathcal{U}_{ad}. \end{aligned} \tag{0.5}$$

For a proof, see Ekeland and Temam[1, Prop. 2.1, pg. 36] □

Let $\Lambda \in \mathcal{L}(Y, F)$ be the space of linear operators from Y to F, where Y and F are Hilbert spaces. We assume some boundary conditions are incorporated into the definition of the space Y and that the associated boundary value problem is well defined, i.e., Λ is an isomorphism from Y onto F.

Let U , the space of controls, be a Hilbert space and $\mathcal{U}_{ad}$, the set of admissible controls, be a closed convex subset of U. Let $B \in \mathcal{L}(U, F)$. For every $v \in U$ and a fixed $f \in F$ we consider the boundary value problem with **linear** control

$$\Lambda y = f + Bv. \tag{0.6}$$

The unique solution of (0.6) defines *the state of the system:*

$$y = y(v) = \Lambda^{-1}(f + Bv). \tag{0.7}$$

Let $C \in \mathcal{L}(Y, H)$ be the "observation" operator. We consider the *cost functional*

$$J(v) = \|Cy(v) - z_d\|^2 + (Nv, v)_U, \tag{0.8}$$

where z_d is a given target function in H and $N \in \mathcal{L}(U, U)$ is a *symmetric positive definite operator.* Once again, the problem is to minimize J on $\mathcal{U}_{ad}$:

$$\inf J(v), \quad v \in \mathcal{U}_{ad}. \tag{0.9}$$

Since $v \to Cy(v) - z_d$ is affine from U to H and $(Nv, v) \geq \nu\|v\|^2$, $\nu > 0$, the function $v \to J(v)$ is continuous, convex and $J(v) \to +\infty$ if $\|v\| \to \infty$. Consequently, there exists a unique element u in $\mathcal{U}_{ad}$ such that

$$J(u) = \inf J(v), \quad v \in \mathcal{U}_{ad}, \tag{0.10}$$

i.e., u is the *optimal control.* It follows directly that J is differentiable; therefore u is characterized by (see Prop. 0.2)

$$(Cy(u) - z_d, C(y(v) - y(u))) + (Nu, v - u)_U \geq 0 \quad \text{for all } v \in \mathcal{U}_{ad}. \tag{0.11}$$

We introduce the adjoint C^* of C:

$$C^* \in \mathcal{L}(H, Y'), \tag{0.12}$$

and the *adjoint state* $p = p(u)$, defined by

$$\Lambda^* p = C^*(Cy(u) - z_d), \tag{0.13}$$

where Λ^* denotes the adjoint operator of Λ.

Then

$$\begin{aligned}
(C^*(Cy(u) - z_d), y(v) - y(u)) &= (Cy(u) - z_d, C(y(v) - y(u))) \\
&= (\Lambda^* p, y(v) - y(u)) \\
&= (p, \Lambda y(v) - \Lambda y(u)) \qquad (0.14) \\
&= (p, B(v - u)) = (B^* p, v - u)
\end{aligned}$$

so that (0.11) is equivalent to $(B^*p + Nu, v - u) \geq 0$ for all $v \in \mathcal{U}_{ad}$. Notice how the linearity of the state problem in terms of the control was exploited in (0.14).

Summing up, we have the optimal control u, which exists and is unique, is given by the solution of the "*optimality system*":

$$\begin{aligned}
&\Lambda y = f + Bv \\
&\Lambda^* p = C^*(Cy - z_d), \\
&u \in \mathcal{U}_{ad}, \\
&(B^* p + Nu, v - u) \geq 0 \text{ for all } v \in \mathcal{U}_{ad}.
\end{aligned}$$

where y and p are subject to the appropriate boundary conditions.

We can explicitly characterize the control if we put some extra conditions on the various operators. For example, if B and N were the identity operators and $\mathcal{U}_{ad} = U$, then clearly

$$u = -p.$$

In Part II, we consider an "optimal control" problem where the state is governed by a system of competitive parabolic (partial) differential equations:

$$\begin{aligned} L_1 u(x,t) &= f(x,t) - u(x,t) \textstyle\int_Q c(x,y,t,\tau) v(y,\tau)\, dy d\tau \\ L_2 v(x,t) &= g(x,t) - v(x,t) \textstyle\int_Q d(x,y,t,\tau) u(y,\tau)\, dy d\tau \end{aligned} \tag{0.15}$$

with suitable initial data and boundary conditions. Here

$$L_k u = u_t - (a_{ij}^k u_{x_i})_{x_j} + b_i^k u_{x_i} + c^k u,\ k = 1, 2.$$

This system has been successfully used to model phenomena in which two competing populations are involved, e.g., opposing armies, chemical reactants and animal species (See Introduction of Part II). The solutions u and v represent the densities of the "two players" involved and the attrition kernels c and d can be the quantitative manifestations of the strategies employed by the players to overwhelm the opposition population. Population u controls d and population v controls c and the objective of u is to maximize $\mathcal{J}$ and that of v is to minimize, $\mathcal{J}$ where

$$\mathcal{J}(c,d) = \frac{1}{2}\int_Q K[u(c,d) - \tilde{u}]^2 - L[v(c,d) - \tilde{v}]^2\, dx\, dt + \frac{1}{2}\int_Q \int_Q (Nc^2 - Md^2)\, dx\, dy\, dt\, d\tau. \tag{0.16}$$

Our goal is to establish the existence of a unique saddle point of the objective functional and then characterize it. The saddle point is defined as a pair of strategies

(c^*, d^*) such that

$$\mathcal{J}(c^*, d^*) = \sup_{d \in C_\Gamma} \mathcal{J}(c^*, d) = \inf_{c \in C_\Gamma} \mathcal{J}(c, d^*).$$

where C_Γ is the control set. Lenhart *et. al*[4] considered the elliptic case, i.e., when the state was governed by a system of elliptic equations. In [10], Szpiro and Protopopescu considered the case when the controls were the initial conditions of the state system. Lenhart and Protopopescu established and characterized the saddle point in a parabolic competitive system when the controls were the source terms of the system in [3].

Problems in optimal control theory, the ones we consider, are actually applications of modern theory of partial differential equations. For example, to prove the existence of the solution of the above system is a non- trivial exercise in the application of the method of monotone iterations, which in turn is dependent on "maximum principle" type arguments. Similarly, the existence of the saddle point is dependent upon the existence of sufficiently regular directional derivatives of the state variables and apriori estimates for justification. Finally the optimality system, which consists of the state system and an adjoint system, is a system of nonlinear partial differential equations, albeit in which the state and adjoint are "time" oriented in opposite directions.

In Part III we take up a problem motivated from the fast emerging environmental remediation technology known as bioremediation. In bioremediation the transformation of contaminants into less hazardous substances is brought about by providing "nutrients" to the bacteria present in the contaminated environment. These bacteria use the externally provided nutrients as "food" and enable the breakdown of the contaminants. Care must be taken about how the nutrients are injected into the subsurface environment because it is known that a haphazard injection of the nutrients inhibits the remediation process. We use tools from optimal control theory to design an "appropriate" nutrient injection strategy (See introduction of Part III).

The state system involved here is unusual, in that , it consists of three nonlinear parabolic partial differential equations coupled with a nonlinear ordinary differential equation:

$$
\begin{aligned}
&u_t - d_h u_{xx} + \nu u_x = -\frac{e\mu_1 v X}{1+\frac{k_1}{u}} - \frac{f\mu_2 v X}{1+\frac{k_2}{u}+\frac{u}{k_3}} \qquad \text{for } (x,t) \in Q_T = (0,L)\times(0,T] \\
&v_t - d_h v_{xx} + \nu v_x = -\frac{\mu_1 v X}{1+\frac{k_1}{u}} - \frac{\mu_2 v X}{1+\frac{k_2}{u}+\frac{u}{k_3}} \\
&w_t - d_h w_{xx} + \nu w_x = -k_3 w X \\
&\tfrac{dX}{dt} = \frac{\mu_2 v X}{1+\frac{k_2}{u}+\frac{u}{k_3}} - \frac{k_4 X}{k_5 + X} \qquad (x\in[0,L],\, t>0)
\end{aligned}
\tag{0.17}
$$

with

$$-d_h u_x(0,t) = \nu(g(t) - u(0,t)), \quad u_x(L,t) = 0.$$

and other suitable boundary and initial conditions.

The functions u and v are concentrations of the nutrients and the function w is the concentration of the contaminant. The function X is the density of the bacteria biomass and because the bacteria is immobile (it is sorbed to the soil), its evolution is governed by an ordinary differential equation. The objective functional is:

$$\mathcal{J}(g) = A\int_Q X(x,t)\phi(x)\,dx\,dt + B\int_0^L w(x,T)\,dx + \frac{1}{2}\int_0^T g^2(t)\,dt,$$

where $\phi(x)$ is a suitably defined "weight" function. Again it is required to characterize g^* such that

$$J(g^*) = \inf_{g \in C_M} J(g),$$

where C_M is the set of admissible controls.

We augment our theoretical results by implementing a numerical simulation of the characterization of the optimal control. We compare our results with those derived by Peterson *et. al* using another method [9].

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PART II

A Minmax Problem

For

Parabolic Systems

With

Competitive Interactions

Abstract

A two dimensional parabolic system with competitive interactions is modeled as a two person zero sum game. The saddle point of the game is established and characterized. The controls are the kernels of the interaction terms.

1 Introduction

In 1914 Lancaster [4] proposed the first analytic model for describing combat between two forces. The Lancaster model, a coupled system of ordinary differential equations, fails to account for the spatial movement of opposing forces on the battlefield. To overcome this obvious shortcoming Protopopescu et al. [9] introduced a more general model, namely, they replaced the system of ordinary differential equations with a system of **semilinear parabolic equations with competitive interactions.** These systems belong to the class of reaction-diffusion systems which lately have become one of the mainstream fields in pure, applied and numerical PDE's [3]. This competition model can be used to represent other phenomenon, e.g., densities of competing biological populations and concentration of chemical reactants.

In this dissertation we consider competitive systems as a two-person zero-sum game which implies that one player's gains necessarily translate to the other players's losses. Each player controls some of the game parameters which the player can manipulate to navigate the evolution of the system towards a desired state. A quantitative measurement of the players performance is modeled in terms of a minimizing(respectively maximizing) functional which depends upon the state of the system and the controls.

We will show that under suitable conditions the game admits a unique saddle point and then we will characterize the saddle point of the game as a solution of an optimality system. The optimality system will consist of the parabolic state equations coupled with two adjoint equations. The controls will be the attrition kernels of the non-local interaction terms. The attrition kernels represent the effect of "weapons" in the combat model case. In general, the interactions between the two populations are non-local and the kernels measure the range over which one population can affect the other population.

Lenhart et al. [8] considered the steady state case with the operator $-\Delta$ and Lenhart et al. [5] have also considered the parabolic case where the controls are the source terms.

The outline of this part of the dissertation is the following. In the next section we give the statement of the problem. The payoff(cost) functional is defined and for given controls, the unique solution of the state system is constructed. The existence of the unique saddle point is established in Section 3. In Section 4 the optimality system is defined and the saddle point is represented as the solution of this optimality system.

2 Statement of the Problem

Throughout this part of the dissertation, C denotes generic constants, unless otherwise indicated.

Let Ω be a bounded domain in $\mathbf{R}^m$ with $\partial\Omega \in C^{1,1}$, let $T > 0$ and $Q = \Omega \times (0, T)$. For $\Gamma > 0$, define the control set,

$$C_\Gamma = \{c \in L^\infty_+(Q \times Q) \mid \|c\| \leq \Gamma\}.$$

where L^∞_+ is the set of positive L^∞ functions.

For any $c, d \in C_\Gamma$, let the pair $(u, v) = (u(c, d), v(c, d))$ denote the solution of the *state system*

$$\begin{aligned}
&L_1 u(x,t) = f(x,t) - u(x,t) \textstyle\int_Q c(x,y,t,\tau) v(y,\tau)\, dy d\tau && \text{on } Q \\
&L_2 v(x,t) = g(x,t) - v(x,t) \textstyle\int_Q d(x,y,t,\tau) u(y,\tau)\, dy d\tau && \\
&u = u^0, \quad v = v^0 && \text{on } \Omega \times \{0\} \\
&u = 0, \quad v = 0 && \text{on } \Sigma = \partial\Omega \times (0,T)
\end{aligned} \tag{2.1}$$

where

$$u, v \in L^2(0, T, H^1_0(\Omega)) = V,$$

$$L_k u = u_t - (a^k_{ij} u_{x_i})_{x_j} + b^k_i u_{x_i} + c^k u, \; k = 1, 2.$$

and we have used the summation convention with respect to repeated indices.

The solutions u, v represent the concentration of the two competing populations. The sources f, g are given and the attrition kernels c, d are the controls. The first player controls d with the purpose of maximizing $\mathcal{J}$ (the payoff); the second player controls c to minimize $\mathcal{J}$ (the cost). Given two target functions, $\tilde{u}$, $\tilde{v} \in L^2$, and constants K, $L \geq 0$ and M, $N > 0$, the *payoff (cost) functional* $\mathcal{J}$ is defined by

$$\mathcal{J}(c,d) = \frac{1}{2}\int_Q \left\{K[u(c,d)-\tilde{u}]^2 - L[v(c,d)-\tilde{v}]^2\right\} dx\,dt + \frac{1}{2}\int_Q\int_Q (Nc^2 - Md^2)\,dx\,dt\,dy\,d\tau. \tag{2.2}$$

The *saddle point* (c^*, d^*) (if it exists) is defined as a pair of *strategies* $(c^*, d^*) \in C_\Gamma \times C_\Gamma$, such that

$$\mathcal{J}(c^*, d^*) = \sup_{d \in C_\Gamma} \mathcal{J}(c^*, d) = \inf_{c \in C_\Gamma} \mathcal{J}(c, d^*)$$

We make the following assumptions:

$$a_{ij}^k, b_i^k, c^k \in L^\infty(Q), k = 1,2,\ i,j = 1, ..., m \tag{2.3}$$

$$\theta \zeta_i \zeta_i \leq a_{ij}^k \zeta_i \zeta_j \leq \theta^{-1} \zeta_i \zeta_i,\ \theta > 0 \text{ for all } \boldsymbol{\zeta} \in \mathbf{R}^\mathbf{m} \tag{2.4}$$

$$u^0, v^0 \in L_+^\infty(\Omega) \tag{2.5}$$

$$c^k(x,t) > c_0 > 0\,, k = 1,2. \tag{2.6}$$

Finally to set up solutions in V, we define the following bilinear form on $H_0^1(\Omega)$:

$$a^k(t,\phi,\psi) = \int_\Omega a_{ij}^k \phi_{x_i} \psi_{x_j}\,dx + \int_\Omega b_i^k \phi_{x_i} \psi\,dx + \int_\Omega c^k \phi\psi\,dx \text{ for each t } \in (0,T). \tag{2.7}$$

Then for all $\phi, \psi \in L^2(0,T,H_0^1(\Omega))$, solutions (u,v) in $V \times V$ of (2.1) satisfy

$$\begin{aligned} \int_0^T (< u_t, \psi > + a^1(t,u,\psi))\,dt &= \textstyle\int_0^T \int_\Omega (f - u(x,t) \int_Q c(x,y,t,\tau) v(y,\tau)\,dy d\tau) \psi\,dx\,dt \\ \int_0^T (< v_t, \phi > + a^2(t,v,\phi))\,dt &= \textstyle\int_0^T \int_\Omega (f - v(x,t) \int_Q d(x,y,t,\tau) u(y,\tau)\,dy d\tau) \phi\,dx\,dt \end{aligned} \tag{2.8}$$

where $<,>$ denotes the duality between $H_0^1(\Omega)$ and $H^{-1}(\Omega)$.

Using an iterative scheme we have the following existence result.

Proposition 2.1 (Existence of solutions of the state system). *Given $c, d \in C_\Gamma$, there exists a solution (u, v) of the state system (2.1) in $V \times V$ and there exists a constant $C_1 > 0$ such that $0 \le u \le C_1$, $0 \le v \le C_1$.*

Proof: Since the bilinear form $a^k(t, \phi, \psi)$ is continuous and coercive for all $\phi,\ \psi \in H_0^1(\Omega)$, we obtain, using standard linear theory [2], positive solutions u_0, $\tilde{v}$ in V to

$$\begin{aligned} L_1 u_0 &= f \quad \text{in } Q, \\ u_0 &= u^0 \quad \text{at } t=0, \\ u_0 &= 0 \quad \text{on } \Sigma, \end{aligned}$$

and

$$\begin{aligned} L_2 \tilde{v} &= g \quad \text{in } Q, \\ \tilde{v} &= v^0 \quad \text{at } t=0, \\ \tilde{v} &= 0 \quad \text{on } \Sigma. \end{aligned}$$

Solution $u_0, \tilde{v}$ will be the supersolutions for the iterates to be constructed. Also, by standard existence theory[2], there exists a constant $C_1 > 0$ such that $\|u_0\|_\infty, \|\tilde{v}\|_\infty \le C_1$.

Now let v_0 be the solution in V of

$$\begin{aligned} L_2 v_0 &= g - \tilde{v} \textstyle\int_Q d(x,y,t,\tau) u_0\, dy d\tau \quad && \text{in } Q, \\ v_0 &= v^0 && \text{at } t=0, \\ v_0 &= 0 && \text{on } \Sigma. \end{aligned}$$

Let (u_k, v_k) be the solutions of the pair of linear Initial - Boundary value problem

$$\begin{aligned} &L_1 u_k + \mu u_k = f - u_{k-1} \textstyle\int_Q c v_{k-1} + \mu u_{k-1} & & \\ &L_2 v_k + \mu v_k = g - v_{k-1} \textstyle\int_Q d u_{k-1} + \mu v_{k-1} & &\text{in } Q, \\ &u_k = u^0, v_k = v^0 & &\text{at } t = 0, \\ &u_k = 0, v_k = 0 & &\text{on } \Sigma, \end{aligned} \tag{2.9}$$

where μ is a constant which makes the right hand side of the first equation in (2.9) an increasing function of u and the right hand side of the second equation an increasing function of v for iterates in the range $0 \leq u_k, v_k \leq C_1$. We have monotone convergence of the iterates,

$$u_k \searrow u,\ v_k \nearrow v \quad \text{pointwise},$$
$$0 \leq u_k \leq C_1, 0 \leq v_k \leq C_1,$$

through comparison results[5]. From *a priori* estimates of u_k, v_k from the system we get uniform bounds on $\|u_k\|_V$, $\|v_k\|_V$. Thus, u_k and v_k converge weakly to u and v in V. Now we show that u, v solve the state system in the sense of (2.8). The uniform bounds on u_k and v_k in V combined with the state equation give uniform bounds for $(u_k)_t$ and $(v_k)_t$ in $L^2(0, T, H^{-1}(\Omega))$. Using compactness results [7, Chapter 4, Prop. 4.2] implies that u_k, v_k converge strongly in $L^2(Q)$. Passing to the limit in the weak formulation of the system (2.9) we obtain $u = u(c, d)$ and $v = v(c, d)$ which solve the system (2.1). □

Proposition 2.2 (Uniqueness of solutions of the state system.) *For a fixed pair (c, d) in $[C_\Gamma]^2$ and for c_0 sufficiently large, the state system (2.1) admits a unique solution.*

Proof. Suppose (u,v) and $(\bar{u},\bar{v})$ solve the state system for given initial conditions u^0 and v^0. Using test functions $(u-\bar{u})$, $(v-\bar{v})$ and then subtracting the $(\bar{u},\bar{v})$ system from (u,v) system

$$\int_Q [(u-\bar{u})_t(u-\bar{u}) + a^1_{ij}(u-\bar{u})_{x_i}(u-\bar{u})_{x_j} + b^1_i(u-\bar{u})_{x_i}(u-\bar{u}) + c^1(u-\bar{u})^2]$$

$$+\int_Q [(v-\bar{v})_t(v-\bar{v}) + a^2_{ij}(v-\bar{v})_{x_i}(v-\bar{v})_{x_j} + b^2_i(v-\bar{v})_{x_i}(v-\bar{v}) + c^2(v-\bar{v})^2]$$

$$= \tag{2.10}$$

$$-\int_Q u(u-\bar{u})\int_Q cv + \int_Q \bar{u}(u-\bar{u})\int_Q c\bar{v} - \int_Q v(v-\bar{v})\int_Q du + \int_Q \bar{v}(v-\bar{v})\int_Q d\bar{u}.$$

We will estimate the various terms in the above equality and show that the resulting relationship can only be satisfied if $u=\bar{u}$ and $v=\bar{v}$. Note that

(i)

$$\int_Q [(u-\bar{u})_t(u-\bar{u}) + (v-\bar{v})_t(v-\bar{v})] = \frac{1}{2}\int_{\Omega\times T}[(u-\bar{u})^2 + (v-\bar{v})^2],$$

(ii)

$$\int_Q a^1_{ij}(u-\bar{u})_{x_i}(u-\bar{u})_{x_j} \geq \theta\int_Q [|\nabla(u-\bar{u})|^2,$$

(iii)

$$\int_Q a^2_{ij}(v-\bar{v})_{x_i}(v-\bar{v})_{x_j} \geq \theta\int_Q [|\nabla(v-\bar{v})|^2,$$

where θ is the ellipticity constant in (2.4),

(iv)

$$\left|\int_Q b^1_i(u-\bar{u})_{x_i}(u-\bar{u})\right| \leq C(\epsilon)\int_Q |\nabla(u-\bar{u})|^2 + C(\frac{1}{\epsilon})\int_Q (u-\bar{u})^2$$

and

(v)

$$\left|\int_Q b_i^2(v-\bar{v})_{x_i}(v-\bar{v})\right| \leq C(\epsilon)\int_Q |\nabla(v-\bar{v})|^2 + C(\frac{1}{\epsilon})\int_Q (v-\bar{v})^2.$$

We choose ϵ such that the $C(\epsilon)$'s in (iv) and (v) equal θ in (ii) and (iii).

