

Optimal Control Applied to Resource Allocation in a PDE Ecosystem Model and a Zika Virus Epidemic Model

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Degree

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*To my parents, Wencel and Yadira, to my siblings, Fidel and Sandra, and to my fiancée,
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Abstract

This dissertation focuses on developing two mathematical models applied to spatial ecology and epidemiology. More specifically, one model considers the spatiotemporal dynamics of a population with its resource while the second model studies the dynamics of a Zika Virus epidemic.

The effects of habitat heterogeneity on a diffusing population are investigated here. We formulate a reaction-diffusion system of partial differential equations to analyze the effect of resource allocation in an ecosystem with resources having their own dynamics in space and time. We show *a priori* estimates to prove the existence of state solutions given a control. We formulate an optimal control problem of our ecosystem model such that the abundance of a single species is maximized while minimizing the cost of inflow resource allocation. In addition, we show the existence and uniqueness of the optimal control as well as the optimal control characterization. We also establish the existence of an optimal diffusion rate. Moreover, we illustrate several numerical simulations with Dirichlet and Neumann boundary conditions with the space domain in 1D and 2D.

Zika virus (ZIKV) is a mostly non-lethal disease in humans transmitted by mosquitoes or humans that can produce severe brain defects such as microcephaly in babies and Guillain-Barré syndrome in elderly adults. The use of optimal control strategies involving information campaigns about insect repellents and condoms alongside an available and effective vaccine can notably prevent the number of infected humans with ZIKV. A system of nonlinear ordinary differential equations is formulated for the transmission dynamics of ZIKV in the presence of three control strategies to evaluate the impact of various scenarios during a ZIKV epidemic. In addition, we estimate parameters using data from previous ZIKV outbreaks in

Colombia and Puerto Rico to capture the dynamics of an epidemic in each country when control measures are available.

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Chapter 1

Introduction

Optimal control theory can illustrate choices of control actions in biological models to achieve desired goals. In this dissertation, this theory is applied to systems of ordinary differential equations and partial differential equations in mathematical epidemiology and ecology. Mathematical epidemiology studies the spread of infectious diseases in a population at the community level. Hence, building epidemic models can help epidemiologist to answer questions such as:

- What are necessary interventions to reduce disease transmission?
- When do we expect the incidence of a disease to peak?

Mathematical ecology studies the behavior of ecosystems by explaining topics like population growth, food webs, group dynamics, population movement, evolution etc. In this case, ecological models are a powerful tool for ecologists to address questions such as:

- What features would impact the total population size of a species?
- How does spatial heterogeneity impact the total population size?

Optimal control theory studies the dynamics of a system with control variables under a given objective functional to optimize. The main idea is to formulate an optimal control problem consisting of a dynamical system, an objective functional, control variables, coefficients or source terms. We will see that these optimal control results can provide advice to public

health policies to alleviate deadly epidemics or to choose management strategies in order to preserve endangered ecosystems.

Motivated by the work of Loreau [31] in connecting population dynamics with ecosystem functioning, the first part of this dissertation focuses on understanding the effect produced by resources that are allowed to vary in time and space on a diffusing population. In order to capture the dynamics of the population and its resources, in Chapter 2 we formulate the following resource allocation model for a diffusing population

$$\begin{aligned}
N_t - d\Delta N &= \alpha_3\alpha_2NR - \mu N && \text{on } Q \\
R_t &= I(x, t) - \alpha_2NR + p\mu N - qR && \text{on } Q \\
N(x, 0) &= N_0(x) && \text{on } \Omega \\
R(x, 0) &= R_0(x) && \text{on } \bar{\Omega} \\
N(x, t) &= 0 && \text{on } \partial\Omega \times [0, T].
\end{aligned}$$

where N and R are the state variables representing the population and resource densities. The function $I(x, t)$ represents the input amount of resources and we think of it as an external factor that could increase growth of the population. In a plant ecosystem, one can think of I as the input amount of inorganic nutrients that impacts the ecosystem through processes such as water flow or nitrogen-containing fertilizers [31]. In Chapter 2 we provide biological interpretations of all other coefficients as well as the meaning of boundary conditions and initial conditions for our problem. Thus, if we are given an external input rate of resources to improve the population size of a species across space and time, what would be the *best* way to do this? Here we understand “best” as the *benefit* for the population while taking into account the *cost* corresponding to the optimal input rate of resource. Motivated by this question, we formulate an optimal control problem subject to the resource allocation model whose goal is to maximize the total population abundance of the species and to minimize the cost associated with the input rate of resources. Therefore, we will require optimal control techniques applied to PDEs to solve the desired optimization problem. We begin by showing the existence of weak solutions corresponding to the state variables. The optimality system consists of the state system, adjoint system and the optimal control characterization.

Then, we prove *a priori* estimates to show the existence and uniqueness of solutions in the optimality system in the corresponding weak sense. In addition, we investigate the effects of different diffusion rates on the values of the objective functional. We provide several numerical examples of the model with control to illustrate its impact in providing management strategies. We implement the Forward-Backward Sweep method in MATLAB to numerically solve the optimality system.

The second part of this dissertation studies the dynamics of a Zika Virus epidemic (ZIKV) when three time dependent control strategies are available in the population. In order to understand the spread of ZIKV in a community, in Chapter 3 we formulate the following system of nonlinear differential equations

$$\begin{aligned}
S'(t) &= \mu N(t) - \beta S(t) \frac{I_v(t)}{N_v(t)} (1 - u_2(t)) - \alpha S(t) \frac{I(t)}{N(t)} (1 - u_1(t)) - \phi(t) f S(t) \\
&\quad + \omega V(t) - \mu S(t), \\
V'(t) &= \phi(t) f S(t) - \omega V(t) - \mu V(t), \\
E'(t) &= \beta S(t) \frac{I_v(t)}{N_v(t)} (1 - u_2(t)) + \alpha S(t) \frac{I(t)}{N(t)} (1 - u_1(t)) - (\kappa + \mu) E(t) \\
I'(t) &= \kappa E(t) - (\gamma + \mu) I(t), \\
R'(t) &= \gamma I(t) - \mu R(t), \\
S'_v(t) &= \mu_v N_v(t) - \mu_v S_v(t) - \beta_v S_v(t) \frac{I(t)}{N(t)}, \\
E'_v(t) &= \beta_v S_v(t) \frac{I(t)}{N(t)} - (\mu_v + \eta) E_v(t), \\
I'_v(t) &= \eta E_v(t) - \mu_v I_v(t).
\end{aligned}$$

to capture the dynamics of human and mosquito classes throughout the course of the epidemic. The state variables S , V , E , I and R correspond to susceptible, vaccinated, exposed, infected and recovered human classes. Similarly, the state variables S_v , E_v and I_v are the susceptible, exposed and infected mosquito classes. The control functions u_1 , u_2 and ϕ represent the effort of implementing information campaigns to promote the use of condoms, insecticides and vaccination to alleviate the human and mosquito transmissions. We find the basic reproductive number of the model to identify the number of secondary cases produced

by one infected individual at the beginning of the epidemic. We also show some existence, uniqueness and positivity results of the solutions to make the model biological feasible. Now, in the scenario that a ZIKV epidemic emerges and these control strategies are available to be implemented under certain constraints, we would like to know if there is a way to optimally deliver personal protection and vaccination campaigns that can minimize the total number of new infections by the end of the epidemic. Motivated by this question, we formulate an optimal control problem subject to our ZIKV epidemic model with the goal to minimize the total number of ZIKV infections while minimizing the costs associated to implementing the controls. In this part, we will require optimal control theory applied to ODEs. We demonstrate the existence of an optimal control and derive necessary conditions for the optimal control problem by using Pontryagin's Maximum Principle [42]. In an effort to apply the optimization problem to a real world ZIKV epidemic, we collect weekly incidence data from two previous ZIKV epidemics in Colombia and Puerto Rico to estimate transmission rates, incubation periods and reporting rates. We want to estimate the reporting rate since most ZIKV cases are not reported due to people with the disease having mild or no symptoms. The parameter estimation scheme consists of minimizing the square error of the incidence between the model and the data. To accomplish this we use MATLAB functions `fmincon` and `MultiStart`. The function `fmincon` solves the minimization problem subject to some constraints and the function `MultiStart` allows us to run the minimization problem multiple times from different start points. Once these key epidemiological parameters are estimated, we illustrate many numerical simulations for each country to realistically capture a ZIKV epidemic in presence of different control strategies. Our simulation results can quantify the number of new infections that could be prevented if timely actions are put in place. These results also report the cost associated with the epidemiological outcomes and the intervention strategies. Based on our results for each country, public health agencies can quickly provide necessary recommendations to mitigate the spread of the disease and prevent ZIKV side effects such as microcephaly in babies and neurological disorders in adults [37, 39, 9].