Now we estimate the double integrals:

$$\begin{aligned}
&-\int_Q u(u-\bar{u})\int_Q cv + \int_Q \bar{u}(u-\bar{u})\int_Q c\bar{v} \\
&\quad = -\int_Q u(u-\bar{u})\int_Q cv + \int_Q \bar{u}(u-\bar{u})\int_Q cv - \int_Q \bar{u}(u-\bar{u})\int_Q cv + \int_Q \bar{u}(u-\bar{u})\int_Q c\bar{v} \\
&\quad = -\int_Q (u-\bar{u})^2\int_Q cv - \int_Q \bar{u}(u-\bar{u})\int_Q c(v-\bar{v}) \\
&\quad \leq -\int_Q \bar{u}(u-\bar{u})\int_Q c(v-\bar{v}) \\
&\quad \leq C\{\int_Q (u-\bar{u})^2 + \int_Q (v-\bar{v})^2\}. \qquad (2.11)
\end{aligned}$$

By choosing c_0 sufficiently large, we absorb the $\int_Q (u-\bar{u})^2$ and $\int_Q (v-\bar{v})^2$ terms on the left hand side in (2.10). Thus we get

$$(c_0 - C)\{\int_Q (u-\bar{u})^2 + \int_Q (v-\bar{v})^2\} \leq 0$$

We conclude that $u = \bar{u}$ and $v = \bar{v}$. □

3 Existence of the Saddle Point

Sufficient conditions for the objective functional $\mathcal{J}(c,d)$ to admit a saddle point are [1]:

(1) The mapping $c \mapsto \mathcal{J}(c,d)$ is strictly convex and lower semi-continuous in the weak toplogy of $L^2(Q \times Q)$.

(2) The mapping $d \mapsto \mathcal{J}(c,d)$ is strictly concave and upper semi-continuous in the weak topology of $L^2(Q \times Q)$.

We will prove (1), *and* (2) follows similarly.

For c, $\bar{c}$ given in C_Γ define a new function $J : [\mathbf{0},\mathbf{1}] \to \mathbf{R}$ as

$$J(\nu) = \mathcal{J}(\nu c + (1-\nu)\bar{c}, d).$$

The strict convexity of the map $c \mapsto \mathcal{J}(c,d)$ is equivalent to showing $J''(\nu) > 0$ for all ν in $[0,1]$.

Since $\mathcal{J}$ is a function of the state variables and the state variables themselves are functions of the controls, we begin by estimating the first and second derivatives of u and v with respected to the control c. The derivatives involved are directional derivatives, in the distributional sense. We begin by deriving a useful apriori estimate.

Consider the Gelfand triple

$$V \subset L^2(Q) \subset V'$$

and for any (c,d) in $[C_\Gamma]^2$ **define** the operator $\mathcal{L} : V^2 \to (V')^2$ by the formula

$$\mathcal{L}\begin{pmatrix} \zeta \\ \chi \end{pmatrix} = \begin{pmatrix} L_1\zeta + u\int_Q c\chi + \zeta\int_Q cv \\ L_2\chi + v\int_Q d\zeta + \chi\int_Q du \end{pmatrix}. \tag{3.12}$$

Proposition 3.1 *For any $\epsilon > 0$, there exists $c_0(\epsilon)$ such that if*

$$c^k(x,t) \geq c_0(\epsilon) > 0, k = 1,2.$$

then for given $\alpha, \beta \in L^2(Q)$, the solution to

$$\mathcal{L}\begin{pmatrix} \zeta \\ \chi \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \tag{3.13}$$

with $\zeta = \chi$ at $t = 0$ and $\zeta = \chi = 0$ on Σ , satisfies the estimate,

$$||\zeta||_{L^2(Q)} + ||\chi||_{L^2(Q)} \leq \epsilon(||\alpha||_{L^2(Q)} + ||\beta||_{L^2(Q)}).$$

Proof: We multiply the first equation in (3.13) by ζ and the second equation by χ. Integrating over Q and using the coercivity of the parabolic operators L_1, L_2, we get,

$$\begin{aligned}\frac{1}{2}\int_{\Omega\times T}(\zeta^2+\chi^2)+\theta\int_Q(|\nabla\zeta|^2+|\nabla\chi|^2)+c_0\int_Q(\zeta^2+\chi^2)&\\ \leq\ -\int_Q u\zeta\int_Q c\chi-\int_Q v\chi\int_Q d\zeta+\int_Q\alpha\zeta+\int_Q\beta\chi&\\ -\int_Q b_i^1\zeta_{x_i}\zeta-\int_Q b_i^2\chi_{x_i}\chi.&\qquad(3.14)\end{aligned}$$

Now we use the L^∞ bounds of u, v, c, d and the ϵ - Cauchy inequality to estimate the right hand side of the above inequality.

(*i*) $\quad -\int_Q u\zeta \int_Q c\chi \leq C\int_Q \zeta \int_Q \chi \leq C\int_Q \zeta^2 + C\int_Q \chi^2$.

(*ii*) $\quad -\int_Q v\chi \int_Q d\zeta \leq C\int_Q \zeta^2 + C\int_Q \chi^2$.

(*iii*) $\quad \int_Q \alpha\zeta \leq \epsilon\int_Q \alpha^2 + C_\epsilon\int_Q \zeta^2$.

(*iv*) $\quad \int_Q \beta\chi \leq \epsilon\int_Q \beta^2 + C_\epsilon\int_Q \chi^2$.

(*v*) $\quad \int_Q b_i^1\zeta_{x_i}\zeta \leq \frac{\theta}{2}\int_Q |\nabla\zeta|^2 + C_\theta\int_Q \zeta^2$.

(*vi*) $\quad \int_Q b_i^2\chi_{x_i}\chi \leq \frac{\theta}{2}\int_Q |\nabla\chi|^2 + C_\theta\int_Q \chi^2$.

Choosing $c0$ sufficiently large and estimating the right hand side of (3.14) by the above estimates, we arrive at our conclusion. □

We now we prove the existence of first derivatives of u, v with respect to the controls. These derivatives satisfy a system with operator $\mathcal{L}$ from (3.12).

Proposition 3.2 *For c_0 sufficiently large, the mapping*

$$c \mapsto (u(c,d), v(c,d)) \in V^2$$

is differentiable in the sense

$$\frac{u(c+\beta\bar{c},d)-u(c,d)}{\beta} \to \zeta \quad \textit{weakly in } V, \tag{3.15}$$

$$\frac{v(c+\beta\bar{c},d)-v(c,d)}{\beta} \to \chi \quad \textit{weakly in } V, \tag{3.16}$$

as $\beta \to 0$, for any $(c,d) \in [C_\Gamma]^2$ and $\bar{c} \in L^\infty(Q)$ such that $c+\beta\bar{c} \in C_\Gamma$.

Also $(\zeta,\chi) \overset{\text{def}}{=} ((\zeta(c,d;\bar{c},0),(\chi(c,d;\bar{c},0))$ is the unique solution of

$$\mathcal{L}\begin{pmatrix}\zeta\\ \chi\end{pmatrix} = -\begin{pmatrix}u(c,d)\int_Q \bar{c}v(c,d)\\ 0\end{pmatrix}. \tag{3.17}$$

with $\zeta=\chi=0$ at $t=0$ and $\zeta=\chi=0$ on Σ.

Proof: Let (u_β, v_β) be the solution of the state system corresponding to the controls $(c+\beta\bar{c},d)$.Then multipling the first equation of the state system by $(u_\beta-u)$ and the second equation by $(v_\beta - v)$ and then integrating over Q, we get

$$\int_Q(u_\beta-u)_t(u_\beta-u)+\int_Q[a^1_{ij}(u_\beta-u)_{x_i}(u_\beta-u)_{x_j}+\int_Q b^1_i(u_\beta-u)_{x_i}(u_\beta-u)+\int_Q c^1(u_\beta-u)^2]$$

$$= -\int_Q u_\beta(u_\beta-u)\int_Q(c+\beta\bar{c})v_\beta + \int_Q u(u_\beta-u)\int_Q cv \tag{3.18}$$

and

$$\int_Q(v_\beta-v)_t(v_\beta-v)+\int_Q a^2_{ij}(v_\beta-v)_{x_i}(v_\beta-v)_{x_j}+\int_Q b^2_i(v_\beta-v)_{x_i}(v_\beta-v)$$

$$+\int_Q c^2(x,y,t,\tau)(v_\beta - v)^2(y,\tau)\,dy\,d\tau$$

$$=$$

$$-\int_Q v_\beta(v_\beta - v)\int_Q du_\beta + \int_Q v(v_\beta - v)\int_Q du. \tag{3.19}$$

After standard manipulations on the left hand side of (3.18) (using coercivity of the a^1_{ij}'s and applying ϵ - Cauchy inequality to separate $\int_Q b^1_i(u_\beta - u)_{x_i}(u_\beta - u)$)

$$\frac{\theta}{2}\int_Q |\nabla(u_\beta - u)|^2 + c_0\int_Q (u_\beta - u)^2 \le -\int_Q u_\beta(u_\beta - u)\int_Q (c+\beta\bar{c})v_\beta + \int_Q u(u_\beta - u)\int_Q cv.$$

Adding and subtracting $\int_Q u_\beta(u_\beta - u)\int_Q (c+\beta\bar{c})v$, we get

$\frac{\theta}{2}\int_Q |\nabla(u_\beta - u)|^2 + c_0\int_Q (u_\beta - u)^2$

$$\le -\int_Q (u_\beta(u_\beta - u)\int_Q (c+\beta\bar{c})(v_\beta - v) - \int_Q (u_\beta - u)^2\int_Q cv - \int_Q u_\beta(u_\beta - u)\int_Q \beta\bar{c}v.$$

Again using the apriori bounds of u, v, c ,

$\frac{\theta}{2}\int_Q |\nabla(u_\beta - u)|^2 + c_0\int_Q (u_\beta - u)^2$

$$\le C\{\|(u_\beta - u)\|^2_{L^2(Q)} + \|(v_\beta - v)\|^2_{L^2(Q)}\} + C\beta^2\|\bar{c}\|^2_{L^2(Q)}. \tag{3.20}$$

Similarly (3.19) yields

$\frac{\theta}{2}\int_Q |\nabla(v_\beta - v)|^2 + c_0\int_Q (v_\beta - v)^2$

$$\le C\{\|(u_\beta - u)\|^2_{L^2(Q)} + \|(v_\beta - v)\|^2_{L^2(Q)}\} \tag{3.21}$$

Combining (3.20) and (3.21), using c_0 large, and dividing across by β, we get

$$\left\|\frac{u_\beta - u}{\beta}\right\|_V + \left\|\frac{v_\beta - v}{\beta}\right\|_V \le C.$$

Since bounded sets in V are weakly compact, we arrive at the required weak limits.

Now writing the weak formulation of the system satisfied by

$$\frac{(u(c+\beta\bar{c},d)-u(c,d))}{\beta},\frac{(v(c+\beta\bar{c},d)-v(c,d))}{\beta}$$

and letting $\beta \to 0$ we get

$$\mathcal{L}\begin{pmatrix} \zeta \\ \chi \end{pmatrix} = -\begin{pmatrix} u(c,d)\int_Q \bar{c}v(c,d) \\ 0 \end{pmatrix}. \tag{3.22}$$

□

We have a similar result for the directional derivative of u, v with respect to the control d.

Proposition 3.3 *For c_0 sufficiently large, the mapping*

$$d \mapsto (u(c,d), v(c,d)) \in V^2$$

is differentiable in the sense

$$\frac{u(c,d+\beta\bar{d})-u(c,d)}{\beta} \to \xi \quad \textit{weakly in } V, \tag{3.23}$$

$$\frac{v(c,d+\beta\bar{d})-v(c,d)}{\beta} \to \sigma \quad \textit{weakly in } V, \tag{3.24}$$

as $\beta \to 0$, for any $(c,d) \in [C_\Gamma]^2$ and $\bar{d} \in L^\infty(Q)$ such that $d+\beta\bar{d} \in C_\Gamma$.

Also $(\xi,\sigma) \stackrel{\text{def}}{=} ((\xi(c,d;0,\bar{d}),(\sigma(c,d;0,\bar{d}))$ is the unique solution of

$$\mathcal{L}\begin{pmatrix} \xi \\ \sigma \end{pmatrix} = -\begin{pmatrix} 0 \\ v(c,d)\int_Q \bar{d}u(c,d) \end{pmatrix}. \tag{3.25}$$

with $\xi = \sigma = 0$ *at* $t = 0$ *and* $\xi = \sigma = 0$ *on* Σ.

We present next the result for the second dervatives of u, v with respect to the controls.

Proposition 3.4 *The mapping*

$$c \mapsto (u(c,d), v(c,d)) \in V^2$$

admits second derivatives with respect to c in the sense

$$\frac{\zeta(c+\beta\bar{c}, d; \bar{c}, 0) - \zeta(c, d; \bar{c}, 0)}{\beta} \to \tau \quad \textit{weakly in } V, \tag{3.26}$$

$$\frac{\chi(c+\beta\bar{c}, d; \bar{c}, 0) - \chi(c, d; \bar{c}, 0)}{\beta} \to \eta \quad \textit{weakly in } V, \tag{3.27}$$

as $\beta \to 0$, *for any* $(c,d) \in [C_\Gamma]^2$ *and* $\bar{c} \in L^\infty(Q)$ *such that* $c + \beta\bar{c} \in C_\Gamma$.
Also $(\tau, \eta) \stackrel{\text{def}}{=} ((\tau(c,d;\bar{c},0;\bar{c},0), \eta(c,d;\bar{c},0;\bar{c},0))$ *is the unique solution of*

$$\mathcal{L}\begin{pmatrix} \tau \\ \eta \end{pmatrix} = -2\begin{pmatrix} \zeta\int_Q c\chi + u\int_Q \bar{c}\chi + \zeta\int_Q \bar{c}v \\ \chi\int_Q d\zeta \end{pmatrix}. \tag{3.28}$$

with $\tau = \eta = 0$ *at* $t = 0$ *and* $\tau = \eta = 0$ *on* Σ.

Proof: We denote by $\zeta_\beta, \chi_\beta, \zeta, \chi$ the solutions of system (3.25) corresponding to $(c+\beta\bar{c}, d; \bar{c}, 0)$ and $(c, d; \bar{c}, 0)$ respectively. Using test functions $(\zeta_\beta - \zeta, \chi_\beta - \chi)$ we subtract the (ζ, χ) system from the $(\zeta_\beta, \chi_\beta)$ system

$$\int_Q [(\zeta_\beta - \zeta)_t(\zeta_\beta - \zeta) + a^1_{ij}(\zeta_\beta - \zeta)_{x_i}(\zeta_\beta - \zeta)_{x_j} + b^1_i(\zeta_\beta - \zeta)_{x_i}(\zeta_\beta - \zeta) + c^1(\zeta_\beta - \zeta)^2]$$

$$+ \int_Q [(\chi_\beta - \chi)_t(\chi_\beta - \chi) + a^2_{ij}(\chi_\beta - \chi)_{x_i}(\chi_\beta - \chi)_{x_j}]$$

$$+\int_Q [b_i^2(\chi_\beta-\chi)_{x_i}(\chi_\beta-\chi)+c^2(\chi_\beta-\chi)^2]$$

$$= \tag{3.29}$$

$$-\int_Q(\zeta_\beta-\zeta)\zeta_\beta\int_Q c(v_\beta-v)-\int_Q(\zeta_\beta-\zeta)^2\int_Q cv-\int_Q(\zeta_\beta-\zeta)u_\beta\int_Q c(\chi_\beta-\chi)$$
$$-\int_Q(\zeta_\beta-\zeta)(u_\beta-u)\int_Q c\chi-\int_Q(\zeta_\beta-\zeta)\zeta_\beta\int_Q\beta\bar{c}v_\beta-\int_Q(\zeta_\beta-\zeta)u_\beta\int_Q\beta\bar{c}\chi_\beta$$
$$-\int_Q(\zeta_\beta-\zeta)u_\beta\int_Q\bar{c}(v_\beta-v)-\int_Q(\zeta_\beta-\zeta)(u_\beta-u)\int_Q\bar{c}v-\int_Q(\chi_\beta-\chi)^2\int_Q du_\beta$$
$$-\int_Q(\chi_\beta-\chi)v_\beta\int_Q d(\zeta_\beta-\zeta)-\int_Q(\chi_\beta-\chi)(v_\beta-v)\int_Q d\zeta-\int_Q(\chi_\beta-\chi)\chi\int_Q d(u_\beta-u).$$

Now we carefully estimate the terms appearing in the above expression.

1.

$$\int_Q(\zeta_\beta-\zeta)_t(\zeta_\beta-\zeta)=\frac{1}{2}\int_\Omega(\zeta_\beta-\zeta)^2(x,T)\,dx.$$

2.

$$\int_Q a_{ij}^1(\zeta_\beta-\zeta)_{x_i}(\zeta_\beta-\zeta)_{x_j}\geq\theta\int_Q|\nabla(\zeta_\beta-\zeta)|^2.$$

3.

$$\int_Q b_i^1(\zeta_\beta-\zeta)_{x_i}(\zeta_\beta-\zeta)$$

is transposed to the right hand side and separated by $\epsilon-$ Cauchy inequality.

4.

$$\begin{aligned}\left|\int_Q(\zeta_\beta-\zeta)\zeta_\beta\int_Q c(v_\beta-v)\right| &= \left|\int_Q\left((\zeta_\beta-\zeta)\zeta_\beta\int_Q c(v_\beta-v)(y,\tau)\,dy\,d\tau\right)(x,t)\,dx\,dt\right|\\ &\leq C\int_Q(\zeta_\beta-\zeta)^2(x,t)\,dx\,dt\\ &\quad+C\int_Q\left(\zeta_\beta\int_Q(v_\beta-v)(y,\tau)\,dy\,d\tau\right)^2dx\,dt \qquad (3.30)\\ &\leq C\int_Q(\zeta_\beta-\zeta)^2(x,t)\,dx\,dt\\ &\quad+C\left(\int_Q\zeta_\beta^2\,dx\,dt\right)\left(\int_Q(v_\beta-v)^2\,dy\,d\tau\right). \qquad (3.31)\end{aligned}$$

Notice how the specific form of the non-local term was used to derive (3.31) from (3.30).