1.1 Optimal Control Problems with ODEs

The basic idea formulating optimal control problem with one ordinary differential equation consists of finding a piecewise continuous control $u(t)$ and the associated state variable $x(t)$ such that a given objective functional can be maximized as follows:

$$\begin{aligned} J(u^*) &= \max_{u \in U} J(u) \\ \text{subject to } x'(t) &= g(t, x(t), u(t)) \\ x(t_0) &= x_0 \text{ and } x(t_1) \text{ free,} \end{aligned} \tag{1.1}$$

where the functions f and g are continuously differentiable in all three arguments, the objective functional is expressed as

$$J(u) = \int_{t_0}^{t_1} f(t, x(t), u(t)) dt$$

in terms of the control u with its corresponding state (denoted by $x(u)$ to show the dependence on u) and the set of admissible controls is given by

$$U = \{u \in L^\infty[t_0, t_1] : a \leq u(t) \leq b\}$$

where $a, b \in \mathbb{R}$.

When an optimal control u^* with associated state x^* exist, one can use Pontryagin's Maximum Principle [28] to derive necessary conditions for the solution of the optimal control problem by formulating the Hamiltonian ($H(t, x, u, \lambda) = f + \lambda g$), the adjoint differential equations (λ') with corresponding transversality conditions ($\lambda(t_1) = 0$) and the optimality equation ($H_u = 0$) to characterize the control in terms of x^* and λ . Thus, we have turned the original maximization problem into maximizing the Hamiltonian with respect to the control u . The state and adjoint differential equations along with the characterization of the optimal control are called the *optimality system*.

In some cases one can show the existence and uniqueness of the optimality system by making assumptions on the functions f, g [19]. For instance, when these functions are

Lipschitz continuous with respect to the state and adjoint variables, then the solution of the optimality system is unique for small time. Later in Chapter 3, we will show the existence of an optimal control triple (u_1^*, u_2^*, ϕ^*) with associated states by showing the existence of a minimizing control sequence that has a weakly convergent subsequence. Then we will use a property of L^2 with respect to the weak convergence to show the limit is a minimizer for the objective functional.

1.2 Optimal Control Problems with PDEs

The basic ideas of optimal control problems involving systems with space and time were first developed by J-L. Lions [30]. The important Pontryagin's Maximum Principle in the ODE case cannot directly be used to study the PDE case. However, Li and Yong [29] present some results involving "maximum principle" type results. Here, we outline the technique of optimal control for one parabolic PDE following the book by Lenhart and Workman [28]. First, it is fundamental to choose a weak solution space for PDEs, since classical solutions may not exist for nonlinear PDEs with L^∞ controls. That is, the state solutions may not have all classical derivatives. Hence, a convenient solution space for most parabolic PDE problems with controls is

$$w \in L^2([0, T]; H_0^1(\Omega)) \cap L^\infty(Q) \text{ and } w_t \in L^2([0, T]; H_0^1(\Omega)^*),$$

where Ω represents the spatial domain and $Q = \Omega \times (0, T)$. Let U be the set of all admissible Lebesgue measurable controls with lower and upper bounds and consider the following problem

$$Aw = f(w, u) \quad \text{in } Q \tag{1.2}$$

with corresponding initial and boundary conditions. Here, A is a parabolic partial differential operator and $u \in U$ is any admissible control. The goal is to find $u^* \in U$ such that

$$J(u^*) = \sup_u J(u)$$

where

$$J(u) = \int_Q g(x, t, w(x, t), u(x, t)) \, dx dt.$$

Observe that we want to maximize J constrained by our problem (1.2). One needs to show that for any given $u \in U$, there exists an associated state solution that depends on u . In this case, we write $w(u)$ showing that w depends on u .

We require *a priori* estimates of states in the solution space to support convergence of a maximizing sequence and finally prove the existence of an optimal control $u^* \in U$. Such estimates provide the existence of a maximizing sequence $u_n \in U$. It has to be shown that indeed $w(u^*) = w^*$, i.e., w^* is the state associated to the optimal control u^* . Furthermore, if one can show that

$$J(u^*) = \sup_{u \in U} J(u)$$

then u^* is an optimal control for problem (1.2).

As in the ODE case, we need to derive the necessary conditions for our optimal control problem with our PDE. We first differentiate the objective functional J with respect to the control u , but since $w = w(u)$ also contributes to J , we also have to differentiate w with respect to u . The two maps to differentiate are

$$u \mapsto J(u) \quad \text{and} \quad u \mapsto w(u).$$

The map $u \mapsto w(u)$ is weakly differentiable on $L^2([0, T]; H_0^1(\Omega))$ such that

$$\lim_{\epsilon \rightarrow 0^+} \frac{w(u + \epsilon k) - w(u)}{\epsilon} = \psi,$$

where k is a variation function that can have any sign and $u + \epsilon k \in U$. The function ψ is called the *sensitivity* of the state w with respect to the control u . One more time we require the use of *a priori* estimates on the difference quotients in the solution space to justify convergence and existence of our sensitivity ψ . The function ψ solves a PDE with corresponding initial and boundary conditions. The linear operator of the sensitivity PDE is a linearized version of the initial PDE operator A . By using the operator in the sensitivity PDE one can derive the operator of the adjoint PDE, the corresponding boundary conditions and adjoint final

time conditions. The adjoint PDE would have a nonhomogeneous term carries the effect of the state on the goal. Finally, we can characterize an optimal control by differentiating the map $u \mapsto J(u)$ at an optimal control u^* and using the adjoint and sensitivity PDEs to simplify the expression. The state and adjoint PDEs together with the optimal control characterization is called the *optimality system*. Note that one must show separately that the optimal control is unique.

1.3 Optimization Tools: fmincon and MultiStart

In Chapter 3, we estimate parameters of the Zika model using the MATLAB functions `fmincon` and `MultiStart`. The `fmincon` function is a nonlinear programming solver that can find a minimum of a multivariate function subject to nonlinear constraints. There are five different large-scale or medium-scale `fmincon` algorithms. In our case, we use the interior-point algorithm (default) since it has a low memory usage and solves large problems quickly. The `MultiStart` function runs a local solver several times from different start points to find multiple local solutions of the objective function that can lead to the solution of a global minimum. Thus, to run the `MultiStart` function we create a global optimization problem consisting of the `fmincon` solver with interior-point algorithm, the objective function to minimize with corresponding upper and lower bounds, and the number of start points to run the solver. The objective function in our case corresponds to the normalized ℓ^2 error between the incidences of the model and the data.

Chapter 2

Resource Allocation in a PDE Ecosystem Model

2.1 Introduction

Heterogeneous habitats impact the dynamics of a diffusing population. Scientists have opted to use reaction-diffusion equations with varying coefficients to model this effect [7, 32, 31, 13, 57, 59, 3]. Some of the advantages of using reaction-diffusion models with spatial heterogeneity is their flexibility in types of rates and boundary conditions. Here, we review some mathematical work over the past few years and discuss some of their results applied to spatial ecology. In this work, we are interested in systems in which the population as well as the resource vary dynamically.

Cantrell and Cosner [6] were motivated by the work done by Skellam [46] to assume that the population can diffuse through the habitat via random walks and the population can have a linear or logistic growth rate with spatially dependent coefficients. The general model proposed by Skellam was

$$u_t = d\Delta u + m(x)u - c(x)u^2 \quad \text{in } \Omega \times (0, \infty) \quad (2.1)$$

subject to necessary boundary and initial conditions. In this model, $u(x, t)$ represents the population density, $m(x)$ is the intrinsic growth rate and $c(x)$ is the carrying capacity.

Hence, in order to model the long term growth and spread of a population, Cosner and Cantrell examined a number of one dimensional cases where the local growth rate $m(x)$ is a piecewise constant function which has positive effect on part of the habitat and negative effect everywhere else. We will discuss later an alternate view of the carrying capacity of this equation.

Cantrell and Cosner [7] discuss the mathematical development of reaction-diffusion theory and its applications to the study of populations and communities of populations in bounded habitats. They consider linear reaction-diffusion models for a single species in an isolated bounded habitat. Subsequently, they considered the steady state analysis of density dependent reaction diffusion models for a single species in a bounded habitat. Some examples included here are cell and molecular biology, immunology and epidemiology as well as ecological and evolutionary dynamics of interacting populations.

Lou in [32] analyzed the effects of migration and spatial heterogeneity of the environment on the total population size at equilibrium of a single species,

$$\begin{aligned}\mu\Delta u + u[m(x) - u] &= 0, \quad u > 0 \quad \text{in } \Omega \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on } \partial\Omega\end{aligned}\tag{2.2}$$

where u is the population density, μ is the migration rate and $m(x)$ is the local intrinsic growth rate. His results showed that the total population size is maximized at some intermediate migration rate and heterogeneity of the environment ($m(x)$) increases the population size. The ideas from a single species case were also applied for a two-species Lotka–Volterra competition model including migration. He concluded that when migration is present, the invading species eliminates the resident species at every point of the habitat. However, without migration, the two species can coexist at every point of the habitat. In Zhang et al. [58], the authors tested experimentally the mathematical results of Lou [32] for a single plant population to measure the impact of diffusion and spatial heterogeneity. They planted duckweed (an aquatic plant) along water containers where resources were heterogeneously and homogeneously distributed. The diffusion rate was controlled manually between the containers. The experimental results showed that duckweed biomass was

maximized at an intermediate diffusion rate which agreed with the theoretical results [32, 43]. With this experiment they found evidence that diffusion in a heterogeneous environment can result in higher population biomass than a population diffusing in a homogeneous environment.

DeAngelis et al. [13] extended the results found by Lou in [32] that population diffusing at any rate in an environment with spatially dependent intrinsic growth rate can reach a higher total equilibrium biomass than the population with constant intrinsic growth rate. Hence, in order to make their model more practical for ecologists, they broke up the local intrinsic growth rate and carrying capacity $m(x)$ in Lou [32] with two new parameters $r(x)$ and $K(x)$. Here, $r(x)$ represents the intrinsic growth rate while $K(x)$ is the carrying capacity. The model proposed in this paper is given by

$$\begin{aligned} d\Delta u + r(x)u \left[1 - \frac{u}{K(x)} \right] &= 0 \quad u > 0 \quad \text{in } \Omega \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on } \partial\Omega. \end{aligned} \tag{2.3}$$

They also studied the case when there is a positive correlation between $r(x)$ and $K(x)$ when dispersal rate d is small. Some implications for population and conservation ecology such as experimental tests for a single plant population exposed to spatial heterogeneity as it diffuses and source-sink experiments were also discussed. Some papers that have tried to test experimentally these implications are in [57, 24, 56]. For instance, Zhang et al. [57] extended the results in DeAngelis et al. [13] and considered a population (budding yeast) with exploitable resource (tryptophan) to test that population diffusing in a heterogeneous environment increases the total population size at equilibrium. Later, He et al. [24] investigated the dynamics of the consumer-resource reaction diffusion model proposed by Zhang et al. [57] for heterogeneous and homogeneous environments. In the case of homogeneous environment, they determined global stability of the constant steady state as well as conditions between the yield rate and resources. For heterogeneous environment, they analyzed the existence and stability of positive steady states as well as the persistence of time-dependent solutions.

Ding et al. [16] were motivated by the work of Cosner and Cantrell [6] on how to find the optimal spatial distribution of resources for species to survive. With this idea in mind, they formulated an optimal control problem to maximize abundance of a single species while a fixed amount of resource is available. Their proposed maximization problem was to find

$$m^* \in U = \left\{ m \in L^\infty : 0 \leq m(x) \leq 1, \int_{\Omega} m(x) dx = \delta \right\}$$

such that

$$\sup_{m \in U} J(m) = J(m^*) \text{ where } J(m) = \int_{\Omega} [u - (Bm^2)] dx$$

subject to

$$\begin{aligned} -\lambda \Delta u &= mu - u^2, & x \in \Omega \\ \frac{\partial u}{\partial n} &= 0 & x \in \partial\Omega. \end{aligned} \tag{2.4}$$

The state $u \in H^1(\Omega)$ represents the population density at equilibrium, λ is the dispersal rate and $m(x)$ is the intrinsic growth rate of species u . They showed the existence and uniqueness of an optimal control as well as its characterization in terms of state and adjoint functions. Numerical simulations of habitats in 1D and 2D domains were also investigated and discussed by the authors. Note that from our current viewpoint, $m(x)$ is a type of carrying capacity, where $u(x) \leq m(x)$ under low rates of dispersal.

Bintz and Lenhart [3] considered an optimal resource allocation for a population with diffusion and logistic growth. They considered a resource function $m(x, t)$ depending on space and time. They formulated and analyzed four different optimal control problems. Here, we only state one of the four control problems. For a fixed amount of resource, the goal is to find

$$m^* \in V = \left\{ m \in L^\infty : 0 \leq m(x, t) \leq M, \int_0^T \int_{\Omega} m(x, t) dx dt = \delta \right\}$$

such that

$$\sup_{m \in V} J(m) = J(m^*) \quad \text{where } J(m) = A \int_{\Omega} u(x, T) \, dx + \int_0^T \int_{\Omega} [u - (Bm^2)] \, dx$$

subject to

$$\begin{aligned} u_t - \mu \Delta u &= u(m - u), & (x, t) \in \Omega \times (0, T) \\ \frac{\partial u}{\partial n} &= 0 & (x, t) \in \partial\Omega \times (0, T). \end{aligned} \tag{2.5}$$

Note that the objective functional J has an extra term $A \int_{\Omega} u(x, T) \, dx$ that was not considered in Ding et al. [16] since their problem did not have time. This integral represents the total abundance at the final time where A is the relative importance of the population level at the final time. Moreover, they performed numerical simulations for the one dimensional case to compare different scenarios of zero-Neumann and zero-Dirichlet boundary conditions. Part of their results showed that in presence of inhospitable boundary, the resource should be allocated further away from the hostile boundary. However, with hospitable boundary, it is required to allocate more resource over the entire domain.

Loreau [31] identified an increasing gap between two subdisciplines of ecology: community ecology and ecosystem ecology. Community ecology mostly considers the population and its interactions with other populations concerning their dynamics, evolution, diversity and complexity of the biological components within the ecosystems. On the other side, ecosystem ecology focuses on the study of the overall system composed of biological organisms and their environment by considering the flow of matter or the energy among functional compartments. The goal of his book is to develop new principles, perspectives and questions connecting these two big branches of ecology and as a result set a new coherent framework relating population, community, ecosystem and evolutionary ecology.

Some of these studies [6, 32, 13] assumed that the resource function is known (either $m(x)$ or $K(x)$) and not varying in time, but this might not be always the case. Inspired by Loreau's work [31] emphasizing the need of including dynamics of the resource as well as

population and by [6, 46, 13, 32, 13, 14, 3], the goal of our work is to formulate a reaction-diffusion population model to study the effect of resource allocation in an ecosystem with resources having their own dynamics in space and time. This is a more realistic scenario than only assuming that the resource function is not changing as population changes. Moreover, motivated by optimal control problems [16, 3] applied to the cost of resource allocation in heterogeneous environment, we also formulate an optimal control problem of our resource allocation model to maximize the abundance of a single species while minimizing the cost of inflow resource allocation. To achieve our goals we require the techniques of optimal control for PDEs.

This chapter is organized as follows: in Section 2.2 we propose the resource allocation model while in Section 2.3 we prove the existence of state solutions. In Section 2.4 we formulate two optimal problems and in Section 2.5 we explore the case when resource is allowed to diffuse. Later, in Sections 2.6 and 2.7 we study several numerical scenarios of the problem without and with control. We conclude and discuss some future directions of our work in Section 2.8.