5.

$$-\int_Q (\zeta_\beta - \zeta)^2 \int_Q cv \le 0.$$

6.

$$\int_Q (\zeta_\beta - \zeta) u_\beta \int_Q c(\chi_\beta - \chi) \le C \int_Q (\zeta_\beta - \zeta)^2 + C \int_Q (\chi_\beta - \chi)^2.$$

7.

$$\int_Q (\zeta_\beta - \zeta)(u_\beta - u) \int_Q c\chi \le C \int_Q (\zeta_\beta - \zeta)^2 + C \int_Q (u_\beta - u)^2.$$

8.

$$\int_Q (\zeta_\beta - \zeta)\zeta_\beta \int_Q \beta \bar{c} v_\beta \le C \int_Q (\zeta_\beta - \zeta)^2 + C\beta^2 \int_Q \zeta_\beta^2.$$

9.

$$\int_Q (\zeta_\beta - \zeta) u_\beta \int_Q \beta \bar{c} \chi_\beta \le C \int_Q (\zeta_\beta - \zeta)^2 + \beta^2 \int_Q \chi_\beta^2.$$

10.

$$\int_Q (\zeta_\beta - \zeta) u_\beta \int_Q \bar{c}(v_\beta - v) \le C \int_Q (\zeta_\beta - \zeta)^2 + C \int_Q (v_\beta - v)^2.$$

11.

$$\int_Q (\zeta_\beta - \zeta)(u_\beta - u) \int_Q \bar{c} v \le C \int_Q (\zeta_\beta - \zeta)^2 + C \int_Q (u_\beta - u)^2.$$

Similar estimates hold for the terms from "the χ" equation. All the terms of the form above $\int_Q (\zeta_\beta - \zeta)^2$ and $\int_Q (\chi_\beta - \chi)^2$ can be combined with the $c_1 \int_Q (\zeta_\beta - \zeta)^2$ and $c_2 \int_Q (\chi_\beta - \chi)^2$ in equation (3.29). Terms above with ζ_β^2, χ_β^2 are estimated as follows:

$$\left(\int_Q \zeta_\beta^2\right)\left(\int_Q (v_\beta - v)^2\right) + \left(\int_Q \chi_\beta^2\right)\left(\int_Q (u_\beta - u)^2\right) \leq$$

$$\left(\|u_\beta - u\|^2_{L^2(Q)}\| + \|v_\beta - v\|^2_{L^2(Q)}\|\right)\left(\|\zeta_\beta\|^2_{L^2(Q)} + \|\chi_\beta\|^2_{L^2(Q)}\right).$$

Other terms include

$$C\beta^2 \int_Q \zeta_\beta^2,\ C\beta^2 \int_Q \chi_\beta^2$$

and

$$C\int_Q (v_\beta - v)^2,\ C\int_Q (u_\beta - u)^2.$$

Now use the estimate in equation (3.20) to get

$$\left(\|u_\beta - u\|^2_{L^2(Q)} + \|v_\beta - v\|^2_{L^2(Q)}\right) \leq C\beta^2 \|\bar{c}\|^2_{L^2(Q\times Q)}.$$

Using proposition (3.1) with $\alpha = \bar{c}$ and $\beta = 0$ we derive

$$\left(\|\zeta_\beta\|^2_{L^2(Q)} + \|\chi_\beta\|^2_{L^2(Q)}\right) \leq C\|\bar{c}\|^2_{L^2(Q\times Q)}.$$

The above estimates provide an *a priori* bound

$$\left\|\frac{\zeta_\beta - \zeta}{\beta}\right\|^2_V + \left\|\frac{\chi_\beta - \chi}{\beta}\right\|^2_V \leq C\|\bar{c}\|^2_{L^2(Q\times Q)}$$

for the second derivative which proves (3.33) and (3.34). These weak convergences of the quotients justify that η and τ satisfy the weak formulation of the system (3.35). □

Remark 1. The estimates in the above Proposition also give us uniform L^2 bounds for the second derivatives of τ and η. Namely,

$$\|\tau\|_{L^2(Q)} + \|\eta\|_{L^2(Q)} \leq C\|\bar{c}\|^2_{L^2(Q\times Q)}.$$

Remark 2. From the proof of previous proposition,

$$\begin{aligned}
&\frac{u_\beta - u}{\beta} \to \zeta \quad \text{strongly in } L^2(Q), \\
&\frac{v_\beta - v}{\beta} \to \chi \quad \text{strongly in } L^2(Q), \\
&\frac{\zeta_\beta - \zeta}{\beta} \to \tau \quad \text{strongly in } L^2(Q), \\
&\frac{\chi_\beta - \chi}{\beta} \to \eta \quad \text{strongly in } L^2(Q).
\end{aligned} \tag{3.32}$$

We have a similar result for the second derivatives of u and v with respect to the control d.

Proposition 3.5 *The mapping*

$$d \mapsto (u(c,d), v(c,d)) \in V^2$$

admits second derivatives with respect to c in the sense

$$\frac{\zeta(c, d+\beta\overline{d}, 0; \overline{d}) - \zeta(c,d;0,\overline{d})}{\beta} \to \kappa \quad \textit{weakly in } V, \tag{3.33}$$

$$\frac{\chi(c, d+\beta\overline{d}, 0; \overline{d}) - \chi(c,d;0,\overline{d})}{\beta} \to \delta \quad \textit{weakly in } V, \tag{3.34}$$

as $\beta \to 0$, for any $(c,d) \in [C_\Gamma]^2$ and $\overline{d} \in L^\infty(Q)$ such that $d + \beta\overline{d} \in C_\Gamma$.

Also $(\kappa, \delta) \overset{\text{def}}{=} ((\kappa(c,d;0,\overline{d};0,\overline{d}), \delta(c,d;0,\overline{d};0,\overline{d}))$ is the unique solution of

$$\mathcal{L}\begin{pmatrix} \kappa \\ \delta \end{pmatrix} = -2 \begin{pmatrix} \sigma \int_Q c\xi \\ \xi \int_Q d\sigma + v \int_Q \overline{d}\sigma + \xi \int_Q \overline{d}u \end{pmatrix}. \tag{3.35}$$

with $\kappa = \delta = 0$ at $t = 0$ and $\kappa = \delta = 0$ on Σ.

Proposition 3.6 *For a fixed $d \in C_\Gamma$, the mapping $c \in C_\Gamma \mapsto \mathcal{J}(c,d)$ is strictly convex, provided c_0 is sufficiently large.*

Proof: As mentioned earlier, it suffices to show that $J''(\nu) > 0$ for $\nu \in [0,1]$.

The justification for differentiating J is a consequence of the above established first and second derivatives of u, v with respect to the control variable c and the strong convergence noted in the previous proposition. Now, for $0 \leq \nu \leq 1$,

$$J(\nu) = \mathcal{J}(\bar{c} + \nu(c - \bar{c}), d).$$

The directional derivative is now in the direction $c - \bar{c}$.

Denoting

$$u = u(\bar{c} + \nu(c - \bar{c}), d),$$

$$v = v(\bar{c} + \nu(c - \bar{c}), d),$$

$$\zeta = \zeta(\bar{c} + \nu(c - \bar{c}), d; c - \bar{c}, 0),$$

$$\chi = \chi(\bar{c} + \nu(c - \bar{c}), d; c - \bar{c}, 0),$$

$$\tau = \chi(\bar{c} + \nu(c - \bar{c}), d; c - \bar{c}, 0; c - \bar{c}, 0),$$

$$\eta = \eta(\bar{c} + \nu(c - \bar{c}), d; c - \bar{c}, 0; c - \bar{c}, 0),$$

$$J(\nu) = \int_Q \left\{K[u - \tilde{u}]^2 - L[v - \tilde{v}]^2\right\} + \int_Q \int_Q \left\{N(\bar{c} + \nu(c - \bar{c}))^2 - Md^2\right\}.$$

Differentiating twice with respect to c

$$\begin{aligned} J''(\nu) &= \int_Q (K\zeta^2 + K[u - \tilde{u}]\tau - L[v - \tilde{v}]\eta - L\chi^2) \\ &\quad + \int_Q \int_Q N(c - \bar{c})^2. \end{aligned} \tag{3.36}$$

$$
\begin{aligned}
J''(\nu) &\geq -K\|u\|_{L^2(Q)}\|\tau\|_{L^2(Q)} - K\|\tilde{u}\|_{L^2(Q)}\|\tau\|_{L^2(Q)} \\
&- L\|\chi\|^2_{L^2(Q)} - L\|v\|_{L^2(Q)}\|\eta\|_{L^2(Q)} \\
&- L\|\tilde{v}\|_{L^2(Q)}\|\eta\|_{L^2(Q)} + N\|c-\bar{c}\|^2_{L^2(Q)}.
\end{aligned}
$$

From proposition 3.5, for $\epsilon > 0$ there exists $c_0(\epsilon)$ such that for $c_k > c_0$, $k = 1, 2$,

$$\|\tau\|_{L^2(Q)} + \|\eta\|_{L^2(Q)} \leq \epsilon\|c-\bar{c}\|^2_{L^2(Q\times Q)}$$

and

$$\|\chi\|^2_{L^2(Q)} \leq \epsilon\|c-\bar{c}\|^2_{L^2(Q\times Q)}.$$

Combining these estimates with above we get

$$J''(\nu) > (N-\tilde{\epsilon})\|c-\bar{c}\|^2_{L^2(Q\times Q)}.$$

□

Proposition 3.7 *For a fixed $d \in C_\Gamma$ the mapping $c \in C_\Gamma \mapsto \mathcal{J}(c,d)$ is lower semicontinuous in the weak topology on $L^2(Q \times Q)$.*

Proof: It is enough to show for every $\alpha \in \mathbf{R}$,

$$S(d,\alpha) = \{h | h \in C_\Gamma, \mathcal{J}(h,d) \leq \alpha\}$$

is closed in the weak topology of $L^2(Q \times Q)$. Let $d \in C_\Gamma$ and $\alpha \in \mathbf{R}$ be fixed such that

$$\mathcal{J}(c_n, d) \leq \alpha$$

and

$$c_n \to \hat{c} \text{ weakly in } L^\infty(Q \times Q).$$

Using the state systems, $u_n(c_n, d), v_n(c_n, d)$ satisfy

$$\|u_n\|_V, \|v_n\|_V \leq C.$$

Then, using compactness results [7, Chapter 4, Prop. 4.2] , we can find subsequences such that

$$u_n \to u \qquad \text{weakly in } V, \text{ strongly in } L^2(Q)$$

$$v_n \to v \qquad \text{weakly in } V, \text{ strongly in } L^2(Q).$$

Standard continuity arguments show that

$$u = u(\hat{c}, d) \qquad v = v(\hat{c}, d).$$

Also using a generalization of Fatou's lemma,

$$\liminf \mathcal{J}(c_n, d) \geq \mathcal{J}(\hat{c}, d).$$

□

Theorem 3.1 *If c_0 is large enough, there exists a unique saddle point* (c^*, d^*).

Proof: Combining Propostion 3.6 and Proposition 3.7 and the existence of saddle point result from Ekeland and Temam [1, Chap.6, Propositions 1.5 and 2.1], we conclude that the cost functional admits a unique saddle point. □

4 The Optimality System

The solution of the optimality system, consisting of the two state equations and two suitably chosen adjoint equations, will be used to characterize the saddle point of the game.

Theorem 4.1 *If $(c,d) \in [C_\Gamma]^2$ is the saddle point and c_0 is sufficiently large, then there exists $(u,v,p,q) \in V^4$ satisfying:*

$$\begin{aligned} L_1u + u\int_Q cv &= f \\ L_2v + v\int_Q du &= g \\ L_1^*p + p\int_Q cv - \int_Q d^T vq &= K(u-\tilde{u}) \\ L_2^*q + q\int_Q du - \int_Q c^T up &= -L(v-\tilde{u}) \quad in\ Q \end{aligned} \tag{4.37}$$

$$\begin{aligned} u(x,t) = u^0, v(x,t) &= v^0 \quad on\ \Omega \times \{0\} \\ u(x,t) = v(x,t) &= 0 \qquad on\ \Sigma \\ p(x,T) = q(x,T) &= 0 \qquad on\ \Omega \times T \\ p(x,t) = q(x,t) &= 0 \qquad on \Sigma, \end{aligned} \tag{4.38}$$

where

$$L_k^*u = -u_t - (a_{ij}^k u_{x_j})_{x_i} - (b_i^k u)_{x_i} + c^k u, \ k = 1,2.$$

Moreover on Q,

$$c(x,y,t,\tau) = \min(\frac{p^+(x,t)u(x,t)v(y,\tau)}{N}, \Gamma),$$

$$d(x,y,t,\tau) = \min(\frac{q^+(x,t)u(y,\tau)v(x,t)}{M}, \Gamma),$$

where $p^+ = max(p,0)$.

Proof: Let $(c, d) \in [C_\Gamma]^2$ be a saddle point. Choose $\bar{c} \in L^\infty(Q \times Q)$ in such a way that for $\beta > 0$ arbitrarily small, $c + \beta\bar{c}$ lies in the set C_Γ. Since (c, d) is a saddle point,

$$\lim_{\beta \to 0} \frac{\mathcal{J}(c + \beta\bar{c}, d) - \mathcal{J}(c, d)}{\beta} \geq 0. \tag{4.39}$$

Substituting the explicit form of the cost functional in (4.39), dividing by β, and noting $\frac{u_\beta - u}{\beta} \to \zeta$ strongly in $L^2(Q)$, and $u_\beta \to u$, we get

$$\int_Q (K(u - \tilde{u})\zeta - L(v - \tilde{v})\chi)\, dx\, dt + \int_Q \int_Q N c \bar{c}\, dx dy\, dt d\tau \geq 0. \tag{4.40}$$

We introduce a new notation:

$$d^T(x, y, t, \tau) := d(y, x, \tau, t),\ c^T(x, y, t, \tau) := c(y, x, \tau, t).$$

Now we define an operator $\mathcal{L}^*$ such that **formally**

$$(p, q)\mathcal{L} \begin{pmatrix} \zeta \\ \\ \chi \end{pmatrix} = (\zeta, \chi)\mathcal{L}^* \begin{pmatrix} p \\ \\ q \end{pmatrix}.$$

We define the adjoint functions (p, q) as the solutions in V of

$$\begin{aligned}
L_1^* p + p \textstyle\int_Q cv - \int_Q d^T vq &= K(u - \tilde{u}), && \text{in } Q \\
L_2^* q + q \textstyle\int_Q du - \int_Q c^T up &= -L(v - \tilde{v}), && \\
p(x, T) = q(x, T) &= 0, && \text{on } \Omega \times T \\
p(x, t) = q(x, t) &= 0, && \text{on } \Sigma.
\end{aligned} \tag{4.41}$$

The solution of the above system, after a change of variable $\hat{p}(x, t) = p(x, T - t)$ and $\hat{q}(x, t) = q(x, T - t)$, is constructed in a manner similar to that of the solution of the original state system. Substituting (4.41) in (4.40), we get

$$\int_Q (\zeta, \chi)\mathcal{L}^* \begin{pmatrix} p \\ q \end{pmatrix} + \int_Q \int_Q N c\bar{c} \geq 0$$

Now, from (3.25)

$$\int_Q (p, q)\mathcal{L} \begin{pmatrix} \zeta \\ \chi \end{pmatrix} + \int_Q \int_Q N c\bar{c} = \int_Q (p, q) \begin{pmatrix} -u \int_Q \bar{c}v \\ 0 \end{pmatrix} + \int_Q \int_Q N c\bar{c} \geq 0$$

This implies

$$\int_Q \int_Q (Nc - puv)\bar{c} \geq 0. \tag{4.42}$$

Since we can choose $\bar{c}$ non-negative and arbitrary, this implies

$$Nc - puv \geq 0.$$

On the set $\{(x, y, t, \tau) | c(x, y, t, \tau) = 0\}$, using $\bar{c} \geq 0$ with support on that set, we get $puv \leq 0$ which gives

$$p^+ = 0.$$

On the set $\{(x, y, t, \tau) | 0 < c(x, y, t, \tau) < \Gamma\}, \bar{c}$ has arbitrary sign with support on that set, which implies $Nc - puv = 0$, $p \geq 0$ and then

$$c = \frac{p^+ uv}{N}.$$

On the set $\{(x, y, t, \tau) | c(x, y, t, \tau) = \Gamma\}, \bar{c}$ must be non-positive with support on that set , which gives

$$Nc - puv \leq 0,$$

and

$$\Gamma \leq \frac{puv}{N}.$$

Combining these results we get

$$c(x,y,t,\tau) = \min(\frac{p^+(x,t)u(x,t)v(y,\tau)}{N}, \Gamma).$$

Similarly,

$$d(x,y,t,\tau) = \min(\frac{q^+(x,t)u(y,\tau)v(x,t)}{M}, \Gamma).$$

$\square$

Theorem 4.2 *For c_0 sufficiently large, bounded solutions of the optimality system:*

$$\begin{aligned} L_1 u + u \int_Q min(\tfrac{p^+uv}{N}, \Gamma) v &= f \\ L_2 v + v \int_Q min(\tfrac{q^+uv}{M}, \Gamma) u &= g \\ L_1^* p + p \int_Q min(\tfrac{p^+uv}{N}, \Gamma) v - \int_Q min(\tfrac{q^+uv}{M}, \Gamma)^T v q &= K(u - \tilde{u}) \\ L_2^* q + q \int_Q min(\tfrac{q^+uv}{M}, \Gamma) u - \int_Q min(\tfrac{p^+uv}{N}, \Gamma)^T u p &= -L(v - \tilde{u}) \quad in\ Q \end{aligned} \tag{4.43}$$

$$\begin{aligned} u(x,t) = u^0, v(x,t) &= v^0 \quad on\ \Omega \times 0 \\ u(x,t) = v(x,t) &= 0 \qquad on\ \Sigma \\ p(x,T) = q(x,T) &= 0 \quad on\ \Omega \times T \\ p(x,t) = q(x,t) &= 0 \qquad on\ \Sigma. \end{aligned} \tag{4.44}$$

exist and are unique in the solution space $[V]^4$.

Proof: The existence of the saddle point implies the existence of u, v and then the existence of p, q. The optimality system for a strictly convex-concave functional completely characterizes its saddle points $\square$

5 Summary

We have proved that a two person zero sum game described by a system of parabolic equations with competitive interactions can be controlled via the non-local kernels of the interacting terms, and the saddle point can be represented in terms of the optimality system.

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PART III

Application of Optimal Control Theory

to

In Situ Bioremediation

Abstract

In situ bioremediation is a remediation technology in which the indigenous subsurface bacteria are stimulated by injecting compounds to provide food and energy. The stimulated bacteria break down the target contaminants into less harmful substances. The way the compounds are injected is a crucial component of the technology. We use techniques from the theory of optimal control of distributed parameter systems to characterize an "optimal" injection function. The state system, the set of equations that govern the the evolution of bioremediation, is a "hybrid" system consisting of both partial and ordinary differential equations.

1 Introduction

In situ bioremediation is a technology for cleaning up subsurface environments contaminated with hazardous materials. Despite the fact that the United States government has spent billions of dollars in environment restoration recent studies have shown, for e.g., that no polluted groundwater site has been restored to conditions fit for drinking [16]. This has fuelled a search for other, less costly, more efficient and safer technologies, among them, in situ bioremediation [16, 17]. Bacteria, microscopic microorganisms that are virtually found everywhere, are the key players in bioremediation. Microorganisms possess enzymes which use environmental contaminants as food and enable the breakdown of the contaminants. Since most of the contaminants of interest to environmentalists are man made, it is a matter of speculation and intense scientific research to determine which bacteria will prey upon which hazardous contaminant.

Organic contaminants undergo microbial transformation because they (the contaminants) are a source of carbon, the basic building block for new cells, and electrons. The transfer of electrons from an electron donor(usually an organic compound) to an electron acceptor(usually oxygen) is accompanied by a release of energy which is used by organisms to multiply(metabolism). For example, under proper conditions metabolism will transform hazardous carbon tetrachloride (CCl_4) to carbon dioxide (CO_2). The electron donor and the electron acceptor are collectively referred to as the *primary substrates.* When the electron acceptor is oxygen, the process is called *aerobic.* When another element besides oxygen plays the role of an electron acceptor the process is referred to as *anaerobic.* A variant of bioremediation in which the contaminant undegoes degradation even though it cannot serve as the primary source of energy and some other compound supplies energy is called *cometabolism*[16, 11].

Plutonium recovery processes carried out at the Department of Energy Hanford site resulted in the discharge of CCl_4 into the surrounding environment. Concentrations of up to 1000 times Environmental Protection Agency's(EPA) drinking water standard of 5 ppb have been measured in the groundwater. In situ bioremediation is one technology that is being developed at Hanford to meet the need for cost effective methods to destroy CCl_4 [16].