2.2 Resource Allocation Model

In this section we formulate a reaction diffusion population model with its resource having explicit dynamics. Consider the following resource allocation model with diffusing population for an ecosystem:

$$\begin{aligned}
N_t - d\Delta N &= \alpha_3\alpha_2NR - \mu N && \text{on } Q \\
R_t &= I(x, t) - \alpha_2NR + p\mu N - qR && \text{on } Q \\
N(x, 0) &= N_0(x) && \text{on } \Omega \\
R(x, 0) &= R_0(x) && \text{on } \bar{\Omega} \\
N(x, t) &= 0 && \text{on } \partial\Omega \times [0, T],
\end{aligned} \tag{2.6}$$

where $\Omega \subset \mathbb{R}^n$ is bounded and $Q = \Omega \times (0, T)$ is the space-time domain. In this model, the state variable $N = N(x, t)$ is measuring the population density while $R = R(x, t)$ represents

the amount of resource, both at certain time and position. Here, d represents the diffusion rate, μ is the natural death rate of the population, α_3 is the conversion of resource into population growth (units: population/resource), $I(x, t)$ is the input amount of resource at location x and time t per unit time, α_2 is the rate of resource uptake by the population (units: $1/(\text{time} \times \text{population})$), $p\mu N$ is the contribution to the resource from the death of the population and q is the resource decay rate. Later we shorthand $\alpha_1 = \alpha_3\alpha_2$. The parameters $d, \mu, \alpha_1, \alpha_2, p$ and q are assumed to be positive constants. The function $I \in U$ with the control set given by

$$U = \left\{ I \in L^\infty(Q) \mid 0 \leq I(x, t) \leq M_1, \text{a.e. } (x, t) \in \bar{\Omega} \times [0, T] \right\}.$$

The value of R at the boundary remains unknown by simply looking at system (2.6). Assuming the ODE for R holds at the spatial boundary one can see that

$$R_t = I(x, t) - qR \text{ on } (x, t) \in \partial\Omega \times [0, T]$$

which solution is given by

$$R(x, t) = R_0(x)e^{-qt} + \int_0^t e^{q(\tau-t)} I(x, \tau) d\tau.$$

Note that $R(x, t) = 0$ at the boundary if and only if $R_0(x) = 0$ and $I(x, \tau) = 0$ on $(0, t)$ are also zero at the boundary.

Remark 2.2.1. *When no flux boundary condition is considered for N , $\frac{\partial N}{\partial \eta} = 0$, and assuming the ODE for R holds at the spatial boundary, we can see that no terms in the R ODE can be dropped. Nonetheless, we can obtain the following form for R at the boundary*

$$R(x, t) = e^{-\int_0^t (\alpha_2 N(x, \tau) + q) d\tau} R_0(x) + \int_0^t e^{\int_t^\tau (\alpha_2 N(x, s) + q) ds} (I(x, \tau) + p\mu N(x, \tau)) d\tau. \quad (2.7)$$

Observe that the above expression doesn't have to be zero at the boundary unless the functions $R_0(x)$, $I(x, \tau)$ and $N(x, \tau)$ are all zero at the boundary with $\tau \in (0, t)$ and $t < T$.

In the next section we present the weak formulation for problem (2.6) and derive some *a priori* estimates.

2.3 Existence of State Solutions

In this section we define the weak formulation for problem (2.6). Let $d, \mu, \alpha_1, \alpha_2, p$ and q be non-negative constants and $I \in U$. The functions $N \in L^2((0, T), H_0^1(\Omega)) \cap L^\infty(Q)$, $N_t \in L^2((0, T), H_0^1(\Omega)^*)$ and $R \in L^2(Q)$ are said to be weak solutions of problem (2.6) if for any test function $\Phi \in L^2((0, T), H_0^1(\Omega)) \cap L^\infty(Q)$

$$\begin{aligned} \int_0^T \langle N_t, \Phi \rangle dt + d \int_0^T \int_\Omega \nabla N \cdot \nabla \Phi \, dx dt &= \int_0^T \int_\Omega \alpha_1 N(x, t) R(x, t) \Phi(x, t) \\ &\quad - \mu N(x, t) \Phi(x, t) \, dx dt \\ R(x, t) - R(x, 0) &= \int_0^t (I(x, s) - \alpha_2 N(x, s) R(x, s) \\ &\quad + p\mu N(x, s) - qR(x, s)) ds \quad x \in \bar{\Omega} \end{aligned} \tag{2.8}$$

with initial and boundary conditions

$$\begin{aligned} N(x, 0) &= N_0(x) \quad \text{on } \Omega \\ R(x, 0) &= R_0(x) \quad \text{on } \bar{\Omega} \\ N(x, t) &= 0 \quad \text{on } \partial\Omega \times (0, T) \end{aligned} \tag{2.9}$$

where $\langle \cdot, \cdot \rangle$ denotes the duality between $H_0^1(\Omega)^*$ and $H_0^1(\Omega)$. Moreover, the initial conditions $N_0(x)$ and $R_0(x)$ are both in $L^\infty(\Omega)$.

Remark 2.3.1. *The weak formulation in system (2.8) also holds when zero Neumann boundary conditions are used instead of zero Dirichlet boundary conditions. In this case the state N and test functions are in the space $L^2((0, T), H^1(\Omega)) \cap L^\infty(Q)$.*

The equation describing the population growth from our resource allocation model in (2.6):

$$N_t - d\Delta N = \alpha_1 NR - \mu N \quad \text{on } Q. \tag{2.10}$$

Using the weak formulation for the population growth equation (2.10) with $\Phi = N$ one can see that

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} N^2 dx + d \int_{\Omega} |\nabla N|^2 dx = \int_{\Omega} N^2 (\alpha_1 R - \mu) dx \quad (2.11)$$

and after dropping the term with the diffusion coefficient

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} N^2 dx \leq \int_{\Omega} N^2 (\alpha_1 R - \mu) dx.$$

From the above inequality it can be seen that when

$$R(x, t) \leq \frac{\mu}{\alpha_1} = R_c \quad \text{on } Q \quad (2.12)$$

the rate of change of the population abundance squared is non-positive

$$\frac{d}{dt} \int_{\Omega} N^2 dx \leq 0$$

which implies that the population abundance squared is always a decreasing function in time,

$$\int_{\Omega} N^2(x, T) dx \leq \int_{\Omega} N^2(x, t) dx \leq \int_{\Omega} N_0^2(x) dx.$$

On the other hand, when $R(x, t) \geq R_c$ one cannot assume that the population abundance is going to grow due to the effect of the diffusion term and boundary conditions. From equation (2.11) we have that

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} N^2 dx = \int_{\Omega} N^2 (\alpha_1 R - \mu) dx - d \int_{\Omega} |\nabla N|^2 dx.$$

In order to $\frac{d}{dt} \int_{\Omega} N^2 dx$ to be non-negative the following condition is required

$$d \int_{\Omega} |\nabla N|^2 dx \leq \int_{\Omega} N^2 (\alpha_1 R - \mu) dx.$$

The critical threshold for the resource, $R_c = \frac{\mu}{\alpha_1}$, is the minimum amount of resource needed for the population to shrink or grow. If the resource levels are below R_c the population

is expected to shrink regardless of how fast or slow it moves. When the resource levels are above the critical threshold, it is unsure whether the population size will increase or decrease due to the population movement decreasing the population size. For example, if the population diffuses too fast, it reaches the hostile boundary and stops any chances of growth. More of this will be discussed in Subsection 2.7.3 when we explore the dynamics of the population and its resource under different levels of diffusion.

The following Theorem shows that given a control, there exists a unique corresponding state solution. We denote the following spaces as $V_1 := L^2((0, T), H_0^1(\Omega)) \cap L^\infty(Q)$ and $V_2 := L^2(Q)$ for writing purposes.

Theorem 2.1. *Given T sufficiently small and $I \in U$, there exists a unique non-negative weak solution $(N, R) \in V_1 \times V_2$. Moreover, there exists a positive constant C such that $0 \leq N(x, t) \leq C$ and $0 \leq R(x, t) \leq C$ a.e. $(x, t) \in Q$.*

Proof. The idea of this proof is to use Banach's fixed point theorem [17]. Given a non-empty complete metric space (X, d) with a contracting mapping $A : X \rightarrow X$, then A has a unique fixed point $u^* \in X$. By Evans [17], we know that if $(N, R) \in V_1 \times V_2$ then $N \in C([0, T]; L^2(\Omega))$ and $R \in L^2(Q)$. Since we require uniform L^∞ bounds for N and R , we define

$$X_1 := C([0, T]; L^2(Q)) \cap \{u \in L^\infty(Q) : 0 \leq u \leq M, \text{ a.e. } (x, t) \in Q\}$$

$$X_2 := L^2(Q) \cap \{u \in L^\infty(Q) : 0 \leq u \leq M, \text{ a.e. } (x, t) \in Q\}$$

for fixed $M \geq 2 \sup\{\|I\|_{L^\infty(Q)}, \|N_0\|_{L^\infty(\Omega)}, \|R_0\|_{L^\infty(\Omega)}\}$. Let $X = X_1 \times X_2$ and define the norm

$$\|(N, R)\|_X = \sup_{0 \leq t \leq T} \|N(\cdot, t)\|_{L^2(\Omega)} + \|R(\cdot, t)\|_{L^2(Q)}.$$