The process by which CCl_4 undergoes biodegradation is cometabolic and anaerobic. Criddle *et al.* [1] have identified the bacterial species *Psuedomonas* as capable of destroying CCl_4 with *acetate* as the electron donor and *nitrate* as the terminal electron acceptor.

Despite many attractive features, fundamental technical constraints must be overcome to fully exploit the benefits of in situ bioremediation. One such constraint is the biofouling of nutrient addition wells. For instance, since the process of degradation of CCl_4 is cometabolic, large amounts of electron donor and electron acceptor have to be injected into the subsurface environment. This can result in rapid microbial growth where the nutrient concentration is highest, i.e., next to the source of injection of the nutrients. Large amounts of biomass will likely clog the injection wells and prevent further remediation. This phenomenon has been observed both in laboratory and field tests[15]. Since the installation of wells constitutes a major portion of the capital costs associated with bioremediation, a carefully designed nutrient addition strategy, that would prevent clogging and allow for the free flow of nutrients across the contaminated site, is crucial for the successful implementation of the technology. We propose to use methods from the theory of optimal control of distributed parameter systems [8, 6, 7], to design a "smart" nutrient addition strategy.

The mathematical model used to determine the effects of various nutrient addition strategies is a simplified version of the model developed by Semprini, *et al* [15]. and modified by Hooker *et. al* [3].

Semprini *et al* [15] developed a model for bioremediation in a tube filled with soil, bacteria, carbon tetrachloride and nutrients. The model has five partial differential equations (PDEs), which are one dimensional in space and four ordinary differential equations (ODEs). The PDEs represent the quantities that can diffuse - acetate, nitrate, second electron donor, carbon tetrachloride and degradation intermediates. The ODEs represent the sorbed quantities that are not transported through the soil - two bacteria biomass populations, sorbed carbon tetrachloride and sorbed degradation intermediates. Hooker *et. al* [3], from Pacific Northwest Laboratory, successfully implemented an optimization procedure designed to choose an "optimal" pulsing pattern for the input of acetate. They solved numerically the nine equation system repeatedly, adjusting the input to minimize the bacteria growth near the inlet. Their technique of "discretizing and then optimizing" with repeated solving of a large system would be difficult to implement for three spatial variables. Our approach, "optimize first on the PDE/ODE system and then discretize" should extend to three spatial dimensions.

Our approach is to apply "control of PDEs" techniques first and then solve only once the resulting optimality system (which is the original system coupled with the adjoint system). We demonstrate this approach here on a simplified model with three PDEs and one ODE. The simplifed model was developed by Lenhart, James Petersen and Rodney Skeen.

Note also that optimal control of this type of hybrid system - PDEs strongly coupled with ODE - is quite unusual in itself. The work on control of hybrid systems is just beginning to be developed.

Nutrients and contaminants are assumed to be injected at the entrance of the flow field, which is assumed to be one dimensional of length L. The process of biological degradation of the contaminants, consumption of the nutrients and the associated microbial growth are described mathematically. Finally it is assumed that the transformed products flow out at the exit of the flow field. The effects of advection, dispersion and sorption in the porous medium are included in the model. In this model we assume that only one microbial population is involved and we ignore the effects of the intermediate products which are likely to be created during the process of biological degradation. The transformation of the CCl_4 is assumed to be governed by Monod kinetics which accounts for the specific interaction terms that appear in the model. Finally it is assumed that the bacteria biomass attaches itself to the soil and is thus immobile [16, 15].

To summarize we assume that we have one electron donor, acetate, one electron acceptor, nitrate and one microbial population. Transport equations govern the flow of the primary substrates, the biomass is immobile and all metabolism and degradation processes are governed by Monod kinetics.

With the above assumptions, the transport equations are as follows [16] :

$$\begin{aligned}
\frac{\partial u}{\partial t} &= d_h \frac{\partial^2 u}{\partial^2 x} - \nu \frac{\partial u}{\partial x} + r_u, \\
\frac{\partial v}{\partial t} &= d_h \frac{\partial^2 v}{\partial^2 x} - \nu \frac{\partial v}{\partial x} + r_v, \\
\frac{\partial w}{\partial t} &= d_h \frac{\partial^2 w}{\partial^2 x} - \nu \frac{\partial w}{\partial x} + r_w, \qquad (1.1)
\end{aligned}$$

where u, v and w are the concentrations of the acetate, nitrate and the contaminant CCl_4 respectively. Here d_h is the hydrodynamic dispersion coefficient and ν is the convective velocity of water through the porous media.

Since the biomass is assumed to be immobile, an ordinary differential equation governs its evolution :

$$\frac{dX}{dt} = r_X, \tag{1.2}$$

where X is the concentration of the biomass [16].

The reaction terms r_u, r_v, r_w and r_X are as follows [3]:

$$r_u = -\frac{.25\mu_1 vX}{1+\frac{k_1}{u}} - \frac{3.5\mu_2 vX}{1+\frac{k_2}{u}+\frac{u}{k_3}}, \tag{1.3}$$

$$r_v = -\frac{\mu_1 vX}{1+\frac{k_1}{u}} - \frac{\mu_2 vX}{1+\frac{k_2}{u}+\frac{u}{k_3}}, \tag{1.4}$$

$$r_w = -k_3 wX, \tag{1.5}$$

$$r_X = \frac{\mu_2 vX}{1+\frac{k_2}{u}+\frac{u}{k_3}} - \frac{k_4 X}{k_5+X}. \tag{1.6}$$

The above terms are at a slight variance from those that appear in Hooker *et al.* [3], due to our simplifying assumption of ignoring the effects of any intermediate products that might be created during the degradation processes.

Our aim is to design a nutrient addition strategy that will dampen the excessive growth of the bacteria at the injection point and at the same time minimize the concentration of carbon tetrachloride at the end of a certain predetermined time period T. We propose to do this by fixing the input flow of the nitrate and the carbon tetrachloride into the flow field and varying the flow of the acetate solution. The flow of the acetate will be our control. Thus boundary conditions at the end points are,

at $x = 0$,

$$-d_h u_x + \nu u = \nu g_1(t), \tag{1.7}$$

$$-d_h v_x + \nu v = \nu g_2(t), \tag{1.8}$$

$$-d_h w_x + \nu w = \nu g_3(t), \tag{1.9}$$

and at $x = L$,

$$u_x = 0, \tag{1.10}$$

$$v_x = 0, \tag{1.11}$$

$$w_x = 0, \tag{1.12}$$

where $g_1(t), g_2(t)$ and $g_3(t)$ are the rate of injection of acetate, nitrate and carbon tetrachloride respectively. A suitable objective functional, the quantity that will measure the perfomance of the nutrient addition strategy, is of the form

$$A \int_Q X(x,t)\phi(x)\,dx\,dt + B \int_0^L w(x,T)\,dx + \frac{1}{2}\int_0^T g_1^2(t)\,dt.$$

where

$$\phi(x) = \begin{cases} \frac{1}{exp(-10)} exp(\frac{1}{(x^2-0.1)}) & 0 \leq x < 0.1 \\ 0 & x \geq 0.1 \end{cases} \tag{1.13}$$

The function $\phi(x)$ is similar to the standard mollifier and we use it to limit the effect of the first term of the objective functional near the injection point of the nutrients. The last term represents the "cost" of exercising the choice of the acetate injection function. A and B are suitable positive constants, weights, assigned to reflect the different needs of each experiment. For example, increasing A means that more emphasis is being placed on reducing the concentration of the microbial population at the injection point.

The paper is organized as follows: In section 2 we formally state the problem and set down the notation. In section 3 we prove the existence and uniqueness of solutions of the *state system*, the set of equations governing the evolution of the degradation process. In section 4 we prove the existence of the *optimal control.* In section 5 the optimal control is characterized in terms of the *optimality system* which consists of the state system and a suitably chosen *adjoint system.* In section 6 the uniqueness of the optimality system is proven for "small" time. In section 7 we use an explicit finite difference scheme to discretize the optimality system coupled with an iteration scheme and get a concrete profile of the optimal injection function. The adjoint system is a "backward" system with data at the final time. Thus the state system and the adjoint system have opposite time orientations and all the equations cannot be " marched forward in time" together. An iteration scheme of solving alternatively the state system forward in time and the adjoint system backwards in time is implemented. We compare this result with that obtained by Petersen *et al.*[17] using numerical optimization. We close in section 8 with a few comments.

2 Statement of the Problem

For $M > 0$ define the control set,

$$C_M = \{g \in L^\infty_+[0,T] \mid \|g\|_\infty \leq M\}.$$

For any $g \in C_M$ define the quadruple

$$(u, v, w, X) = (u(g), v(g), w(g), X(g))$$

as a solution of the *state system*

$$u_t - d_h u_{xx} + \nu u_x = -\frac{e\mu_1 vX}{1+\frac{k_1}{u}} - \frac{f\mu_2 vX}{1+\frac{k_2}{u}+\frac{u}{k_3}}, \qquad \text{for } (x,t) \in Q = (0,L) \times (0,T)$$

$$v_t - d_h v_{xx} + \nu v_x = -\frac{\mu_1 vX}{1+\frac{k_1}{u}} - \frac{\mu_2 vX}{1+\frac{k_2}{u}+\frac{u}{k_3}},$$

$$w_t - d_h w_{xx} + \nu w_x = -k_3 wX,$$

$$\frac{dX}{dt} = \frac{\mu_2 vX}{1+\frac{k_2}{u}+\frac{u}{k_3}} - \frac{k_4 X}{k_5 + X}, \qquad (x \in [0,L], t > 0)$$

$$-d_h u_x(0,t) = \nu(g(t) - u(0,t)), \quad u_x(L,t) = 0,$$

$$-d_h v_x(0,t) = \nu(g_1(t) - v(0,t)), \quad v_x(L,t) = 0,$$

$$-d_h w_x(0,t) = \nu(g_2(t) - w(0,t)), \quad w_x(L,t) = 0,$$

$$u(x,0) = U_0(x),\ v(x,0) = V_0(x),\ w(x,0) = W_0(x),$$

$$X(x,0) = X_0(x), \tag{2.14}$$

where k_i, $i = 1, \ldots 5$, d_h, ν, μ_1, μ_2, e, f are positive constants. The boundary functions $g_1(t)$ and $g_2(t)$ are positive fixed functions. The **cost functional** is

$$\mathcal{J}(g) = A \int_Q X(x,t)\phi(x)\, dx\, dt + B \int_0^L w(x,T)\, dx + \frac{1}{2}\int_0^T g^2(t)\, dt,$$

where A and B are positive constants. We define the optimal control g^* as an element in the set C_M such that

$$\mathcal{J}(g^*) = \min_{g \in C_M} \mathcal{J}(g).$$

We need the following assumptions:

$$U_0(x), V_0(x), W_0(x), X_0(x) \in L^2[0,L]. \tag{2.15}$$

By a change of notation we simplify the presentation of the state system (2.14).

1. Define an operator L such that $Lu = u_t - d_h u_{xx} + \nu u_x$.

2. Rewrite, $-\frac{e\mu_1 v X}{1+\frac{k_1}{u}} - \frac{f\mu_2 v X}{1+\frac{k_2}{u}+\frac{u}{k_3}}$ as $-\frac{e\mu_1 uvX}{k_1+u} - \frac{fk_3\mu_2 uvX}{k_2k_3+k_3u+u^2}$.

3. Set $R_1(u,v,X) = \frac{\mu_1 uvX}{k_1+u}$.

4. Set $R_2(u,v,X) = \frac{k_3\mu_2 uvX}{k_2k_3+k_3u+u^2}$.

5. Set $F(u,v,X) = -eR_1(u,v,X) - fR_2(u,v,X)$.

6. Set $G(u,v,X) = -R_1(u,v,X) - R_2(u,v,X)$.

7. Set $H(w,X) = -k_3 wX$.

8. Set $M(u,v,X) = R_2(u,v,X) - \frac{k_4 X}{k_5+X}$.

9. In the new notation defined above the state system now appears as

$$\begin{aligned}
Lu &= F(u,v,X),\\
Lv &= G(u,v,X),\\
Lw &= H(w,X),\\
\tfrac{dX}{dt} &= M(u,v,X),
\end{aligned} \tag{2.16}$$

   with the appropriate boundary and initial conditions.

10. Set $H = L^2[0,T,H^1(0,L)]$.

11. We will look for solution for the state system in the space

$$V = (H)^3 \times L^2(Q).$$

Define the bilinear form on H,

$$a(u, \phi, t) = d_h \int_0^L u_x \phi_x + \nu \int_0^L u_x \phi.$$

Definition of weak solution:

(u, v, w, X) solve the state system if for any $(\phi, \psi, \chi) \in (H)^3$

$$\begin{aligned}
\textstyle\int_0^T < u_t, \phi > + \int_0^T a(u, \phi, t) = &\quad \textstyle\int_Q F(u, v, X)\phi + \nu \int_0^T (g(t) - u(0,t))\phi(0,t), \\
\textstyle\int_0^T < v_t, \psi > + \int_0^T a(v, \psi, t) = &\quad \textstyle\int_Q G(u, v, X)\psi + \nu \int_0^T (g_1(t) - v(0,t))\psi(0,t), \\
\textstyle\int_0^T < w_t, \chi > + \int_0^T a(w, \chi, t) = &\quad \textstyle\int_Q H(w, X)\chi + \nu \int_0^T (g_2(t) - w(0,t))\chi(0,t), \\
X(x,t) = &\quad \textstyle X_0(x) + \int_0^t M(u, v, X)(x, s)\, ds \quad x \in [0, L],
\end{aligned} \tag{2.17}$$

where $<,>$ denotes the duality between $(H^1(0,L))^*$ and $H^1(0,L)$.

Since $u(x,t), v(x,t) \in L^2[0,T,H^1(0,L)]$, $u(x,.), v(x,.) \in L^2[0,T]$. Thus the integral representation of X(x,t) is well defined.

3 Existence and Uniqueness of the State System

We begin by showing that F, G, H and M are Lipschitz. Then the uniqueness of the state system is proved. We then show existence for a modified state system and finally we use limit arguments to show that the solutions of the modified system converge to the solution of the original system.

Proposition 3.1 *If u, v, w and X are positive and take values in a bounded set, then F, G, H and M as defined above are Lipschitz.*

Proof: We will show that F is Lipschitz, the others follow similarly. The partial derivatives of F with respect to u, v and X are bounded, hence

$$\begin{aligned}
F(u,v,X)-F(\bar{u},\bar{v},\bar{X}) &= -\frac{e\mu_1 uvX}{k_1+u}-\frac{fk_3\mu_2 uvX}{k_2k_3+k_3u+u^2}+\frac{e\mu_1\bar{u}\bar{v}\bar{X}}{k_1+\bar{u}}+\frac{fk_3\mu_2\bar{u}\bar{v}\bar{X}}{k_2k_3+k_3\bar{u}+\bar{u}^2} \\
&= -\frac{e\mu_1 uvX}{k_1+u}+\frac{e\mu_1\bar{u}vX}{k_1+u}-\frac{e\mu_1\bar{u}vX}{k_1+u}+\frac{e\mu_1\bar{u}\bar{v}X}{k_1+u} \\
&\quad -\frac{e\mu_1\bar{u}\bar{v}X}{k_1+u}+\frac{e\mu_1\bar{u}\bar{v}\bar{X}}{k_1+u}-\frac{e\mu_1\bar{u}\bar{v}\bar{X}}{k_1+u}+\frac{e\mu_1\bar{u}\bar{v}\bar{X}}{k_1+\bar{u}} \\
&\quad -\frac{fk_3\mu_2 uvX}{k_2k_3+k_3u+u^2}+\frac{fk_3\mu_2\bar{u}vX}{k_2k_3+k_3u+u^2}-\frac{fk_3\mu_2\bar{u}vX}{k_2k_3+k_3u+u^2} \\
&\quad +\frac{fk_3\mu_2\bar{u}\bar{v}X}{k_2k_3+k_3u+u^2}-\frac{fk_3\mu_2\bar{u}\bar{v}X}{k_2k_3+k_3u+u^2}+\frac{fk_3\mu_2\bar{u}\bar{v}\bar{X}}{k_2k_3+k_3u+u^2} \\
&\quad -\frac{fk_3\mu_2\bar{u}\bar{v}\bar{X}}{k_2k_3+k_3u+u^2}+\frac{fk_3\mu_2\bar{u}\bar{v}\bar{X}}{k_2k_3+k_3\bar{u}+\bar{u}^2}.
\end{aligned}$$

Therefore

$$|F(u,v,X)-F(\bar{u},\bar{v},\bar{X})| \le C\{|u-\bar{u}|+|v-\bar{v}|+|X-\bar{X}|\}.$$

where C is a constant depending on the constant coefficients and the range of the bounded set of the state variables. □

Now we will prove the uniqueness of solution of the state system. We will first show that the solution is unique for "small" time T and then use a "stacking" argument to prove uniqueness for arbitrarily large but finite time.

Theorem 3.1 *If the solution of the state system exists and is bounded then it is unique.*

Proof Substituting $ue^{\lambda t}, ve^{\lambda t}, we^{\lambda t}$ and $Xe^{\lambda t}$ instead of u, v, w and X, we can, without loss of generality, consider the system

$$\begin{aligned} Lu + \lambda u &= F(ue^{\lambda t}, ve^{\lambda t}, Xe^{\lambda t})e^{-\lambda t}, \\ Lv + \lambda v &= G(ue^{\lambda t}, ve^{\lambda t}, Xe^{\lambda t})e^{-\lambda t}, \\ Lw + \lambda w &= H(we^{\lambda t}, Xe^{\lambda t})e^{-\lambda t}, \\ \tfrac{dX}{dt} + \lambda X &= M(ue^{\lambda t}, ve^{\lambda t}, Xe^{\lambda t})e^{-\lambda t}. \end{aligned} \tag{3.18}$$

with the appropriate boundary and initial conditions.

Suppose (u, v, w, X) and $(\bar{u}, \bar{v}, \bar{w}, \bar{X})$ are two solutions of (3.18). Use test functions $(u - \bar{u}, v - \bar{v}, w - \bar{w})$ for the u, v, w and $\bar{u}, \bar{v}, \bar{w}$ equations and multiply the X and $\bar{X}$ equations by $X - \bar{X}$. Subtracting the "u" system from the "$\bar{u}$" system and integrating over Q we get

$$\begin{aligned} &\textstyle\int_0^T < (u-\bar{u})_t, u - \bar{u} > + \\ &\textstyle\int_0^T a((u-\bar{u}), (u-\bar{u}), t) + \lambda \int_Q (u-\bar{u})^2 \;=\; \int_Q F(ue^{\lambda t}, ve^{\lambda t}, Xe^{\lambda t})e^{-\lambda t}(u-\bar{u}) \\ &\qquad\qquad - \textstyle\int_Q F(\bar{u}e^{\lambda t}, \bar{v}e^{\lambda t}, \bar{X}e^{\lambda t})e^{-\lambda t}(u-\bar{u}), \end{aligned} \tag{3.19}$$

$$\begin{aligned} &\textstyle\int_0^T < (v-\bar{v})_t, v - \bar{v} > + \\ &\textstyle\int_0^T a((v-\bar{v}), (v-\bar{v}), t) + \lambda \int_Q (v-\bar{v})^2 \;=\; \int_Q G(ue^{\lambda t}, ve^{\lambda t}, Xe^{\lambda t})e^{-\lambda t}(v-\bar{v}) \\ &\qquad\qquad - \textstyle\int_Q G(\bar{u}e^{\lambda t}, \bar{v}e^{\lambda t}, \bar{X}e^{\lambda t}))e^{-\lambda t}(v-\bar{v}), \end{aligned} \tag{3.20}$$

$$\int_0^T < (w-\bar{w})_t, w-\bar{w} > +$$

$$\begin{aligned}
\int_0^T a((w-\bar{w}),(w-\bar{w}),t) + \lambda \int_Q (w-\bar{w})^2 &= \int_Q H(we^{\lambda t}, Xe^{\lambda t})e^{-\lambda t}(w-\bar{w}) \\
&- \int_Q H(\bar{w}e^{\lambda t}, \bar{X}e^{\lambda t}))e^{-\lambda t}(w-\bar{w}),
\end{aligned}$$

$$\begin{aligned}
\int_Q (X-\bar{X})_t(X-\bar{X}) + \lambda \int_Q (X-\bar{X})^2 &= \int_Q (M(ue^{\lambda t}, ve^{\lambda t}, Xe^{\lambda t})e^{-\lambda t}(X-\bar{X}) \\
&- \int_Q M(\bar{u}e^{\lambda t}, \bar{v}e^{\lambda t}, \bar{X}e^{\lambda t})e^{-\lambda t}(X-\bar{X}).
\end{aligned} \tag{3.21}$$

Since u, v and X are bounded and $M(u,v,X)$ is a bounded function of u, v and X, we have, for each $x, X(x,t)$ absolutely continuous in t. This implies X_t exists a.e. and $X_t(x,t) \in L^2(Q)$.

Define $Q_1 = [0,L] \times (0,T_1)$, for $0 \le T_1 \le T$. Using the fact that

$$\int_{Q_1} uu_t = \frac{1}{2}\int_0^L u^2(x,T_1) - \frac{1}{2}\int_0^L u^2(x,0)$$

and F, G, H and M are Lipschitz, one arrives, after standard manipulations, at the following set of inequalities.

$$\begin{aligned}
\frac{1}{2}\int_0^L (u-\bar{u})^2(x,T_1) + \frac{d_h}{2}\int_{Q_1}(u-\bar{u})_x^2 &+ (\lambda - \frac{\nu^2}{2d_h} - C_1 e^{4\lambda T_1})\int_{Q_1}(u-\bar{u}^2) \\
&\le C_2\left(\int_{Q_1}(v-\bar{v})^2 + \int_{Q_1}(X-\bar{X})^2\right). \\
\frac{1}{2}\int_0^L (v-\bar{v})^2(x,T_1) + \frac{d_h}{2}\int_{Q_1}(v-\bar{v})_x^2 &+ (\lambda - \frac{\nu^2}{2d_h} - C_1 e^{4\lambda T_1})\int_{Q_1}(v-\bar{v})^2 \\
&\le C_2\left(\int_{Q_1}(u-\bar{u})^2 + \int_{Q_1}(X-\bar{X})^2\right). \\
\frac{1}{2}\int_0^L (w-\bar{w})^2(x,T_1) + \frac{d_h}{2}\int_{Q_1}(w-\bar{w})_x^2 &+ (\lambda - \frac{\nu^2}{2d_h} - C_1 e^{2\lambda T_1})\int_{Q_1}(w-\bar{w}^2) \\
&\le C_2\int_{Q_1}(X-\bar{X})^2.
\end{aligned}$$

$$\frac{1}{2}\int_0^L (X-\bar{X})^2(x,T_1) \quad + \quad (\lambda - C_1 e^{4\lambda T_1})\int_{Q_1}(X-\bar{X})^2$$

$$\leq \quad C_2\left(\int_{Q_1}(u-\bar{u})^2 + \int_{Q_1}(v-\bar{v})^2\right).$$

where C_1 and C_2 are computable constants, independent of the state variables.

Dropping the first and the second term on the left hand side of the first three of the above four inequalites(they are positive) and then adding the four inequalities we get

$$\Big\{(\lambda - \frac{\nu^2}{2d_h} - C_1 e^{4\lambda T_1} - 3C_2)\|u-\bar{u}\|_{L^2(Q_1)}$$

$$+$$

$$(\lambda - \frac{\nu^2}{2d_h} - C_1 e^{4\lambda T_1} - 3C_2)\|v-\bar{v}\|_{L^2(Q_1)}$$

$$+$$

$$(\lambda - \frac{\nu^2}{2d_h} - C_1 e^{4\lambda T_1})\|w-\bar{w}\|_{L^2(Q_1)}$$

$$+$$

$$(\lambda - C_1 e^{4\lambda T_1} - 4C_2)\|X-\bar{X}\|_{L^2(Q_1)}\Big\}$$

$$\leq 0.$$

Now choose λ first and then T_1 such that

$$\frac{(\lambda - \frac{\nu^2}{2d_h} - 4C_2)}{C_1} > 1$$

and

$$T_1 < \frac{1}{4\lambda}\ln\left(\frac{(\lambda - \frac{\nu^2}{2d_h} - 4C_2)}{C_1}\right).$$

Now we can conclude that $u=\bar{u}$, $v=\bar{v}$, $w=\bar{w}$ and $X=\bar{X}$. on $[0,L]\times(0,T_1)$.

Since the solutions are bounded and the bounds are independent of T_1, we can "stack" the solutions. We then get uniqueness on $(T_1, 2T_1)$, etc. $\square$

Theorem 3.2 *For a given g in the control set, the state system (2.14) admits a solution in V.*

Proof: The proof is divided into two parts. We first modify R_2 as defined above to make it a monotone function of u and use the method of monotone iteration scheme to construct a solution for the modified state system. This modified system admits a unique solution, the proof being similar to that which we have shown above for the original system. In the second step we vary R_2 as a function of u and then show that the solutions of the modified system converge to the solution of the original system.

For a fixed function $A > 0$ define

$$R_2^A = \frac{k_3 \mu_2 u v X}{k_2 k_3 + k_3 u + A^2}.$$

R_2^A is an increasing function of u. Set

$$F^A(u, v, X) = -eR_1 - fR_2^A,$$

$$G^A(u, v, X) = -R_1 - R_A^2,$$

$$M^A(u, v, X) = R_2^A - \frac{k_4 X}{k_5 + X}.$$

The modified system is

$$
\begin{aligned}
Lu &= F^A(u, v, X), \\
Lv &= G^A(u, v, X), \\
Lw &= H(w, X), \\
\tfrac{dX}{dt} &= M^A(u, v, X),
\end{aligned}
\tag{3.22}
$$

with the appropriate boundary and initial conditions.

Note that F^A and G^A are decreasing functions of u, v and X and M^A is an increasing function of u and v.

Since $F^A(0, v, X) = G^A(u, 0, X) = H(0, X) = M^A(u, v, 0) = 0$ and the initial and boundary data is nonnegative, $(0, 0, 0, 0)$ is a *lower solution* of the modified state system (3.22). let $\rho_u > 0$ be a constant such that $\rho_u > \max(M, U_0)$. Then since $F^A(\rho_u, v, X) < 0$ for positive v and X, ρ_u is an *upper solution* for $Lu = F^A(u, v, X)$. Similarly we can construct upper solutions ρ_v, ρ_w and ρ_X.

We will construct a solution of the modified system using monotone iteration scheme. Choose $K > 0$ large enough such that

$$|F^A(u_1, v, X) - F^A(u_2, v, X)| \leq K|u_1 - u_2|,$$

$$|G^A(u, v_1, X) - G^A(u, v_2, X)| \leq K|v_1 - v_2|,$$

$$|H(w_1, X) - H(w_2, X)| \leq K|w_1 - w_2|,$$

$$|M^A(u, v, X_1) - M^A(u, v, X_2)| \leq K|X_1 - X_2|,$$

for $0 < u_1, u_2 < \rho_u$, $0 < v_1, v_2 < \rho_v$, $0 < w_1, w_2 < \rho_w$, $0 < X_1, X_2 < \rho_X$.

Consider the following iteration scheme with solutions in V,

$$\begin{aligned}
L\bar{u}^k + K\bar{u}^k &= K\bar{u}^{k-1} + F^A(\bar{u}^{k-1}, \underline{v}^{k-1}, \underline{X}^{k-1}), \\
L\underline{u}^k + K\underline{u}^k &= K\underline{u}^{k-1} + F^A(\underline{u}^{k-1}, \bar{v}^{k-1}, \bar{X}^{k-1}).
\end{aligned}$$

$$\begin{aligned}
L\bar{v}^k + K\bar{v}^k &= K\bar{v}^{k-1} + G^A(\underline{u}^{k-1}, \bar{v}^{k-1}, \underline{X}^{k-1}), \\
L\underline{v}^k + K\underline{v}^k &= K\underline{v}^{k-1} + G^A(\bar{u}^{k-1}, \underline{v}^{k-1}, \bar{X}^{k-1}).
\end{aligned}$$

$$\begin{aligned}
L\bar{w}^k + K\bar{w}^k &= K\bar{w}^{k-1} + H(\bar{w}^{k-1}, \underline{X}^{k-1}), \\
L\underline{w}^k + K\underline{w}^k &= K\underline{w}^{k-1} + H(\underline{w}^{k-1}, \bar{X}^{k-1}).
\end{aligned}$$

$$\begin{aligned}
\frac{d\bar{X}^k}{dt} &= K\bar{X}^k + M^A(\bar{u}^{k-1}, \bar{v}^{k-1}, \bar{X}^{k-1}), \\
\frac{d\underline{X}^k}{dt} &= K\underline{X}^k + M^A(\underline{u}^{k-1}, \underline{v}^{k-1}, \underline{X}^{k-1}).
\end{aligned}$$

where the initial iterates

$$\underline{u}^0 = \underline{v}^0 = \underline{w}^0 = \underline{X}^0 = 0,$$

and

$$\bar{u}^0 = \rho_u\,, \bar{v}^0 = \rho_v\,, \bar{w}^0 = \rho_w\,, \bar{X}^0 = \rho_X.$$

The iterates satisfy the boundary and initial conditions from (2.14). The terms with K were added to make the right hand sides increasing in u, v, w, X respectively. Now using the comparison principle (Krylov [5]) and induction we can show (Pao [13] and Lenhart [7]):

$$\underline{u}^0 \le \underline{u}^k \le \underline{u}^{k+1} \quad \ldots \quad \bar{u}^{k+1} \le \bar{u}^k \le \bar{u}^0, \tag{3.23}$$

$$\underline{v}^0 \le \underline{v}^k \le \underline{v}^{k+1} \quad \ldots \quad \bar{v}^{k+1} \le \bar{v}^k \le \bar{v}^0, \tag{3.24}$$

$$\underline{w}^0 \le \underline{w}^k \le \underline{w}^{k+1} \quad \ldots \quad \bar{w}^{k+1} \le \bar{w}^k \le \bar{w}^0, \tag{3.25}$$

$$\underline{X}^0 \le \underline{X}^k \le \underline{X}^{k+1} \quad \ldots \quad \bar{X}^{k+1} \le \bar{X}^k \le \bar{X}^0. \tag{3.26}$$

This implies that

$$(\bar{u}^k, \bar{v}^k, \bar{w}^k, \bar{X}^k) \searrow (\check{u}, \check{v}, \check{v}, \check{X}) \text{ pointwise} \tag{3.27}$$

$$(\underline{u}^k, \underline{v}^k, \underline{w}^k, \underline{X}^k) \nearrow (\hat{u}, \hat{v}, \hat{v}, \hat{X}) \text{ pointwise.} \tag{3.28}$$

Apriori estimates, similar to those estimates in the proof of Theorem (3.1), yield uniform bounds on all the iterates in V. This implies that $\{\bar{u}^k, \bar{v}^k, \bar{w}^k, \bar{X}^k\}$ converges weakly in V to $(\check{u}, \check{v}, \check{w}, \check{X})$ and $\{\underline{u}^k, \underline{v}^k, \underline{w}^k, \underline{X}^k\}$ converge weakly in V to $(\hat{u}, \hat{v}, \hat{w}, \hat{X})$.

The uniform apriori estimates on the iterates in V combined with the state equations, give us uniform bounds on the time derivatives $||\bar{u}_t||, ||\bar{v}_t||, ||\bar{w}_t||$ and $||\underline{u}_t||, ||\underline{v}_t||, ||\underline{w}_t||$ in the space H^*. A compactness result of Lions [9, chapter 4, proposition 4.2] implies that the $\{\bar{u}^k, \bar{v}^k, \bar{w}^k\}$ converge strongly to $(\check{u}, \check{v}, \check{w})$ in $L^2(Q)$. This implies that the $(\check{u}, \check{v}, \check{w}, \check{X})$ solves the modified system weakly in sense of (2.17). A similar conclusion holds for $(\hat{u}, \hat{v}, \hat{w}, \hat{X})$. A uniqueness result similar to that proved above guarantees that

$$(\check{u}, \check{v}, \check{w}, \check{X}) = (\hat{u}, \hat{v}, \hat{w}, \hat{X}) := (u, v, w, X),$$

solve the modified system (3.22).

Now, let (u^1, v^1, w^1, X^1) be the solution of the modified system (3.22) with

$$(F^A, G^A, H, M^A) = (F^{u_0}, G^{u_0}, H, M^{u_0}),$$

where

$$u_0 = \bar{u}_0, v_0 = \bar{v}_0, w_0 = \bar{w}_0, X_0 = \bar{X}_0.$$

Let u^k, v^k, w^k and X^k solve

$$\begin{aligned} Lu^k &= F^{u^{k-1}}(u^k, v^k, X^k), \\ Lv^k &= G^{u^{k-1}}(u^k, v^k, X^k), \\ Lw^k &= H(w^k, X^k), \\ \frac{dX^k}{dt} &= M^{u^{k-1}}(u^k, v^k, X^k), \end{aligned} \tag{3.29}$$

with the appropriate boundary conditions for $k = 2, 3...$

Clearly

$$\begin{aligned} 0 \leq \quad & u^k & \leq u_0, \\ 0 \leq \quad & v^k & \leq v_0, \\ 0 \leq \quad & w^k & \leq w_0, \\ 0 \leq \quad & X^k & \leq X_0, \end{aligned}$$

for all $k = 1, 2, 3...$. Now $R_2^{u^{k-1}}$ is a decreasing function of u^{k-1}. Therefore $F^{u^{k-1}}, G^{u^{k-1}}$ are increasing functions of u^{k-1} (Note as functions of u^{k-1} and not u^k). $M^{u^{k-1}}$ is a decreasing function of u^{k-1}. By the comparison principle

$$\begin{aligned} u^k \searrow u \quad & \text{pointwise}, \\ v^k \searrow v \quad & \text{pointwise}, \\ w^k \searrow w \quad & \text{pointwise}, \\ X^k \nearrow X \quad & \text{pointwise}. \end{aligned} \tag{3.30}$$

In the weak formulation (2.17) of the modified system (3.22) for each

$k = 1, 2, 3 \ldots$, we get

$$\begin{aligned}
\int_0^T < u_t^k, \phi > + \int_0^T a(u^k, \phi, t) = & \quad \int_Q F^{u^{k-1}}(u^k, v^k, X^k)\phi + \nu \int_0^T (g(t) - u^k(0,t))\phi(0,t), \\
\int_0^T < v_t^k, \psi > + \int_0^T a(v^k, \psi, t) = & \quad \int_Q G^{u^{k-1}}(u^k, v^k, X^k)\psi + \nu \int_0^T (g_1(t) - v^k(0,t))\psi(0,t), \\
\int_0^T < w_t^k, \chi > + \int_0^T a(w^k, \chi, t) = & \quad \int_Q H(w^k, X^k)\chi + \nu \int_0^T (g_2(t) - w^k(0,t))\chi(0,t), \\
X^k(x,t) = & \quad X_{0x} + \int_0^t M^{u^{k-1}}(u^k, v^k, X^k)(x,s)\, ds \quad x \in [0, L].
\end{aligned} \tag{3.31}$$

Now because of the apriori bounds for the iterates in H and their time derivatives in H^* , (3.30) and the continuity of F, G, H and M with respect to state variables, we can conclude that u, v, w and X indeed satisfy the state system (2.14). □

4 Existence of the Optimal Control

To prove the existence of the optimal control we first use a minimizing argument to obtain a sequence of functions that converge to the infimum of the cost functionals taken over the control set. We then establish apriori bounds for the state variables corresponding to the members of the minimizing sequence. Finally we use the lower semicontinuity of the cost functional to establish the existence of the optimal control.

Theorem 4.1 *There exists a $g^* \in C_M$ such that $\mathcal{J}(g^*) = \inf_{g \in C_M} \mathcal{J}(g)$ and $(u(g^*), v(g^*), w(g^*), X(g^*))$ satisfy the state system (2.14).*

Proof Let $\{g_n\}$ be a minimizing sequence for J in C_M,

$$\lim_{n \to \infty} \mathcal{J}(g^n) = \inf_{g \in C_M} \mathcal{J}(g).$$

Let (u_n, v_n, w_n, X_n) be the solution of the state system corresponding to the control g^n. Then

$$\begin{aligned}
\textstyle\int_0^T < (u_n)_t, \phi > + \int_0^T a(u_n, \phi, t) &= \textstyle\int_Q F(u_n, v_n, X_n)\phi + \nu \int_0^T (g^n(t) - u_n(0,t))\phi(0,t), \\
\textstyle\int_0^T < (v_n)_t, \psi > + \int_0^T a(v_n, \psi, t) &= \textstyle\int_Q G(u_n, v_n, X_n)\psi + \nu \int_0^T (g_1(t) - v_n(0,t))\psi(0,t), \\
\textstyle\int_0^T < (w_n)_t, \chi > + \int_0^T a(w_n, \chi, t) &= \textstyle\int_Q H(w_n, X_n)\chi + \nu \int_0^T (g_2(t) - w_n(0,t))\chi(0,t), \\
X_n(x,t) &= \textstyle X_0(x) + \int_0^t M(u_n, v_n, X_n)(x,s)\, ds.
\end{aligned} \tag{4.32}$$

Using (u_n, v_n, w_n) as test functions and standard estimation techniques, which include Cauchy inequality and the trace inequality, we get

$$\begin{aligned}
\int_0^L u_n^2(x,T)\, dx + \int_Q u_n^2 + \int_Q ((u_n)_x)^2 &\leq C_1 \int_0^T u_n^2(x,0)\, dx + C_2 \int_0^T (g^n(t))^2\, dt, \\
\int_0^L v_n^2(x,T)\, dx + \int_Q v_n^2 + \int_Q ((v_n)_x)^2 &\leq C_1 \int_0^T v_n^2(x,0)\, dx + C_2 \int_0^T (g_1(t))^2\, dt, \\
\int_0^L w^2(x,T)\, dx + \int_Q w_n^2 + \int_Q ((w_n)_x)^2 &\leq C_1 \int_0^T w_n^2(x,0)\, dx + C_2 \int_0^T (g_2(t))^2\, dt.
\end{aligned}$$

From above and the fact that $\|g^n\|_\infty \leq M$, we conclude

$\|u_n\|, \|v_n\|$ and $\|w_n\|$ are uniformly bounded independent of n in the norm of H.

We can now extract subsequences with the following convergence properties:

$$\begin{aligned}
u_n &\rightharpoonup u \quad \text{weakly in } H, \\
v_n &\rightharpoonup v \quad \text{weakly in } H, \\
w_n &\rightharpoonup w \quad \text{weakly in } H,.
\end{aligned} \tag{4.33}$$

Now, dropping the decay term in the X equation, we have

$$X_n(x,t) \le X_0(x) + \int_0^t R_2(u_n, v_n, X_n)$$

implies

$$X_n(x,t) \le X_0(x) + C\int_0^t v_n X_n$$

because

$$\frac{k_3\mu_2 u_n}{k_2k_3 + k_3u_n + u_n^2} \le C.$$

By Gronwall's inequality [12]

$$X_n(x,t) \le X_0(x)exp(C\int_0^t v_n(x,s)\,ds).$$

By Sobolev's embedding theorem [12], v_n is continous in x, (space dimension $= 1$),

$$\sup_Q |X_n(x,t)| \le C.$$

Furthermore,

$$|X_n(x,t_2) - X_n(x,t_1)| \le \int_{t_1}^{t_2} |M(u_n, v_n, X_n)(x,s)|\,ds$$

and

$$\begin{aligned} |M(u_n, v_n, X_n)| &\le \left|\frac{k_3\mu_2 u_n v_n X_n}{k_2k_3 + k_3u_n + u_n^2} + \frac{k_4 X_n}{k_5 + X_n}\right| \\ &\le |X_n|\left|\frac{\mu_2 u_n v_n}{k_2} + k_4\right| \\ &\le C(\text{ independent of n }) \end{aligned}$$

imply

$$|X_n(x,t_2) - X_n(x,t_1)| \le C|t_2 - t_1|.$$

where C is a constant independent of n. The above estimate and Arzela - Ascoli theorem [12] imply that for each x, $X_n(x,t) \rightarrow X(x,t)$ uniformly(as a function of t). To summarize, we now have

$$
\begin{aligned}
u_n &\rightharpoonup u && \text{weakly in H,} \\
v_n &\rightharpoonup v && \text{weakly in H,} \\
w_n &\rightharpoonup w && \text{weakly in H,} \\
g^n &\rightharpoonup g^* && \text{weakly in } L^2(0,T), \\
X_n &\rightharpoonup X && \text{weakly in } L^2(Q), \\
& && \text{for each } x \text{, uniformly in } t.
\end{aligned}
\tag{4.34}
$$

From the above weak convergences, uniform bounds and the PDE's we can extract weakly convergent subsequences,

$$
\begin{aligned}
(u_n)_t &\rightharpoonup u_t && \text{weakly in } H^*, \\
(v_n)_t &\rightharpoonup v_t && \text{weakly in } H^*, \\
(w_n)_t &\rightharpoonup v_t && \text{weakly in } H^*.
\end{aligned}
\tag{4.35}
$$

We now have enough regularity to use the compactness result of Lion's [9] and pass to limits in (4.32). We thus conclude that (u, v, w, X) is indeed the solution of the state system corresponding to the control g^*.