Assume that $I \in U$ and consider the following change of functions $w = e^{-\lambda t}N$ and $z = e^{-\lambda t}R$. Under the substitution, system (2.6) can be written as

$$\begin{aligned}
w_t - d\Delta w + \lambda w &= \alpha_1 e^{\lambda t} w z - \mu w && \text{on } Q \\
z_t + \lambda z &= I(x, t) e^{-\lambda t} - \alpha_2 e^{\lambda t} w z + p\mu w - qz && \text{on } Q \\
w(x, 0) &= N_0(x) && \text{on } \Omega \\
z(x, 0) &= R_0(x) && \text{on } \Omega \\
w(x, t) &= 0 && \text{on } \partial\Omega \times [0, T].
\end{aligned} \tag{2.13}$$

Let $(h_1, h_2) \in X$ and consider the following system of linear equations

$$\begin{aligned}
w_t - d\Delta w + \lambda w &= \alpha_1 e^{\lambda t} w h_2 - \mu w && \text{on } Q \\
z_t + \lambda z &= I(x, t) e^{-\lambda t} - \alpha_2 e^{\lambda t} h_1 z + p\mu h_1 - qz && \text{on } Q \\
w(x, 0) &= N_0(x) && \text{on } \Omega \\
z(x, 0) &= R_0(x) && \text{on } \Omega \\
w(x, t) &= 0 && \text{on } \partial\Omega \times [0, T].
\end{aligned} \tag{2.14}$$

By techniques from Evans [17], the w PDE has a solution and then the uncoupled system (2.14) has a unique weak solution $(w, z) \in V_1 \times V_2$. We will have to show that $(w, z) \in X$ in order to use our fixed point argument. By Evans, we know that $w \in C([0, T]; L^2(\Omega))$ and $z \in L^2(Q)$. However, we still require to show that $0 \leq w(x, t) \leq M$ and $0 \leq z(x, t) \leq M$ a.e. $(x, t) \in Q$.

Claim 1. $0 \leq w(x, t)$ and $0 \leq z(x, t)$ a.e in Q .

Proof. Rearranging the terms in system (2.14) we see that

$$\begin{aligned}
w_t - d\Delta w + (\lambda - \alpha_1 e^{\lambda t} h_2 - \mu)w &= 0 && \text{on } Q \\
z_t + (\lambda + \alpha_2 e^{\lambda t} h_1 + q)z &= I(x, t) e^{-\lambda t} + p\mu h_1 \geq 0 && \text{on } Q \\
w(x, 0) &= N_0(x) && \text{on } \Omega \\
z(x, 0) &= R_0(x) && \text{on } \Omega \\
w(x, t) &= 0 && \text{on } \partial\Omega \times [0, T].
\end{aligned} \tag{2.15}$$

Since the term with λ is L^∞ bounded and by the weak maximum principle of parabolic equations, we have that $0 \leq w(x, t)$ a.e in Q . By simple ODE techniques we can also obtain that $0 \leq z(x, t)$. Let $a(x, t) = \lambda + \alpha_2 e^{\lambda t} h_1 + q$ then $z_t + a(x, t)z \geq 0$. Note that $a(x, t)$ is bounded. Hence, using integrating factor

$$z(x, t) \geq e^{-\int_0^t a(x, s) ds} z(x, 0) \geq 0.$$

□

Claim 2. $w(x, t) \leq M$ and $z(x, t) \leq M$ a.e. in Q .

Proof. Note that since $\|I\|_{L^\infty(Q)} \leq \frac{M}{2}$ and $h_1 \in X_1$, then

$$\|I(x, t)e^{-\lambda t} + p\mu h_1\| \leq \|I(x, t)\|_{L^\infty(Q)} + p\mu \|h_1\|_{X_1} \leq \frac{M}{2}(1 + 2p\mu) = C.$$

Hence, both of the equations in system (2.14) satisfy that

$$\begin{aligned} w_t - d\Delta w + (\lambda - \alpha_1 e^{\lambda t} h_2 - \mu)w &\leq 0 && \text{on } Q \\ z_t + (\lambda + \alpha_2 e^{\lambda t} h_1 + q)z &\leq C && \text{on } Q \\ w(x, 0) &= N_0(x) && \text{on } \Omega \\ z(x, 0) &= R_0(x) && \text{on } \Omega \\ w(x, t) &= 0 && \text{on } \partial\Omega \times [0, T]. \end{aligned} \tag{2.16}$$

Let $W(x, t) = w(x, t) - Ct$ and $Z(x, t) = z(x, t) - Ct$. Then, the new functions W and Z satisfy the following problem

$$\begin{aligned} W_t - d\Delta W + (\lambda - \alpha_1 e^{\lambda t} h_2 + \mu)W &\leq -Ct(\lambda - \alpha_1 e^{\lambda t} h_2 + \mu) - C && \text{on } Q \\ Z_t + (\lambda + \alpha_2 e^{\lambda t} h_1 + q)Z &\leq -Ct(\lambda + \alpha_2 e^{\lambda t} h_1 + q) && \text{on } Q \\ W(x, 0) &= N_0(x) && \text{on } \Omega \\ Z(x, 0) &= R_0(x) && \text{on } \Omega \\ W(x, t) &= -Ct && \text{on } \partial\Omega \times [0, T]. \end{aligned} \tag{2.17}$$

Choose $\lambda > \alpha_1 h_2 - \mu$ and T sufficiently small such that $\lambda - \alpha_1 e^{\lambda t} h_2 + \mu > 0$. This implies that

$$\begin{aligned} W_t - d\Delta W + (\lambda - \alpha_1 e^{\lambda t} h_2 + \mu)W &\leq 0 \quad \text{on } Q \\ Z_t + (\lambda + \alpha_2 e^{\lambda t} h_1 + q)Z &\leq 0 \quad \text{on } Q \end{aligned} \tag{2.18}$$

One more time, using the weak maximum principle for parabolic equations, we obtain that

$$W(x, t) \leq \|N_0\|_{L^\infty(\Omega)}.$$

Furthermore, we can show that

$$Z(x, t) \leq \|R_0\|_{L^\infty(\Omega)}$$

by using simple ODE techniques. Therefore, it can be seen that w and z satisfy the following estimates

$$w(x, t) \leq \|N_0\|_{L^\infty(\Omega)} + CT \leq \frac{M}{2} + \frac{M}{2}T(1 + 2p\mu)$$

and

$$z(x, t) \leq \|R_0\|_{L^\infty(\Omega)} + CT \leq \frac{M}{2} + \frac{M}{2}T(1 + 2p\mu).$$

Upon taking $T < \frac{1}{1 + 2p\mu}$ the claim is proven. $\square$

The claims 1 and 2 guarantee also that $(w, z) \in X$.

Let $A : X \rightarrow X$ be a map such that $A(h_1, h_2) = (w, z)$. We will show that A is a contraction. Let $(h_1, h_2), (\hat{h}_1, \hat{h}_2) \in X$ such that $A(h_1, h_2) = (w, z)$ and $A(\hat{h}_1, \hat{h}_2) = (\hat{w}, \hat{z})$. Consider the differences $w - \hat{w}$ and $z - \hat{z}$. These differences satisfy the following system:

$$\begin{aligned} (w - \hat{w})_t - d\Delta(w - \hat{w}) + \lambda(w - \hat{w}) &= \alpha_1 e^{\lambda t}(wh_2 - \hat{w}\hat{h}_2) \\ &\quad - \mu(w - \hat{w}) \quad \text{on } Q \\ (z - \hat{z})_t + \lambda(z - \hat{z}) &= -\alpha_2 e^{\lambda t}(h_1 z - \hat{h}_1 \hat{z}) \\ &\quad + p\mu(h_1 - \hat{h}_1) - q(z - \hat{z}) \quad \text{on } Q \end{aligned} \tag{2.19}$$

with initial and boundary conditions

$$\begin{aligned}
(w - \hat{w})(x, 0) &= 0 && \text{on } \Omega \\
(z - \hat{z})(x, 0) &= 0 && \text{on } \Omega \\
(w - \hat{w})(x, t) &= 0 && \text{on } \partial\Omega \times [0, T].
\end{aligned}$$

Multiply the first equation of system (2.19) by $(w - \hat{w})$ and integrate over $Q_t = \Omega \times (0, t)$ with $t < T$

$$\begin{aligned}
\frac{1}{2} \int_{\Omega} (w - \hat{w})^2 dx + d \int_0^t \int_{\Omega} |\nabla(w - \hat{w})|^2 dx ds \\
+ \int_0^t \int_{\Omega} (\lambda + \mu)(w - \hat{w})^2 dx ds = \alpha_1 \int_0^t \int_{\Omega} e^{\lambda s} (wh_2 - \hat{w}\hat{h}_2)(w - \hat{w}) dx ds
\end{aligned} \tag{2.20}$$