We will now verify that g^* is an optimal control. The above apriori estimate (following equation (4.32)) also give us a uniform bound for

$$\|w_n(x,T)\|_{L^2(0,L)},$$

and we can extract a weakly convergent subsequence from those traces on the top $t = T$ [6].

Now, using the lower semicontinuity of the cost functional with respect to the weak convergences of w and g and uniform convergence with respect to X we get

$$\begin{aligned}
\inf_{h \in C_M} \mathcal{J}(h) &= \lim_{n\to\infty} \mathcal{J}(g^n) \\
&= \lim_{n\to\infty} \left[A \int_Q X_n(x,t)\phi(x)\,dx\,dt + B\int_0^L w_n(x,T)\,dx + \frac{1}{2}\int_0^T (g^n)^2\,dt \right] \\
&\geq A\int_Q X(x,t)\phi(x,t) + B\int_0^L w(x,T)\,dx + \frac{1}{2}\int_0^T (g^*)^2\,dt \\
&= \mathcal{J}(g^*).
\end{aligned}$$

5 Derivation of the Optimality System

The optimal control will be represented in terms of the solution of the optimality system, (OS), consisting of the original state system and a suitably defined adjoint system. The form of the OS depends on the form of the objective functional $\mathcal{J}(g)$. Since we will differentiate $\mathcal{J}(g)$ with respect to g and the state variables are involved in $\mathcal{J}$, we must first differentiate the state variables with respect to g.

Lemma 5.1 *The mapping*

$$g \in C_M \to (u(g), v(g), w(g), X(g)) \in V$$

is differentiable in the sense that

$$\frac{u^\epsilon - u}{\epsilon} \rightharpoonup \zeta_1 \qquad \text{weakly in } H,$$

$$\frac{v^\epsilon - v}{\epsilon} \rightharpoonup \zeta_2 \qquad \text{weakly in } H,$$

$$\frac{w^\epsilon - w}{\epsilon} \rightharpoonup \zeta_3 \qquad \text{weakly in } H,$$

$$\frac{X^\epsilon - X}{\epsilon} \rightharpoonup \zeta_4 \qquad \text{weakly in } L^2(Q).$$

Also

$$\text{for each } x, \ \frac{X^\epsilon(x,t) - X(x,t)}{\epsilon} \to \zeta_4 \text{ uniformly in } t.$$

Furthermore $(\zeta_1, \zeta_2, \zeta_3, \zeta_4)$ *satisfy (in the weak sense):*

$$\begin{aligned} L\zeta_1 &= F_u\zeta_1 + F_v\zeta_2 + F_X\zeta_4, \\ L\zeta_2 &= G_u\zeta_1 + G_v\zeta_2 + G_X\zeta_4, \\ L\zeta_3 &= H_w\zeta_3 + H_X\zeta_4, \\ \tfrac{d\zeta_4}{dt} &= M_u\zeta_1 + M_v\zeta_2 + M_X\zeta_4. \end{aligned} \tag{5.36}$$

With the boundary conditions

$$\begin{aligned} -d_h(\zeta_1)_x &= \nu(\bar{g} - \zeta_1) \quad \text{at } x = 0, \ (\zeta_1)_x = 0 \text{ at } x = L, \\ -d_h(\zeta_2)_x &= -\nu\zeta_2 \quad \text{at } x = 0, \ (\zeta_2)_x = 0 \text{ at } x = L, \\ -d_h(\zeta_3)_x &= -\nu\zeta_3 \quad \text{at } x = 0, \ (\zeta_3)_x = 0 \text{ at } x = L, \end{aligned} \tag{5.37}$$

and initial condition

$$\zeta_1 = \zeta_2 = \zeta_3 = \zeta_4 = 0 \text{ at } t = 0,$$

where $F_u, F_v, F_X, G_u, G_v, G_X, H_w, H_X, M_u, M_v$ and M_X denote partial derivatives with respect to the subscripted variable.

Proof: For a given g in C_M, fix a $\bar{g}$ in C_M such that $g + \epsilon\bar{g} \in C_M$.

Let $(u^\epsilon, v^\epsilon, w^\epsilon, X^\epsilon)$ be the solution of the state system (2.17) corresponding to the control $g + \epsilon\bar{g}$.

$$
\begin{aligned}
\int_0^T < u_t^\epsilon, \phi > + \int_0^T a(u^\epsilon, \phi, t) &= \int_Q F(u^\epsilon, v^\epsilon, X^\epsilon)\phi \\
&= \quad + \nu \int_0^T ((g(t) + \epsilon\bar{g}(t)) - u^\epsilon(0,t))\phi(0,t), \\
\int_0^T < v_t^\epsilon, \psi > + \int_0^T a(v^\epsilon, \psi, t) &= \int_Q G(u^\epsilon, v^\epsilon, X^\epsilon)\psi + \nu \int_0^T (g_1(t) - v^\epsilon(0,t))\psi(0,t), \\
\int_0^T < w_t^\epsilon, \chi > + \int_0^T a(w^\epsilon, \chi, t) &= \int_Q H(w^\epsilon, X^\epsilon)\chi + \nu \int_0^T (g_2(t) - w^\epsilon(0,t))\chi(0,t), \\
X^\epsilon(x,t) &= X_0(x) + \int_0^t M(u^\epsilon, v^\epsilon, X^\epsilon)(x,s)\, ds.
\end{aligned}
\tag{5.38}
$$

Subtracting the original system, i.e., one corresponding to (u, v, w, X), we get

$$
\begin{aligned}
\int_0^T < (u^\epsilon - u)_t, \phi > + \int_0^T a(u^\epsilon - u, \phi, t) &= \int_Q (F(u^\epsilon, v^\epsilon, X^\epsilon) - F(u, v, X))\phi \\
&+ \quad \nu \int_0^T (\epsilon\bar{g}(t) - (u^\epsilon - u)(0,t))\phi(0,t). \\
\int_0^T < (v^\epsilon - v)_t, \psi > + \int_0^T a(v^\epsilon - v, \psi, t) &= \int_Q (G(u^\epsilon, v^\epsilon, X^\epsilon) - G(u, v, X))\psi \\
&- \quad \nu \int_0^T (u^\epsilon - u)(0,t))\psi(0,t). \\
\int_0^T < (w^\epsilon - w)_t, \chi > + \int_0^T a(w^\epsilon - w, \chi, t) &= \int_Q (H(w^\epsilon, X^\epsilon) - H(w, X))\chi \\
&- \quad \nu \int_0^T (w^\epsilon - w)(0,t))\chi(0,t). \\
X^\epsilon(x,t) - X(x,t) &= \int_0^t (M(u^\epsilon, v^\epsilon, X^\epsilon) - M(u, v, X))(x,s)\, ds.
\end{aligned}
\tag{5.39}
$$

Apriori estimates(using F, G, H, M are Lipschitz) lead to

$$\|u^\epsilon - u\|_H^2 + \|v^\epsilon - v\|_H^2 + \|w^\epsilon - w\|_H^2 + \|X^\epsilon - X\|_{L^2(Q)}^2 \leq \epsilon^2 \|\bar{g}\|_{L^2[0,T]}^2.$$

From the above apriori bounds we can extract subsequences such that

$$\frac{u^\epsilon - u}{\epsilon} \rightharpoonup \zeta_1 \qquad \text{weakly in } H,$$

$$\frac{v^\epsilon - v}{\epsilon} \rightharpoonup \zeta_2 \qquad \text{weakly in } H,$$

$$\frac{w^\epsilon - w}{\epsilon} \rightharpoonup \zeta_3 \qquad \text{weakly in } H,$$

$$\frac{X^\epsilon - X}{\epsilon} \rightharpoonup \zeta_4 \qquad \text{weakly in } L^2(Q).$$

Also, as in (4.34), we can show that that for each x

$$\frac{X^\epsilon(x,t) - X(x,t)}{\epsilon} \to \zeta_4,$$

uniformly in t.

Now given the fact that F, G, H and M are Lipschitz and rational functions of u, v, w and X and the general result that [12]

$$f_n \rightharpoonup \bar{f} \qquad \text{weakly in } L^2(\Omega)$$

$$g_n \to \bar{g} \qquad \text{strongly in } L^2(\Omega)$$

implies

$$f_n g_n \to \bar{f}\bar{g} \qquad \text{in } L^2(\Omega),$$

we can pass limits (as $\epsilon \to 0$) in (5.39) and arrive at (5.36).

We illustrate our notation in (5.36) by illustrating one case:

$$F_u(u,v,X) = -e(R_1)_u(u,v,X) - f(R_2)_u(u,v,X).$$

where

$$(R_1)_u = \frac{k_1\mu_1 vX}{(k_1+u)^2}$$

and

$$(R_2)_u = \frac{k_3\mu_2 vX(k_2k_3-u^2)}{(k_2k_3+k_3u+u^2)^2}.$$

□

Now we derive the optimality system by differentiating $\mathcal{J}$ with respect to g.

Theorem 5.1 *Given an optimal control g in C_M, there exists a solution (p_1, p_2, p_3, p_4) in V to the adjoint problem*

$$\begin{aligned}
L^1 p_1 &= F_u p_1 + G_u p_2 + M_u p_4,\\
L^1 p_2 &= F_v p_1 + G_v p_2 + M_v p_4,\\
L^1 p_3 &= H_w p_3,\\
-\frac{dp_4}{dt} &= F_X p_1 + G_X p_2 + H_X p_3 + M_X p_4 + \frac{A}{B}\phi(x), \quad x \in [0,L],
\end{aligned}$$

with boundary conditions

$$\begin{aligned}
d_h(p_i)_x(L,t) + \nu p_i(L,t) &= 0 \quad i = 1,2,3,\\
(p_i)_x(0,t) &= 0 \quad i = 1,2,3,\\
p_i(x,T) &= 0 \quad i = 1,2,4, \textit{ for all } x,\\
p_3(x,T) &= 1 \quad \textit{for all } x,
\end{aligned} \tag{5.40}$$

and where L^1 is the operator

$$L^1 = -\frac{\partial}{\partial t} - d_h \frac{\partial^2}{\partial^2 x} - \nu \frac{\partial}{\partial x}.$$

Moreover

$$g(t) = \min\left(-B\nu p_1^-(0,t), M\right). \tag{5.41}$$

Proof Notice that the adjoint system (5.40) is a linear system and the right hand side is globally Lipschitz in p_1, p_2, p_3, p_4. Furthermore p_4 satisfies a first order linear ordinary differential equation and thus we can get an explicit representation of p_4 in terms of the other adjoint variables:

$$p_4(x,t) = e^{\int_t^T M_X(x,s)\,ds} \int_t^T e^{-\int_s^T M_X(x,y)\,dy} \left\{F_X p_1 + G_X p_2 + H_X p_3 + \frac{A}{B}\phi\right\}(x,s)\,ds$$

We can substitute this representation of p_4 into the adjoint system (5.40). We now have a coupled parabolic system consisting of three PDE's with the right hand side globally Lipschitz. Using a contraction fixed point argument in $C([0,T]; L^2(0,L)]$ adapted from Evans[2, chapter 9, pg. 463, Thm. 2], we can prove the existence of solution of the coupled PDE system in $(H)^3$ and thus the adjoint system.

Suppose $g(t)$ is an optimal control. Let $\bar{g} \in L^\infty(0,T)$ such that $g + \epsilon\bar{g} \in C_M$ for $\epsilon > 0$. The derivative of $J(g)$ with respect to g in the direction $\bar{g}$ satisfies

$$\begin{aligned}
0 &\le \lim_{\epsilon\to 0} \frac{J(g+\epsilon\bar{g}) - J(g)}{\epsilon} \\
&= \lim_{\epsilon\to 0}\left(A\int_Q \frac{(X^\epsilon - X)}{\epsilon}(x,t)\phi(x)\,dx\,dt + B\int_0^L \frac{(w^\epsilon - w)}{\epsilon}(x,T)\,dx\right) \qquad (5.42) \\
&+ \lim_{\epsilon\to 0}\frac{1}{2}\left(\int_0^T \frac{((g+\epsilon\bar{g})^2 - g^2)}{\epsilon}(t)\,dt\right) \\
&= A\int_Q \zeta_4(x,t)\phi(x) + B\int_0^L \zeta_3(x,T)\,dx + \int_0^T g(t)\bar{g}(t)\,dt. \qquad (5.43)
\end{aligned}$$

We used the weak convergence of $\frac{w^\epsilon - w}{\epsilon}$ at $t = T$.

Let $\mathbf{p} = (p_1, p_2, p_3, p_4)$ and $\boldsymbol{\zeta} = (\zeta_1, \zeta_2, \zeta_3, \zeta_4)$.

Proceeding **formally**, we explain how to obtain the form of the adjoint system. Let

$$\mathbf{R} = \begin{pmatrix} L - F_u & -F_v & 0 & -F_X \\ \\ -G_u & L - G_v & 0 & -G_X \\ \\ 0 & 0 & L - H_w & -H_X \\ \\ -M_u & -M_v & 0 & \frac{d}{dt} - M_X \end{pmatrix}. \tag{5.44}$$

Then (5.36) can we formally written as

$$\mathbf{R}\boldsymbol{\zeta}^T = 0,$$

with boundary conditions

$$\begin{aligned} -d_h(\zeta_1)_x &= \nu(\bar{g} - \zeta_1) \quad \text{at } x = 0, \quad (\zeta_1)_x = 0 \text{ at } x = L, \\ -d_h(\zeta_2)_x &= -\nu\zeta_2 \qquad\quad \text{at } x = 0, \quad (\zeta_2)_x = 0 \text{ at } x = L, \\ -d_h(\zeta_3)_x &= -\nu\zeta_3 \qquad\quad \text{at } x = 0, \quad (\zeta_3)_x = 0 \text{ at } x = L, \end{aligned} \tag{5.45}$$

and initial condition

$$\zeta_1 = \zeta_2 = \zeta_3 = \zeta_4 = 0 \text{ at } t = 0.$$

Taking the "adjoint-transpose" of R, set

$$\mathbf{S} = \begin{pmatrix} L^1 - F_u & -G_u & 0 & -M_u \\ \\ -F_v & L^1 - G_v & 0 & -M_v \\ \\ 0 & 0 & L^1 - H_w & 0 \\ \\ -F_X & -G_X & -H_X & -\frac{d}{dt} - M_X \end{pmatrix}. \tag{5.46}$$

Now

$$\int_Q (L^1 p_1)\zeta_1 = \int_Q (L\zeta_1)p_1 + \nu \int_0^T p_1(0,t)\bar{g}(t)\,dt \tag{5.47}$$

and

$$\int_Q (L^1 p_3)\zeta_3 = \int_Q (L\zeta_3)p_3 - \int_0^L \zeta_3(x,T)\,dx.$$

Thus

$$B\int_Q \boldsymbol{\zeta}\mathbf{S}\mathbf{p}^{\mathbf{T}} = B\int_Q \mathbf{p}\mathbf{R}\boldsymbol{\zeta}^T + B\nu\int_0^T p_1(0,t)\bar{g}(t)\,dt - B\int_0^L \zeta_3(x,T)\,dx. \tag{5.48}$$

Also

$$B\int_Q \boldsymbol{\zeta}\mathbf{S}\mathbf{p}^{\mathbf{T}} = A\int_Q \zeta_4(x,t)\phi(x) \tag{5.49}$$

Therefore

$$\begin{aligned} 0 &\le A\int_Q \zeta_4(x,t)\phi(x) + B\int_0^L \zeta_3(x,T)\,dx + \int_0^T 2g(t)\bar{g}(t)\,dt \\ &= B\nu\int_0^T p_1(0,t)\bar{g}(t)\,dt + \int_0^T g(t)\bar{g}(t)\,dt. \end{aligned}$$

Using standard control arguments

$$g(t) = \min\left(-B\nu p_1^-(0,t), M\right),$$

where $p^- = \min(p,0)$.

Though the above calculations are formal, they can be easily verified. For example equation (5.47): In the weak formulation the left hand side of (5.47) is

$$\int_0^T < -(p_1)_t, \zeta_1 > + d_h\int_Q (p_1)_x(\zeta_1)_x - \nu\int_Q (p_1)_x\zeta_1 + \nu\int_0^T p_1(L,t)\zeta_1(L,t)\,dt \tag{5.50}$$

The specific form of the weak formulation is a consequence of the boundary conditions imposed on the adjoint system. Similarly, the weak formulation of first term on the right hand side of (5.47) is

$$\int_0^T < (\zeta_1)_t, p_1 > +d_h \int_Q (\zeta_1)_x (p_1)_x + \nu \int_Q (\zeta_1)_x p_1 + \nu \int_0^T p_1(0,t)(\zeta_1(0,t) - \bar{g}(t))\, dt. \tag{5.51}$$

Now

$$-\nu \int_Q (p_1)_x \zeta_1 = \nu \int_Q (\zeta_1)_x p_1 - \nu \int_0^T \zeta_1(L,t) p_1(L,t)\, dt + \nu \int_0^T \zeta_1(0,t) p_1(0,t)\, dt.$$

Also

$$\int_0^T < -(p_1)_t, \zeta_1 >= \int_0^T < (\zeta_1)_t, p_1 >$$

because $\zeta_1(x,0) = 0$ and $p_1(x,T) = 0$. Therfore if we subtract (5.51) from (5.50) we get

$$\nu \int_0^T p_1(0,t)\bar{g}(t)\, dt$$

which is the second term on the right hand side of (5.47).

Remark The optimality system(OS) is obtained by substituting the characterization of an optimal control $g(t)$ (5.41) in the state system (2.14). Then the state system and the adjoint system (5.40) constitute the optimality system (OS)

$$
\begin{aligned}
Lu &= F(u,v,X),\\
Lv &= G(u,v,X),\\
Lw &= H(w,X),\\
\tfrac{dX}{dt} &= M(u,v,X), \quad x \in [0,L],\\
L^1 p_1 &= F_u p_1 + G_u p_2 + M_u p_4,\\
L^1 p_2 &= F_v p_1 + G_v p_2 + M_v p_4,\\
L^1 p_3 &= H_w p_3,\\
-\tfrac{dp_4}{dt} &= F_X p_1 + G_X p_2 + H_X p_3 + M_X p_4 + \tfrac{A}{B}\phi(x) \quad x \in [0,L].
\end{aligned}
\tag{5.52}
$$

With initial and boundary conditions

$$
\begin{aligned}
-d_h u_x(0,t) - \nu\left(\min\left(-B\nu p_1^-(0,t), M\right) - u(0,t)\right) &= 0,\\
u_x(L,t) &= 0,\\
-d_h v_x(0,t) - \nu(g_1(t) - v(0,t)) &= 0,\\
v_x(L,t) &= 0,\\
-d_h w_x(0,t) - \nu(g_2(t) - w(0,t)) &= 0,\\
w_x(L,t) &= 0,\\
u(x,0) = U_0(x),\ v(x,0) &= V_0(x)\\
w(x,0) = W_0(x),\ X(x,0) &= X_0(x)
\end{aligned}
\tag{5.53}
$$

$$
\begin{aligned}
d_h (p_i)_x(L,t) + \nu p_i(L,t) &= 0 \quad i = 1,2,3.\\
(p_i)_x(0,t) &= 0 \quad i = 1,2,3.\\
p_i(x,T) &= 0 \quad i = 1,2,4, \text{ for all } x.\\
p_3(x,T) &= 1 \quad \text{for all } x.
\end{aligned}
\tag{5.54}
$$

6 Uniqueness of the Optimality System

Unlike the state system the uniqueness of the optimality system can only be established for a small time period. This is because solutions cannot be "stacked" as in the case of the state system because the adjoint system evolves backward in time as opposed to the state system which moves forward in time.