Observe that we can estimate the right hand side of equation (2.20) as

$$\begin{aligned}
\int_{Q_t} \alpha_1 e^{\lambda t} (wh_2 - \hat{w}\hat{h}_2)(w - \hat{w}) dx ds &= \int_{Q_t} \alpha_1 e^{\lambda s} (w(h_2 - \hat{h}_2) + (w - \hat{w})\hat{h}_2)(w - \hat{w}) dx ds \\
&= \int_{Q_t} \alpha_1 e^{\lambda s} w(h_2 - \hat{h}_2)(w - \hat{w}) dx ds \\
&\quad + \int_{Q_t} \alpha_1 e^{\lambda s} \hat{h}_2(w - \hat{w})^2 dx ds \\
&\leq \frac{1}{2} \int_{Q_t} \alpha_1^2 e^{2\lambda s} w^2 (w - \hat{w})^2 dx ds + \frac{1}{2} \int_{Q_t} (h_2 - \hat{h}_2)^2 dx ds \\
&\quad + \frac{\alpha_1 M}{2} \int_{Q_t} e^{2\lambda s} (w - \hat{w})^2 dx ds \\
&= \left(\frac{\alpha_1 M + \alpha_1^2 M^2}{2} \right) \int_{Q_t} e^{2\lambda s} (w - \hat{w})^2 dx ds \\
&\quad + \frac{1}{2} \int_{Q_t} (h_2 - \hat{h}_2)^2 dx ds \\
&\leq \left(\frac{(\alpha_1 M + \alpha_1^2 M^2) e^{2\lambda T}}{2} \right) \int_{Q_t} (w - \hat{w})^2 dx ds \\
&\quad + \frac{1}{2} \int_{Q_t} (h_2 - \hat{h}_2)^2 dx ds
\end{aligned}$$

Thus, equation (2.20) can be estimated as

$$\begin{aligned}
\frac{1}{2} \int_{\Omega} (w - \hat{w})^2 dx + d \int_{Q_t} |\nabla(w - \hat{w})|^2 dx ds \\
+ \left(\lambda + \mu - \frac{\alpha_1(M + \alpha_1 M^2) e^{2\lambda T}}{2} \right) \int_{Q_t} (w - \hat{w})^2 dx ds \leq \frac{1}{2} \int_{Q_t} (h_2 - \hat{h}_2)^2 dx ds
\end{aligned} \tag{2.21}$$

and by taking λ large and T sufficiently small such that $\lambda + \mu - \frac{\alpha_1(M + \alpha_1 M^2)e^{2\lambda T}}{2} > 0$, we have that

$$\int_{\Omega} (w - \hat{w})^2 dx \leq \int_0^t \int_{\Omega} (h_2 - \hat{h}_2)^2 dx ds. \quad (2.22)$$

Similarly, multiply the second equation of system (2.19) by $(z - \hat{z})$ and integrate over Q_t ,

$$\begin{aligned} \frac{1}{2} \int_{\Omega} (z - \hat{z})^2 dx + (\lambda + q) \int_{Q_t} (z - \hat{z})^2 dx ds &= -\alpha_2 \int_{Q_t} e^{\lambda t} (h_1 z - \hat{h}_1 \hat{z})(z - \hat{z}) dx ds \\ &\quad + p\mu \int_{Q_t} (h_1 - \hat{h}_1)(z - \hat{z}) dx ds. \end{aligned} \quad (2.23)$$

The two integrals on the right hand side of equation (2.23) can be estimated as follows

$$\int_{Q_t} p\mu (h_1 - \hat{h}_1)(z - \hat{z}) dx ds \leq \frac{1}{2} \int_{Q_t} (h_1 - \hat{h}_1)^2 dx ds + \frac{(p\mu)^2}{2} \int_{Q_t} (z - \hat{z})^2 dx ds$$

and

$$\begin{aligned} \int_{Q_t} e^{\lambda s} \alpha_2 (h_1 z - \hat{h}_1 \hat{z})(z - \hat{z}) dx ds &= \int_{Q_t} \alpha_2 e^{\lambda s} (h_1(z - \hat{z}) + (h_1 - \hat{h}_1)\hat{z})(z - \hat{z}) dx ds \\ &= \int_{Q_t} \alpha_2 e^{\lambda s} h_1 (z - \hat{z})^2 dx ds + \int_{Q_t} \alpha_2 e^{\lambda s} \hat{z} (h_1 - \hat{h}_1)(z - \hat{z}) dx ds \\ &\leq \frac{\alpha_2 M e^{2\lambda T}}{2} \int_{Q_t} (z - \hat{z})^2 dx ds + \frac{\alpha_2^2}{2} \int_{Q_t} e^{2\lambda s} (\hat{z})^2 (z - \hat{z})^2 dx ds \\ &\quad + \frac{1}{2} \int_{Q_t} (h_1 - \hat{h}_1)^2 dx ds \\ &\leq \frac{\alpha_2 e^{2\lambda T} (M + \alpha_2 M^2)}{2} \int_{Q_t} (z - \hat{z})^2 dx ds + \frac{1}{2} \int_{Q_t} (h_1 - \hat{h}_1)^2 dx ds \end{aligned}$$

Putting together the latter two estimates in equation (2.23), we obtain the following estimate

$$\begin{aligned} \frac{1}{2} \int_{\Omega} (z - \hat{z})^2 dx ds + (\lambda + q) \int_{Q_t} (z - \hat{z})^2 dx ds &\leq \frac{\alpha_2 e^{2\lambda T} (M + \alpha_2 M^2) + (p\mu)^2}{2} \int_{Q_t} (z - \hat{z})^2 dx ds \\ &\quad + \int_{Q_t} (h_1 - \hat{h}_1)^2 dx ds \end{aligned} \quad (2.24)$$

and rearranging the terms in inequality (2.24) we see that

$$\frac{1}{2} \int_{\Omega} (z - \hat{z})^2 dx ds + \left(\lambda + q - \frac{\alpha_2 e^{2\lambda T} (M + M^2) + (p\mu)^2}{2} \right) \int_{Q_t} (z - \hat{z})^2 dx ds \leq \int_{Q_t} (h_1 - \hat{h}_1)^2 dx ds. \quad (2.25)$$

Taking λ large and T sufficiently small such that $\lambda + q - \frac{\alpha_2 e^{2\lambda T}(M + M^2) + p\mu}{2} > 0$, we note that

$$\int_{\Omega} (z - \hat{z})^2 dx ds \leq 2 \int_{Q_t} (h_1 - \hat{h}_1)^2 dx ds. \quad (2.26)$$

Taking square roots of inequalities (2.22) and (2.26) and then the supremum over all $t \in [0, T]$ yields

$$\sup_{0 \leq t \leq T} \|w - \hat{w}\|_{L^2(\Omega)} \leq \sqrt{T} \|h_2 - \hat{h}_2\|_{L^2(Q)} \leq \sqrt{2T} \|h_2 - \hat{h}_2\|_{L^2(Q)}$$

and

$$\|z - \hat{z}\|_{L^2(Q)} \leq \sqrt{2T} \sup_{0 \leq t \leq T} \|h_1 - \hat{h}_1\|_{L^2(\Omega)}.$$

It is clear that also

$$\sup_{0 \leq t \leq T} \|w - \hat{w}\|_{L^2(\Omega)} \leq \sqrt{2T} \left(\|h_2 - \hat{h}_2\|_{L^2(Q)} + \sup_{0 \leq t \leq T} \|h_1 - \hat{h}_1\|_{L^2(\Omega)} \right)$$

$$\|z - \hat{z}\|_{L^2(Q)} \leq \sqrt{2T} \left(\|h_2 - \hat{h}_2\|_{L^2(Q)} + \sup_{0 \leq t \leq T} \|h_1 - \hat{h}_1\|_{L^2(\Omega)} \right).$$