Theorem 6.1 *The optimality system (OS)(5.52 - 5.54) admits a unique solution in V^2 for small time T.*

Proof Let $\mathbf{u} = (u, v, w, X)$ and $\mathbf{p} = (p_1, p_2, p_3, p_4)$. Let $(\mathbf{u}, \mathbf{p})$ and $(\bar{\mathbf{u}}, \bar{\mathbf{p}})$ be solutions of the optimality system. First we will verify that the integral

$$\int_Q (p_4 - \bar{p_4})_t (p_4 - \bar{p_4})$$

is well defined. Note that

$$(p_4-\bar{p_4})(x,t) = \int_t^T (F_X(p_1-\bar{p_1})+G_X(p_2-\bar{p_2})+H_X(p_3-\bar{p_3})+M_X(p_4-\bar{p_4}))(x,s)\,ds.$$

F_X, G_X, H_X and M_X are uniformly bounded and since p_1, p_2 and $p_3 \in L^2[0,T,H^1(0,L)]$, they are continous and thus bounded. Thus the first three terms in the above integral can be uniformly bounded. Now, using Gronwall's inequality we get

$$|p_4(x,t)| \le C_1 e^{C_2 T},$$

where C_1 and C_2 are independent of p_4. Also, it can be shown that

$$|p_4(x,t_1) - p_4(x,t_2)| \le C|t_1 - t_2|,$$

for some constant C. This implies that $(p_4 - \bar{p_4})_t$ exists a.e. and is also uniformly bounded.

Now the uniqueness proof for the optimality system(OS) is very similar in character to the uniqueness proof of the state system (2.14), except for the fact that we cannot "stack" the solutions as in the case of the solutions of the state system. This is because the data for the state system and the adjoint system, which constitute the optimality system, are given on opposite ends of the time horizon. So as before we make a change of variable

$$\mathbf{u} = \mathbf{z}e^{\lambda t}$$

$$\mathbf{p} = \mathbf{q}e^{-\lambda t}$$

Using test functions $(\mathbf{z}-\bar{\mathbf{z}}), (\mathbf{q}-\bar{\mathbf{q}})$ we get

$$\int_0^T < (z_1-\bar{z}_1),(z_1-\bar{z}_1)_t > + \int_0^T a(z_1-\bar{z}_1, z_1-\bar{z}_1, t) + \lambda\int_Q (z_1-\bar{z}_1)^2 =$$
$$\int_Q [F(z_1e^{\lambda t}, z_2e^{\lambda t}, z_4e^{\lambda t}) - F(\bar{z}_1e^{\lambda t}, \bar{z}_2e^{\lambda t}, \bar{z}_4e^{\lambda t})]e^{-\lambda t}(z-\bar{z}_1)$$
$$+\nu\int_0^T \left(\min(-B\nu(q_1e^{-\lambda t})^-(0,t), M) - \min(-B\nu(\bar{q}_1e^{-\lambda t})^-(0,t), M)\right)(z_1-\bar{z}_1)(0,t)$$
$$-\nu\int_0^T (z_1-\bar{z}_1)^2\,dt. \tag{6.55}$$

$$\int_0^T < (z_2-\bar{z}_2),(z_2-\bar{z}_2)_t > + \int_0^T a(z_2-\bar{z}_2, z_2-\bar{z}_2, t) + \lambda\int_Q (z_2-\bar{z}_2)^2 =$$
$$\int_Q [G(z_1e^{\lambda t}, z_2e^{\lambda t}, z_4e^{\lambda t}) - G(\bar{z}_1e^{\lambda t}, \bar{z}_2e^{\lambda t}, \bar{z}_4e^{\lambda t})]e^{-\lambda t}(z_2-\bar{z}_2)$$
$$-\nu\int_0^T (z_2-\bar{z}_2)^2(0,t)\,dt. \tag{6.56}$$

$$\int_0^T < (z_3-\bar{z}_3),(z_3-\bar{z}_3)_t > + \int_0^T a(z_3-\bar{z}_3, z_3-\bar{z}_3, t) + \lambda\int_Q (z_3-\bar{z}_3)^2 =$$

$$\int_Q [H(z_3 e^{\lambda t}, z_4 e^{\lambda t}) - H(\bar{z}_3 e^{\lambda t}, \bar{z}_4 e^{\lambda t})] e^{-\lambda t}(z_3 - \bar{z}_3)$$
$$- \nu \int_0^T (z_3 - \bar{z}_3)^2(0,t)\, dt. \tag{6.57}$$

$$\int_Q (z_4 - \bar{z}_4)_t (z_4 - \bar{z}_4) + \lambda \int_Q (z_4 - \bar{z}_4)^2 =$$
$$\int_Q [M(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) - M(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t})] e^{-\lambda t}(z_4 - \bar{z}_4) \tag{6.58}$$

$$\int_0^T < -(q_1 - \bar{q_1})_t, (q_1 - \bar{q_1}) > + d_h \int_Q (q_1 - \bar{q_1})_x^2 - \nu \int_Q (q_1 - \bar{q_1})_x (q_1 - \bar{q_1}) + \lambda \int_Q (q_1 - \bar{q_1})^2 =$$
$$\int_Q (F_u(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_1 - F_u(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t}) \bar{q_1})(q_1 - \bar{q_1})$$
$$+ \int_Q [(G_u(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_2 - G_u(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t}) \bar{q_2})](q_1 - \bar{q_1})$$
$$+ \int_Q (M_u(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_4 - M_u(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t}) \bar{q_4})(q_1 - \bar{q_1})$$
$$- \nu \int_0^T (q_1 - \bar{q_1})^2(L,t)\, dt. \tag{6.59}$$

$$\int_0^T < -(q_2 - \bar{q_2})_t, (q_2 - \bar{q_2}) > + d_h \int_Q (q_2 - \bar{q_2})_x^2 - \nu \int_Q (q_2 - \bar{q_2})_x (q_2 - \bar{q_2}) + \lambda \int_Q (q_2 - \bar{q_2})^2 =$$
$$\int_Q (F_v(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_1 - F_v(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t}) \bar{q_1})(q_2 - \bar{q_2})$$
$$+ \int_Q (G_v(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_2 - G_v(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t}) \bar{q_2})(q_2 - \bar{q_2})$$
$$+ \int_Q (M_v(z_1, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_4 - M_v(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t}) \bar{q_4})(q_2 - \bar{q_2})$$
$$- \nu \int_0^T (q_2 - \bar{q_2})^2(L,t)\, dt. \tag{6.60}$$

$$\int_0^T < -(q_3-\bar{q_3})_t, (q_3-\bar{q_3}) > +d_h \int_Q (q_3-\bar{q_3})_x^3 - \nu \int_Q (q_3-\bar{q_3})_x (q_3-\bar{q_3}) + \lambda \int_Q (q_3-\bar{q_3})^2 =$$

$$\int_Q (H_w(z_3, z_4) q_3 - H_w(\bar{z}_3, \bar{z}_4)\bar{q_3})(q_3 - \bar{q_3}). \tag{6.61}$$

$$\int_Q -(q_4 - q_4)_t (q_4 - q_4) =$$

$$\int_Q (F_X(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_1 - F_X(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t})\bar{q_1})(q_4 - \bar{q_4})$$

$$+ \int_Q (G_X(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_2 - G_X(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t})\bar{q_2})(q_4 - \bar{q_4})$$

$$+ \int_Q (H_X(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_3 - H_X(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t})\bar{q_3})(q_4 - \bar{q_4})$$

$$+ \int_Q (M_X(z_1 e^{\lambda t}, z_2 e^{\lambda t}, z_4 e^{\lambda t}) q_4 - M_X(\bar{z}_1 e^{\lambda t}, \bar{z}_2 e^{\lambda t}, \bar{z}_4 e^{\lambda t})\bar{q_4})(q_4 - \bar{q_4}). \tag{6.62}$$

Now we will use

the ϵ - Cauchy inequality

$$ab \le \frac{1}{2}(\epsilon^2 a^2 + \frac{1}{\epsilon^2} b^2),$$

the trace inequality

$$\int_0^T u^2(0,t) \le C_1 \int_Q u^2 + C_2 \int_Q u_x^2,$$

if f and g are positive functions and M is a positive constant then

$$|\min(f, M) - \min(g, M)| \le |f - g|,$$

and A_b is Lipschitz, where $A \in \{F, G, H, M\}$ and $b \in \{u, v, w, X\}$, to estimate the above integrals. For example, estimating a term from (6.55) yields

$$\nu \int_0^T \left(\min(-B\nu(q_1 e^{-\lambda t})^-(0,t), M) - \min(-B\nu(\bar{q_1} e^{-\lambda t})^-(0,t), M)\right)(z_1 - \bar{z}_1)(0,t) \le$$

$$\begin{aligned}
B\nu^2\int_0^T |(q_1^- - \bar{q_1}^-)||z_1-\bar{z}_1|(0,t) &\le C_1\int_0^T (z-\bar{z}_1)^2(0,t) + C_2\int_0^T (q_1^- - \bar{q_1}^-)^2(0,t)\\
&\le C_1\int_0^T (z-\bar{z}_1)^2(0,t) + C_2\int_0^T (q_1-\bar{q}_1)^2(0,t)\\
&\le C_3\int_Q (z_1-\bar{z}_1)^2 + C_4\int_Q (z_1-\bar{z}_1)_x^2\\
&\quad + C_5\int_Q (q_1-\bar{q}_1)^2 + C_6\int_Q (q_1-\bar{q}_1)_x^2.
\end{aligned}$$

Now, like before, we can absorb these terms on the left hand side.

Similarly from (6.59), we obtain

$$\begin{aligned}
&\int_Q (F_u(z_1e^{\lambda t}, z_2e^{\lambda t}, z_4e^{\lambda t})q_1 - F_u(\bar{z}_1e^{\lambda t}, \bar{z}_2e^{\lambda t}, \bar{z}_4e^{\lambda t})\bar{q}_1)(q_1-\bar{q}_1) =\\
&\int_Q (F_u(z_1e^{\lambda t}, z_2e^{\lambda t}, z_4e^{\lambda t})q_1 - F_u(\bar{z}_1e^{\lambda t}, \bar{z}_2e^{\lambda t}, \bar{z}_4e^{\lambda t})q_1)(q_1-\bar{q}_1)\\
&+\int_Q (F_u(\bar{z}_1e^{\lambda t}, \bar{z}_2e^{\lambda t}, \bar{z}_4e^{\lambda t})q_1) - F_u(\bar{z}_1e^{\lambda t}, \bar{z}_2e^{\lambda t}, \bar{z}_4e^{\lambda t})\bar{q}_1)(q_1-\bar{q}_1)\\
&\le Ce^{\lambda t}\left\{\int_Q (z_1-\bar{z}_1)^2 + \int_Q (z_2-\bar{z}_2)^2 + \int_Q (z_4-\bar{z}_4)^2\right\} + C\int_Q (q_1-\bar{q}_1)^2.
\end{aligned}$$

From this we get

$$(\lambda - C_1 - Ce^{\lambda T})\left(\int_Q (z_1-\bar{z}_1)^2 + \int_Q (z_2-\bar{z})^2 + \int_Q (w-\bar{w})^2 + \int_Q (X-\bar{X})^2\right)$$
$$+\sum_{i=1}^{4} C\int_Q (p_i-\bar{p}_i)^2 \le 0.$$

Now choose λ such that

$$\lambda > C_1$$

and then T such that

$$T < \frac{1}{\lambda}\ln\left(\frac{\lambda - C_1}{C}\right).$$

Thus we conclude that for small T

$$u=\bar{u}, v=\bar{v}, w=\bar{w}, X=\bar{X}, p_i=\bar{p}_i, i=1,2,3,4.$$

$\square$

7 Numerical Results

The optimality system(OS)(5.52) consists of the state system(2.14) and the adjoint system(5.40). Thesse two systems are oriented in the opposite directions. The state is oriented forward in time and the adjoint backward in time. Therefore it is not possible to solve the optimality system directly. At each step, the PDE system (state system or adjoint system) has been solved by finite differences solution technique. We will use the following algorithm (See Appendix for the program):

1. Guess the solution of the adjoint system. Since the optimal control only consists of adjoint variable p_1 we only guess the value of p_1.

2. Substitute the guessed value into the discretized state system and solve forward in time. Save the values of the state variables at each time step.

3. Using the stored values of the state variables, solve the discretized adjoint system backward in time.

4. Substitute the new value of p_1 into the optimal control representation, and again solve the state system forward in time.

5. Repeat the process and stop after the difference between the values of the present iteration and previous iteration become neglibly small.

In Table 1 the values of the different model parameters used are extracted from refrences [14] and [15]. Figure 1 gives the optimal injection profile for acetate. Our profile is comparable in shape to that shown in Petersen et. al ([17]).

Table 1: Model Parameters

Parameter	**Value**	**Units**
μ_1	15.4	L/(gmolmin)
μ_2	3.0	L/(gmolmin)
k_1	5.2×10^{-6}	gmol/L
k_2	3.0×10^{-3}	gmol/L
k_3	2.72×10^{-3}	gmol/L
k_4	4.86×10^{-6}	gmol/(lmin)
k_5	0.1	gmol/L
d_h	0.32	m^2/d
ν	2.7	m/d

Table 2: Initial Concentration

Acetate	100.0 mg/L
Nitrate	26.0 mg/L
Carbon Tetrachloride	0.0396 mg/L
Bacteria Biomass	1.9 mg/L

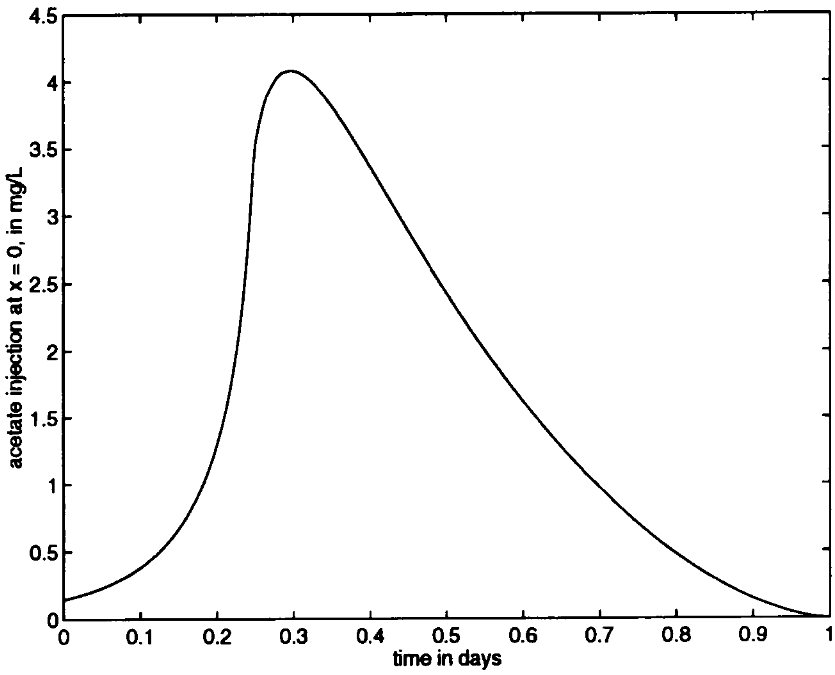

Figure 1: optimal injection profile

8 Conclusions

The approach here worked well to compute the optimal strategy of acetate input, comparing our input profile (figure 1) with the input profile shown in Petersen et. al [17]. The profiles are very similar in shape. The key point to note is that the acetate injection profile attains a sharp peak near time $t = 0$. Since the bioremediation process is cometabolic, large quantities of the primary substrates are required to initiate the process. Therefore the acetate profile in figure 1 is compatible with theoretical expectations.

We plan to use this approach to model bioremediation and optimizing nutrient input for a more realisitic model with three spatial dimensions.