Finally, adding the latter two inequalities and choosing $T < \frac{1}{8}$ we are able to see that

$$\begin{aligned} \sup_{0 \leq t \leq T} \|w - \hat{w}\|_{L^2(\Omega)} + \|z - \hat{z}\|_{L^2(Q)} &\leq 2\sqrt{2T} \left(\|h_2 - \hat{h}_2\|_{L^2(Q)} \right. \\ &\quad \left. + \sup_{0 \leq t \leq T} \|h_1 - \hat{h}_1\|_{L^2(\Omega)} \right) \\ &\leq \gamma \left(\|h_2 - \hat{h}_2\|_{L^2(Q)} + \sup_{0 \leq t \leq T} \|h_1 - \hat{h}_1\|_{L^2(\Omega)} \right) \end{aligned} \quad (2.27)$$

where $\gamma < 1$. The last inequality shows that the operator A is a strict contraction. Hence, by Banach's fixed point theorem, there exists a unique solution $(w, z) \in (X_1 \times X_2) \cap (V_1 \times V_2)$ that solves system (2.15). Thus, for T sufficiently small, there exist non-negative solutions $(N, R) \in V_1 \times V_2$ of system (2.6). Moreover, it follows that

$$0 \leq N(x, t) \leq Me^{\lambda T} \quad \text{and} \quad 0 \leq R(x, t) \leq Me^{\lambda T} \quad \text{a.e. } (x, t) \in Q.$$

□

Remark 2.3.2. By Theorem 2.1 one can see that N and R are also uniformly bounded in $L^2(Q)$ since N and R are in $L^\infty(Q)$ and $Q = \Omega \times [0, T]$ is a bounded set. Thus, there exists a positive constant C such that

$$\|R\|_{L^2(Q)} \leq C \quad \text{and} \quad \|N\|_{L^2(Q)} \leq C.$$

Although Theorem 2.1 guarantees the existence of state solutions when T is sufficiently small, one can use the interval stacking methods to extend the existence of solutions for larger T . The method consists of applying Banach's fixed point theorem to find a solution on $[0, T_1]$. After that, we repeat the same process to extend the solution to $[T_1, T_2]$. This process can be continued several times to extend the existence of state solutions to longer time intervals.

Remark 2.3.3. The existence of weak solutions given in Theorem (2.1) also holds if zero Neumann boundary condition is chosen.

2.3.1 *A priori* Estimates

The following lemmas prove our *a priori* estimates. These estimates will be used later to show the existence and uniqueness of the optimal control with its corresponding state solutions and to obtain the adjoint equations and an optimal control characterization.

Lemma 2.2. Let N and R be weak solutions of problem (2.8)-(2.9) with $N_0(x) \geq 0$, then there exists a constant $B > 0$ depending only on given coefficients and final time T such that

$$\|N\|_{L^2(0,T;H_0^1(\Omega))} \leq B \|N_0\|_{L^\infty(\Omega)}.$$

Proof. Using the weak formulation in (2.8) with N as a test function, it can be seen that

$$\begin{aligned} \int_{\Omega} N_t N \, dx + d \int_{\Omega} |\nabla N|^2 \, dx &= \int_{\Omega} \alpha_1 R N^2 - \mu N^2 \, dx \\ &\leq C \alpha_1 \int_{\Omega} N^2 \, dx. \end{aligned}$$

From the above inequality we have that

$$\frac{d}{dt} \int_{\Omega} (N)^2 \, dx \leq 2C \alpha_1 \int_{\Omega} N^2 \, dx$$

and by Gronwall's inequality

$$\int_{\Omega} (N)^2(x, t) \, dx \leq e^{2C \alpha_1 T} \int_{\Omega} N_0^2 \, dx$$

and integrating over $[0, T]$ yields

$$\int_0^T \int_{\Omega} (N)^2(x, t) \, dx \leq T e^{2C \alpha_1 T} \int_{\Omega} N_0^2 \, dx \quad (2.28)$$

Similarly, from our first inequality on this proof, we see that

$$\int_{\Omega} |\nabla N|^2 \, dx \leq \frac{C \alpha_1}{d} \int_{\Omega} N^2 \, dx$$

and integrating over $[0, T]$ as well as using our estimate in (2.28)

$$\int_0^T \int_{\Omega} |\nabla N|^2 \, dx \leq \frac{T C \alpha_1}{d} e^{2C \alpha_1 T} \int_{\Omega} N_0^2 \, dx. \quad (2.29)$$

Combining inequalities (2.28) and (2.29) we obtain our desire inequality

$$\|N\|_{L^2(0, T; H_0^1(\Omega))}^2 \leq \left(\frac{C \alpha_1}{d} + 1\right) T e^{2C \alpha_1 T} |\Omega| \|N_0\|_{L^\infty(\Omega)}^2 \quad (2.30)$$

with $B = \left(\frac{C \alpha_1}{d} + 1\right) T e^{2C \alpha_1 T} |\Omega|$. □

Remark 2.3.4. *If we assume that $d \in [d_{\min}, d_{\max}]$, with $0 < d_{\min} < d_{\max}$, then the constant in Lemma 2.2 is given by $B = \left(\frac{C \alpha_1}{d_{\min}} + 1\right) T e^{2C \alpha_1 T} |\Omega|$.*

Lemma 2.3. *Let N and R be weak solutions of problem (2.8)-(2.9) with $N_0(x) \geq 0$, then there exists a constant $B_1 > 0$ depending on given data such that*

$$\|N_t\|_{L^2(0,T;H_0^1(\Omega)^*)} \leq B_1.$$

Proof. Let Φ be any test function. Using the weak formulation in (2.8) for the state N

$$\begin{aligned} \left| \int_0^T \langle N, \Phi \rangle dt \right| &= \left| \int_0^T \int_{\Omega} \alpha_1 N R \Phi - \mu N \Phi \, dx dt - d \int_0^T \int_{\Omega} \nabla N \cdot \nabla \Phi \, dx dt \right| \\ &\leq (\alpha_1 C + \mu) \int_0^T \int_{\Omega} |N \Phi| \, dx dt + d \int_0^T \int_{\Omega} |\nabla N \cdot \nabla \Phi| \, dx dt \\ &\leq (\alpha_1 C + \mu) \left(\int_0^T \int_{\Omega} |N|^2 \, dx dt \right)^{\frac{1}{2}} \left(\int_0^T \int_{\Omega} |\Phi|^2 \, dx dt \right)^{\frac{1}{2}} \\ &\quad + d \left(\int_0^T \int_{\Omega} |\nabla N|^2 \, dx dt \right)^{\frac{1}{2}} \left(\int_0^T \int_{\Omega} |\nabla \Phi|^2 \, dx dt \right)^{\frac{1}{2}}. \end{aligned}$$

Let $M = \max\{\alpha_1 C + \mu, d\}$ and using the estimate found in (2.30), we obtain

$$\left| \int_0^T \langle N, \Phi \rangle dt \right| \leq MB \|N_0\|_{L^\infty(\Omega)} \|\Phi\|_{L^2(0,T;H_0^1(\Omega))}$$

and hence we conclude that

$$\|N_t\|_{L^2(0,T;H_0^1(\Omega)^*)} \leq MB \|N_0\|_{L^\infty(\Omega)} \quad (2.31)$$

with $B_1 = MB \|N_0\|_{L^\infty(\Omega)}$. □

Remark 2.3.5. *The a priori estimates in Lemmas 2.2 and 2.3 also hold when zero Neumann boundary condition is applied.*

In the next section we formulate the optimal control problem and derive the necessary conditions for an optimal control.

2.4 Optimal Control Problem Formulation

Here, we present an optimal control problem applied to the resource allocation problem (2.6). Later, we derive necessary conditions for the solution of the optimal control. The maximization problem to analyze is

$$\sup_{I \in U} J(I) \quad \text{where } J(I) = \int_{\Omega} C_4 N(x, T) dx + \int_0^T \int_{\Omega} C_1 N - (C_3 + C_2 I) I dx dt$$

subject to

$$\begin{aligned} N_t - d\Delta N &= \alpha_1 N R - \mu N && \text{on } Q \\ R_t &= I(x, t) - \alpha_2 N R + p\mu N - qR && \text{on } Q \\ N(x, 0) &= N_0(x) && \text{on } \Omega \\ R(x, 0) &= R_0(x) && \text{on } \Omega \\ N(x, t) &= 0 && \text{on } \partial\Omega \times [0, T], \end{aligned} \tag{2.32}$$

where $Q = \Omega \times (0, T)$ with fixed final time T . The state variable $N = N(x, t)$ is measuring the population density while $R = R(x, t)$ represents the amount of resource available for the population, both at time t and position x . The set of admissible controls is

$$U = \left\{ I \in L^\infty(Q) \mid 0 \leq I(x, t) \leq M_1, \text{ a.e.} \right\}.$$

The objective functional $J(I)$ maximizes the total abundance of the population inside the habitat Ω and at the final time while minimizing the cost related to the input amount of resource. The constants C_i for $i = 1, 2, 3, 4$ represent the weight parameters associated with each term in the objective functional. These parameters determine the relative importance of each term in J . The two terms with N 's in the integrand in the objective functional,

$$\int_{\Omega} C_4 N(x, T) dx + \int_0^T \int_{\Omega} C_1 N dx dt,$$

represent the total *benefit* of maximizing the total population abundance at all times. And, the other two terms left with I 's inside the integrand represent the *cost* associated with the implementation of the optimal control.