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APPENDIX

```
*
********          BEGIN MAIN PROGRAM
        program main
        integer m,n
        double precision L, T
        double precision dh, nu, sstep, tstep
        double precision check
        parameter( dh = 0.32, nu = 2.7)
        parameter(L = 1.0d0, T = 1.0d0)
        parameter( m = 40, n = 1250)
        parameter(sstep = 0.025d0 , tstep = 0.0008d0) !space,time  step
        double precision u(0:m,0:n), v(0:m,0:n), ! state variables
     +                    w(0:m,0:n), X(0:m,0:n)
        double precision p1(0:m,0:n), p2(0:m,0:n), !adjoint variables
     +                    p3(0:m,0:n), p4(0:m,0:n)
        double precision  inj(0:n),inj1(0:n) !injection functions
        double precision q1side(0:n), qinj(0:n) ! initial guess
        double precision temp1(0:m,0:n), check1(0:m,0:n)
        double precision check2(0:m-1,0:n),check3(0:n-1)
        integer i,j
        integer iterate
        integer  ct, bct
                    do  j = 0, n
*           q1side(j) = - (3.0d3*dble(j)/dble(n) + 1000.0d0)
*              q1side(j) = 1.0d0*(dble(j)/dble(n) -1.0d0)
*         q1side(j) = -10.0d3*(1.0d0 - dble(j)/dble(n))
             q1side(j) =- 0.0d1
                  end do
****** calculating the injection function
*
             call g1(q1side,inj,inj1,n,nu)
*
******
******* initializing  state and adjoint varibales
*
        call initial(u,v,w,X,inj,m,n,ssize,tsize,dh,nu)
        call pinitial(p1,p2,p3,p4,m,n)
*
******  setting up flags to decide number of iterations
*
```

```
        check = 5.0d0
        iterate = 0
*
*******
 10     if ((check .gt. 0.5d-15) .and. (iterate .lt. 10)) then
        iterate = iterate + 1
        print*, iterate
                do  j = 0, n
                        do i = 0, m
                        templ(i,j) = p1(i,j)
                        end do
                end do
                call g1(q1side,inj,inj1,n,nu)
*
******* calling subroutine to march the state variables
******* forward in time.
*
                do  ct = 0, n-1
                call tforward(u,v,w,X,m,n,ct,
     +                  inj,sstep,tstep,dh,nu)
                end do
*
****** calling subroutine to march the adjoint variables
****** backward i time
*
                do  bct = n, 1, -1
                call tbackward(p1,p2,p3,p4,
     +          u,v,w,X,m,n,bct,sstep,tstep,
     +          dh,nu)
                end do
*
                do  j = 0, n
                q1side(j) = p1(0,j)
                end do
*
***** calling subroutine to compare the present and
***** the previous iteration value
*
                call compare(p1,temp1,check1,check2,check3,
     +                          m,n,check )
*
                goto 10
```

```
            endif
65      open(100,file = 'inject.m')
        open(110,file = 'acetate.m')
        open(120,file = 'CCl4.m')
        open(130,file = 'nitrate.m')
        open(140,file = 'biomass.m')
        open(150,file = 'u.m')
        open(160,file = 'v.m')
        open(170,file = 'w.m')
        open(180,file = 'X.m')
        open(190,file = 'wend.m')
        open(191,file = 'p1.m')
        open(192,file = 'p4.m')
        open(193,file = 'q1.m')
        open(194,file = 'p2.m')
        open(195,file = 'p3.m')
        do  j = 0, n
        write(100,200)  inj(j)
        write(110,200)  u(m,j)
        write(130,200)  v(m,j)
        write(140,200)  X(0,j)
        write(190,200)  w(m,j)
        write(193,200) q1side(j)
        end do
        do j = 0, n, 10
        do i = 0, m
        write(150,200)  u(i,j)
        write(160,200)  v(i,j)
        write(170,200)  w(i,j)
        write(180,200)  X(i,j)
        write(191,200) p1(i,j)
        write(192,200) p4(i,j)
        write(194,200) p2(i,j)
        write(195,200) p3(i,j)
        end do
        end  do
        do i = 0, m
        write(120,200) w(i,n)
        end do
        close(100)
        close(110)
        close(120)
```

```
      close(130)
      close(140)
      close(150)
      close(160)
      close(170)
      close(180)
      close(190)
      close(191)
      close(192)
      close(193)
200   format(x,f14.7)
      stop
      end
*******          END MAIN PROGRAM
********
      subroutine tforward(u,v,w,X,m,n,ct,
     +                    inj,sstep,tstep,
     +                    dh,nu)
            integer m,n, ct
            integer i
      double precision u(0:m,0:n), v(0:m,0:n),
     +                 w(0:m,0:n), X(0:m,0:n)
      double precision  inj(0:n)
      double precision a, b, c, e, dh, nu
      double precision f, g, hx, mx
      double precision g2,g3
      double precision sstep, tstep
      double precision minu
      parameter(minu = 0.175d0)
      a = tstep*(dh/sstep**2 - nu/(2*sstep))
      b = tstep*(-2*dh/sstep**2 + 1/tstep)
      c = tstep*(dh/sstep**2 + nu/(2*sstep))
      e = dh/sstep + nu
      do  i = 1, m-1
        u(i, ct +1) =dmax1(minu,a*u(i+1,ct) + b*u(i,ct)
     +            + c*u(i-1,ct) + tstep*f(u,v,X,m,n,i,ct))
            v(i, ct +1) = a*v(i+1,ct) + b*v(i,ct)
     +            + c*v(i-1,ct) + tstep*g(u,v,X,m,n,i,ct)
           w(i, ct +1) = a*w(i+1,ct) + b*w(i,ct)
     +          + c*w(i-1,ct) + tstep*hx(w,X,m,n,i,ct)
      end do
      u(m,ct+1) =   dmax1(minu,(a+c)*u(m-1,ct+1) + b*u(m,ct)+
```

```
+                       tstep*f(u,v,X,m,n,m,ct))
      u(0,ct+1) = dmax1(minu,(a+c)*u(1,ct) + (b-2*sstep*nu*c/dh)*
+                       u(0,ct) + 2*sstep*nu*c*inj(ct)/dh +
+                       tstep*f(u,v,X,m,n,0,ct))
             v(m,ct+1) = (a+c)*v(m-1,ct+1) + b*v(m,ct)+
+                         tstep*g(u,v,X,m,n,m,ct)
             v(0,ct+1) = (a+c)*v(1,ct) + (b-2*sstep*nu*c/dh)*
+                         v(0,ct) + 2*sstep*nu*c*g2(ct)/dh +
+                         tstep*g(u,v,X,m,n,0,ct)
             w(m,ct+1) = (a+c)*w(m-1,ct+1) + b*w(m,ct)+
+                         tstep*hx(w,X,m,n,m,ct)
             w(0,ct+1) = (a+c)*w(1,ct) + (b-2*sstep*nu*c/dh)*
+                         w(0,ct) + 2*sstep*nu*c*g3(ct)/dh +
+                         tstep*hx(w,X,m,n,0,ct)
      do  i = 0,  m
             X(i,ct+1) = X(i,ct) + tstep*mx(u,v,X,m,n,i,ct)
      end do
      return
      end
*******
      subroutine tbackward(p1,p2,p3,p4,u,v,
+                         w,X,m,n,bct,sstep,tstep,
+                         dh,nu)
      integer i,m,n,bct
      double precision sstep, tstep
      double precision a,b,c,e
      double precision dh, nu
      double precision fu, fv, fx
      double precision gu, gv, gxp
      double precision hw, hxp
      double precision mu, mv, mxp
      double precision p1(0:m,0:n), p2(0:m,0:n),
+                      p3(0:m,0:n), p4(0:m,0:n)
      double precision u(0:m,0:n), v(0:m,0:n),
+                      w(0:m,0:n), X(0:m,0:n)
      a = tstep*(dh/sstep**2 - nu/(2*sstep))
      b = tstep*(-2*dh/sstep**2 + 1/tstep)
      c = tstep*(dh/sstep**2 + nu/(2*sstep))
      e = dh/sstep + nu
      do  i = 1, m-1
             p1(i,bct-1) = c*p1(i+1,bct) +
+            (b + fu(u,v,X,m,n,i,bct)*tstep)*p1(i,bct) +
```

```
     +          a*p1(i-1,bct) +
     +          tstep*gu(u,v,X,m,n,i,bct)*p2(i,bct) +
     +  tstep*mu(u,v,X,m,n,i,bct)*p4(i,bct)
*
                p2(i,bct-1) = c*p2(i+1,bct) +
     +          (b + gv(u,v,X,m,n,i,bct)*tstep)*p2(i,bct) +
     +          a*p2(i-1,bct) +
     +          tstep*fv(u,v,X,m,n,i,bct)*p1(i,bct) +
     +  tstep*mv(u,v,X,m,n,i,bct)*p4(i,bct)
*
                p3(i,bct-1) = c*p3(i+1,bct) +
     +          (b + hw(X,m,n,i,bct)*tstep)*p3(i,bct) +
     +          a*p3(i-1,bct)
        end do
                p1(0,bct-1) = (c+a)*p1(1,bct) +
     +          (b + tstep*fu(u,v,X,m,n,1,bct))*p1(0,bct)+
     +          tstep*gu(u,v,X,m,n,1,bct)*p2(0,bct)+
     +          tstep*mu(u,v,X,m,n,1,bct)*p4(0,bct)
                p1(m,bct-1) = (b + tstep*
     +          fu(u,v,X,m,n,m-1,bct) - 2.0*nu*sstep*c/dh)*
     +          p1(m,bct) + (a+c)*p1(m-1,bct) +
     +          tstep*gu(u,v,X,m,n,m-1,bct)*p2(m,bct) +
     +          tstep*mu(u,v,X,m,n,m-1,bct)*p4(m,bct)

                p2(0,bct-1) = (c+a)*p2(1,bct) +
     +          (b + tstep*gv(u,v,X,m,n,1,bct))*p2(0,bct)+
     +          tstep*fv(u,v,X,m,n,1,bct)*p1(0,bct)+
     +          tstep*mv(u,v,X,m,n,1,bct)*p4(0,bct)
                p2(m,bct-1) = (b + tstep*
     +          gv(u,v,X,m,n,m,bct) - 2.0*nu*sstep*c/dh)*
     +          p2(m,bct) + (a+c)*p2(m-1,bct) +
     +          tstep*fv(u,v,X,m,n,m-1,bct)*p1(m,bct) +
     +          tstep*mv(u,v,X,m,n,m-1,bct)*p4(m,bct)

                p3(0,bct-1) = (c+a)*p3(1,bct) +
     +          (b + tstep*hw(X,m,n,1,bct))*p3(0,bct)
                p3(m,bct-1) = (b + tstep*
     +          hw(X,m,n,m-1,bct) - 2.0*nu*sstep*c/dh)*
     +          p3(m,bct) + (a+c)*p3(m-1,bct)

*
          do   i = 0, m
```

```
      if (i .le. 4) then
                p4(i,bct-1) = p4(i,bct) +
     +          tstep*(fx(u,v,m,n,i,bct)*p1(i,bct) +
     +          gxp(u,v,X,m,n,i,bct)*p2(i,bct) +
     +          hxp(w,m,n,i,bct)*p3(i,bct) +
     + mxp(u,v,X,m,n,i,bct)*p4(i,bct) + (1-i/4.0))
      else
                p4(i,bct-1) = p4(i,bct) +
     +           tstep*(fx(u,v,m,n,i,bct)*p1(i,bct) +
     +           gxp(u,v,X,m,n,i,bct)*p2(i,bct) +
     +           hxp(w,m,n,i,bct)*p3(i,bct) +
     +  mxp(u,v,X,m,n,i,bct)*p4(i,bct))
      endif

      end do
      return
      end
******
      double precision  function f(u, v, X,m,n, cs, ct)
      integer  cs, ct, m, n
      double precision  mu1,mu2,k1,k2,k3,theta
      parameter( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +              mu1 = 15.4, mu2 = 3.0,theta =1.0)
      double precision  u(0:m,0:n), v(0:m,0:n), X(0:m,0:n)
                f =
     +           -  (0.25d0*mu1*u(cs,ct)*v(cs,ct)*X(cs,ct)/
     +          (k1 + u(cs,ct)) +
     +          3.5d0*k3*mu2*u(cs,ct)*v(cs,ct)*X(cs,ct)/
     +  (k2*k3 + k3*u(cs,ct) + u(cs,ct)*u(cs,ct)))/theta
      return
      end
*****
      double precision  function g(u,v,X,m,n, cs, ct)
      integer  cs, ct, m, n
      double precision mu1,mu2,k1,k2,k3,theta
      parameter( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +              mu1 = 15.4, mu2 = 3.0,theta = 1.0)
      double precision u(0:m,0:n), v(0:m,0:n), X(0:m,0:n)
                g =
     +            - ( mu1*u(cs,ct)*v(cs,ct)*X(cs,ct)/
     +          (k1 + u(cs,ct)) +
     +          k3*mu2*u(cs,ct)*v(cs,ct)*X(cs,ct)/
```

```
     +     (k2*k3 + k3*u(cs,ct) + u(cs,ct)*u(cs,ct)))/theta
      return
      end
*****
      double precision function hx(w,X,m,n,cs,ct)
      integer cs,ct,m,n
      double precision k3, theta
      parameter(k3 =  2.72D-3,theta = 1.0)
      double precision w(0:m,0:n) , X(0:m,0:n)
            hx = -k3*w(cs,ct)*X(cs,ct)/theta
      return
      end
*****
      double precision function mx(u,v,X,m,n,cs,ct)
      integer  cs,ct,m,n
      double precision  mu2,k1,k2,k3,k4,k5,theta
      parameter ( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +             k4 = 4.8d-6, k5 = 0.1d0,
     +              mu1 = 15.4, mu2 = 3.0,theta =1.0)
      double precision u(0:m,0:n), v(0:m,0:n), X(0:m,0:n)
           mx  =  (k3*mu2*u(cs,ct)*v(cs,ct)*X(cs,ct)/
     +        (k2*k3 + k3*u(cs,ct) + u(cs,ct)*u(cs,ct)) -
     +       k4*X(cs,ct)/(k5 + X(cs,ct)))/theta
      return
      end
******
      subroutine g1(p1side,inj,inj1,n,nu)
      integer n,j
      double precision p1side(0:n), inj(0:n)
      double precision inj1(0:n)
      double precision nu
      do  j = 0, n
      inj1(j) = dmin1(-nu*4.0d0*dmin1(p1side(j),0.0d0)
     + , 3.0d3)
      inj(j) = inj1(j)
*     print*, inj(j)
      end do
      return
      end
******
      double precision function g2(ct)
      double precision const2
```

```
      parameter(const2 = 26.0d0)
      integer ct
      g2 = const2
      return
      end
******
      double precision function  g3(ct)
      double precision const3
      parameter(const3 = 0.0d0)
      integer ct
      g3 = const3
      return
      end
******
      double precision function  fu(u,v,X,m,n,bcs,bct)
      integer m,n,bcs,bct
      double precision k1,k2,k3,mu1,mu2,theta
      double precision u(0:m,0:n), v(0:m,0:n),
     +                  X(0:m,0:n)
      PARAMETER( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +              mu1 = 15.4, mu2 = 3.0,theta =1.0)
*     common /param/ k1,k2,k3,mu1,mu2
*
      fu = -(0.25*k1*mu1*v(bcs,bct)*X(bcs,bct)/
     +        (k1 + u(bcs,bct))**2 +
     +        3.5*k3*mu2*v(bcs,bct)*X(bcs,bct)*
     +         (k2*k3 - u(bcs,bct)**2)/
     + (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2)**2)/theta
      return
      end
******
      double precision function  fv(u,v,X,m,n,bcs,bct)
      integer m,n,bcs,bct
      double precision k1,k2,k3,mu1,mu2,theta
      double precision u(0:m,0:n), v(0:m,0:n),
     +                  X(0:m,0:n)
      PARAMETER( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +              mu1 = 15.4, mu2 = 3.0,theta = 1.0)
*     common /param/ k1,k2,k3,mu1,mu2
*
      fv = -(0.25*k1*mu1*u(bcs,bct)*X(bcs,bct)/
     +        (k1 + u(bcs,bct)) +
```

```
     +       3.5*k3*mu2*u(bcs,bct)*X(bcs,bct)/
     + (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2))/theta
*       if((bcs .eq. 1) .and.  (bct .gt. 9850)) then
*       print*,bct, fv
*       endif
        return
        end
*******
        double precision function fx(u,v,m,n,bcs,bct)
        integer m,n,bcs,bct
        double precision k1,k2,k3,mu1,mu2,theta
        double precision u(0:m,0:n), v(0:m,0:n)
        PARAMETER( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +             mu1 = 15.4, mu2 = 3.0,theta =1.0)
*       common /param/ k1,k2,k3,mu1,mu2
*
        fx = -(0.25*k1*mu1*u(bcs,bct)*v(bcs,bct)/
     +       (k1 + u(bcs,bct)) +
     +       3.5*k3*mu2*u(bcs,bct)*v(bcs,bct)/
     +        (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2))/theta
        return
        end
********
        double precision function  gu(u,v,X,m,n,bcs,bct)
        integer m,n,bcs,bct
        double precision k1,k2,k3,mu1,mu2,theta
        double precision u(0:m,0:n), v(0:m,0:n),
     +                         X(0:m,0:n)
        PARAMETER( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +             mu1 = 15.4, mu2 = 3.0,theta =1.0)
*       common /param/ k1,k2,k3,mu1,mu2
*
        gu = -(k1*mu1*v(bcs,bct)*X(bcs,bct)/
     +       (k1 + u(bcs,bct))**2 +
     +       k3*mu2*v(bcs,bct)*X(bcs,bct)*
     +        (k2*k3 - u(bcs,bct)**2)/
     + (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2)**2)/theta
        return
        end
*********
        double precision function gv(u,v,X,m,n,bcs,bct)
        integer m,n,bcs,bct
```

```
      double precision k1,k2,k3,mu1,mu2,theta
      double precision u(0:m,0:n), v(0:m,0:n),
     +                 X(0:m,0:n)
      PARAMETER( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +           mu1 = 15.4, mu2 = 3.0,theta =1.0)
*     common /param/ k1,k2,k3,mu1,mu2
*
      gv = -(k1*mu1*u(bcs,bct)*X(bcs,bct)/
     +       (k1 + u(bcs,bct)) +
     +       k3*mu2*u(bcs,bct)*X(bcs,bct)/
     +       (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2))/theta
      return
      end
********
      double precision function  gxp(u,v,X,m,n,bcs,bct)
      integer m,n,bcs,bct
      double precision k1,k2,k3,mu1,mu2,theta
      double precision u(0:m,0:n), v(0:m,0:n),
     +                 X(0:m,0:n)
      PARAMETER( k1 = 5.2D-6, k2 =  3.0D-3, k3 = 2.72D-3,
     +           mu1 = 15.4, mu2 = 3.0,theta =1.0)
*     common /param/ k1,k2,k3,mu1,mu2
*
      gxp = -(k1*mu1*u(bcs,bct)*v(bcs,bct)/
     +       (k1 + u(bcs,bct)) +
     +       k3*mu2*u(bcs,bct)*v(bcs,bct)/
     +       (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2))/theta
      return
      end
********
      double precision function  hw(X,m,n,bcs,bct)
      integer m,n,bcs,bct
      double precision k3,theta
      double precision  X(0:m,0:n)
      parameter(k3 = 2.72d-3,theta =1.0)
*     common /param/ k3
      hw = -k3*X(bcs,bct)/theta
      return
      end
*********
      double precision function  hxp(w,m,n,bcs,bct)
      integer m,n,bcs,bct
```

```
      double precision k3,theta
      parameter(k3 = 2.72d-3,theta =1.0)
      double precision w(0:m,0:n)
*     common /param/ k3
      hxp = -k3*w(bcs,bct)/theta
      return
      end
*********
      double precision function  mu(u,v,X,m,n,bcs,bct)
      integer m,n,bcs,bct
      double precision k2,k3,mu2,theta
      double precision u(0:m,0:n), v(0:m,0:n),
     +                    X(0:m,0:n)
      parameter(k2 = 3.0d-3, k3 = 2.72d-3,
     +           mu2 = 3.0d0,theta =1.0)
*     common /param/ k3,k4,k5,mu2
       mu =  (k3*mu2*v(bcs,bct)*X(bcs,bct)*
     +       (k2*k3 - u(bcs,bct)**2)/
     + (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2)**2)/theta
      return
      end
*********
      double precision function  mv(u,v,X,m,n,bcs,bct)
      integer m,n,bcs,bct
      double precision k2,k3,mu2,theta
      double precision u(0:m,0:n), v(0:m,0:n),
     +                   X(0:m,0:n)
      parameter(k2 = 3.0d-3, k3 = 2.72d-3,
     +            mu2 = 3.0d0,theta = 1.0)
*     common /param/k2,k3,mu2
       mv =  k3*mu2*u(bcs,bct)*X(bcs,bct)/
     +       (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2)/theta
      return
      end
*********
      double precision function  mxp(u,v,X,m,n,bcs,bct)
      integer m,n,bcs,bct
      double precision k2,k3,k5,mu2,theta
      double precision u(0:m,0:n), v(0:m,0:n),
     +                    X(0:m,0:n)
      PARAMETER(  k2 =  3.0D-3, k3 = 2.72D-3,
     +              k5 = 0.1d0,
```

```
     +                mu2 = 3.0,theta = 1.0)
*     common /param/ k2,k3,k5,mu2
      mxp =  (k3*mu2*u(bcs,bct)*v(bcs,bct)/
     +       (k2*k3 + k3*u(bcs,bct) + u(bcs,bct)**2)-
     +        k5/(k5 +X(bcs,bct))**2)/theta
      return
      end
*******
        subroutine initial(u,v,w,X,inj,m,n,sstep,tstep,
     +                     dh,nu)
      integer m, n
      integer i,j
      double precision const1, const2, const3, const4
*     double precision  g2, g3
      double precision nu, dh
      double precision e
      double precision sstep, tstep
      parameter(const1 =  1.000d2, const2 = 26.0D0,
     +               const3 = 0.0396D0, const4 = 1.9D0)
      double precision u(0:m,0:n), v(0:m,0:n),
     +                   w(0:m,0:n), X(0:m,0:n),
     +                   inj(0:n)
            end do
            end do
            do i = 0, m
            if (i .eq. 0) then
            u(i,0) = const1
            else
            u(i,0) = const1
            endif
            v(i,0) = const2
            w(i,0) = const3
            X(i,0) = const4
            end do
      return
      end
*******
      subroutine pinitial(p1,p2,p3,p4,m,n)
      integer i,j
      integer m, n
      double precision p1(0:m,0:n), p2(0:m,0:n),
     +                  p3(0:m,0:n), p4(0:m,0:n)
```

```
          do  i = 0, m
                  p3(i,n) =1.0d0
                  p1(i,n) =0.0d0
                  p2(i,n) = 0.0d0
                  p4(i,n) = 0.0d0
          end do
      return
      end
*******
      subroutine compare(cp1,ctemp1,dum1,dum2,dum,m,n,residue)
      integer m,n
      double precision cp1(0:m,0:n), ctemp1(0:m,0:n)
      double precision dum1(0:m,0:n), dum2(0:m-1,0:n)
      double precision dum(0:n-1), residue
      do j = 0, n
              do i = 0, m
              dum1(i,j) = dabs(cp1(i,j) - ctemp1(i,j))
              end do
      end do
       do j = 0, n
       dum2(0,j) = dmax1(dum1(0,j), dum1(1,j))
       do i = 1,m-1
              dum2(i,j) = dmax1(dum2(i-1,j),dum1(i+1,j))
      end do
      end do
       dum(0) = dmax1(dum2(m-1,0), dum2(m-1,1))
      do j = 1, n-1
              dum(j) = dmax1(dum(j-1),dum2(m-1,j+1))
      end do
      residue = dum(n-1)
      return
      end
```

Vita

Sanjay Chawla was born on the 29th of May 1966, in New Delhi, India. He attended St. Columba's High School in New Delhi and graduated from High School in 1984. In July 1987 he received his B.A.(Hons) from Hindu College, Delhi University. In 1988 he came to the United States of America to pursue his graduate studies. He received his M.A. in Mathematics from Central Michigan University in August 1990 and his Ph.d in Mathematics from the University of Tennessee in August 1995. He is married to Preeti Singh and they are blessed with a son, Ishaan Gobind.