2.4.1 Existence of an Optimal Control

We must show that there is a connection between a given control I and the state equations N and R . In other words, for any given admissible control $I \in U$ there exists a unique state solution (N, R) in their corresponding solution space using references [17, 26, 5].

Theorem 2.4. *There exist an optimal control $I^* \in U$ and corresponding states (N^*, R^*) that maximizes the objective functional*

$$J(I) = \int_{\Omega} C_4 N(x, T) dx + \int_0^T \int_{\Omega} C_1 N - (C_3 + C_2 I) I dx dt.$$

Proof. Observe that I is uniformly bounded in $L^\infty(Q)$. Also, N and R are uniformly bounded in $L^\infty(Q)$ by Theorem 2.1. It can be seen that

$$\begin{aligned} \sup_{I \in U} J(I) &= \sup_{I \in U} \int_{\Omega} C_4 N(x, T) dx + \sup_{I \in U} \int_0^T \int_{\Omega} C_1 N - (C_3 + C_2 I) I dx dt \\ &\leq \sup_{I \in U} \int_{\Omega} C_4 N(x, T) dx + \sup_{I \in U} \int_0^T \int_{\Omega} C_1 N dx dt \\ &\leq (C_4 + C_1 T) |\Omega| M e^{\lambda T} < \infty. \end{aligned}$$

Thus, there exist a maximizing sequence $I^n \in U$ such that

$$\lim_{n \rightarrow \infty} J(I^n) = \sup J(I).$$

By Theorem 2.1, we can guarantee the existence of a sequence of state solutions

$$(N^n, R^n) = (N(I^n), R(I^n))$$

given $I^n \in U$ for every n .

The next step is to determine uniform bounds for $\|N^n\|_{L^2(0,T;H_0^1(\Omega))}$, $\|N_t^n\|_{L^2(0,T;H_0^1(\Omega)^*)}$ and $\|R^n\|_{L^2(Q)}$ for all n . Since N^n is a weak solution of problem (2.8), we can apply Lemmas 2.2 and 2.3 to obtain uniform bounds for $\|N^n\|_{L^2(0,T;H_0^1(\Omega))}$ and $\|N_t^n\|_{L^2(0,T;H_0^1(\Omega)^*)}$. Similarly,

we can use remark 2.3.2 (since R^n is a weak solution of problem (2.8)) to obtain an uniform bound for $\|R^n\|_{L^2(Q)}$.

Due to $\|N^n\|_{L^2(0,T;H_0^1(\Omega))}$, $\|N_t^n\|_{L^2(0,T;H_0^1(\Omega)^*)}$ and $\|R^n\|_{L^2(Q)}$ are uniformly bounded independently of n and $I^n \in L^\infty(Q)$, there exist subsequences N^n , R^n and I^n such that

$$\begin{aligned} N^n &\rightharpoonup N^* \text{ weakly in } L^2(0, T; H_0^1(\Omega)) \\ N_t^n &\rightharpoonup N_t^* \text{ weakly in } L^2(0, T; H_0^1(\Omega)^*) \\ R^n &\rightharpoonup R^* \text{ weakly in } L^2(Q) \\ I^n &\rightharpoonup I^* \text{ weakly in } L^2(Q) \end{aligned}$$

One must show next that N^* and R^* are the corresponding state solutions associated with the optimal control I^* . The weak formulation of system (2.8) satisfied by N^n and R^n with a test function Φ is given by

$$\begin{aligned} \int_0^T \langle N_t^n, \Phi \rangle dt + d \int_0^T \int_\Omega \nabla N^n \cdot \nabla \Phi \, dx dt &= \int_0^T \int_\Omega \alpha_1 N^n(x, t) R^n(x, t) \Phi(x, t) \\ &\quad - \mu N(x, t) \Phi(x, t) \, dx dt \\ R^n(x, t) - R(x, 0) &= \int_0^t I^n(x, s) - \alpha_2 N^n(x, s) R^n(x, s) \\ &\quad + p \mu N^n(x, s) - q R^n(x, s) ds. \end{aligned} \tag{2.33}$$

We require stronger convergence results in system (2.33) in order to pass the limit. A compactness result of Simon in [45] guarantees that

$$N^n \rightarrow N^* \text{ strongly in } L^2(Q).$$

Observe that from the weak convergences, we have that

$$\begin{aligned} \lim_{n \rightarrow \infty} \int_0^T \langle N_t^n, \Phi \rangle dt &= \int_0^T \langle N_t^*, \Phi \rangle dt \\ \lim_{n \rightarrow \infty} \int_0^T \int_\Omega \nabla N^n \cdot \nabla \Phi \, dx dt &= \int_0^T \int_\Omega \nabla N^* \cdot \nabla \Phi \, dx dt \end{aligned}$$

and using the strong convergence of N and weak convergence of R we can see that

$$\begin{aligned}
& \left| \int_0^T \int_{\Omega} \alpha_1 \left(N^n(x, t) R^n(x, t) - N^*(x, t) R^*(x, t) \right) \Phi(x, t) \, dx dt \right| \\
& \leq \int_0^T \int_{\Omega} \alpha_1 \left| N^n(x, t) - N^*(x, t) \right| R^n(x, t) \Phi(x, t) \, dx dt \\
& \quad + \alpha_1 \left| \int_0^T \int_{\Omega} \left(R^n(x, t) - R^*(x, t) \right) N^*(x, t) \Phi(x, t) \, dx dt \right| \\
& \leq \alpha_1 C \|\Phi\|_{L^2(Q)} \|N^n - N^*\|_{L^2(Q)} + \alpha_1 \left| \int_0^T \int_{\Omega} \left(R^n(x, t) - R^*(x, t) \right) N^*(x, t) \Phi(x, t) \, dx dt \right| \\
& \rightarrow 0 \text{ as } n \rightarrow \infty.
\end{aligned}$$

Note that $N^* \Phi \in L^2(Q)$ since $N^* \in L^\infty(Q)$. Now, we can pass the limit as $n \rightarrow \infty$ in (2.33) and obtain that $(N^*, R^*) = (N(I^*), R(I^*))$. Finally, by the strong convergence of the sequence N^n and since the function

$$I \mapsto \int_0^T \int_{\Omega} (C_3 + C_2 I) I \, dx dt$$

is weakly lower semi-continuous in $L^2(Q)$ [20], we have that

$$\begin{aligned}
\int_0^T \int_{\Omega} (C_3 + C_2 I^*) I^* \, dx dt & \leq \liminf_{n \rightarrow \infty} \int_0^T \int_{\Omega} C_3 I^n \, dx dt + \liminf_{n \rightarrow \infty} \int_0^T \int_{\Omega} C_2 (I^n)^2 \, dx dt \\
& \leq \liminf_{n \rightarrow \infty} \int_0^T \int_{\Omega} (C_3 + C_2 I^n) I^n \, dx dt
\end{aligned}$$

which implies that

$$\begin{aligned}
-\int_0^T \int_{\Omega} (C_3 + C_2 I^*) I^* \, dx dt & \geq -\liminf_{n \rightarrow \infty} \int_0^T \int_{\Omega} C_3 I^n \, dx dt - \liminf_{n \rightarrow \infty} \int_0^T \int_{\Omega} C_2 (I^n)^2 \, dx dt \\
& = \limsup_{n \rightarrow \infty} \int_0^T \int_{\Omega} -C_3 I^n \, dx dt + \limsup_{n \rightarrow \infty} \int_0^T \int_{\Omega} -C_2 (I^n)^2 \, dx dt \\
& \geq \limsup_{n \rightarrow \infty} \int_0^T \int_{\Omega} -(C_3 + C_2 I^n) I^n \, dx dt.
\end{aligned}$$

Thus,

$$\begin{aligned} J(I^*) &= \int_{\Omega} C_4 N^*(x, T) \, dx + \int_0^T \int_{\Omega} C_1 N^* - (C_3 + C_2 I^*) I^* \, dx dt \\ &\geq \limsup_{n \rightarrow \infty} \int_{\Omega} C_4 N^n(x, T) \, dx + \limsup_{n \rightarrow \infty} \int_0^T \int_{\Omega} C_1 N^n - (C_3 + C_2 I^n) I^n \, dx dt, \end{aligned}$$

but our choice of the maximizing sequence I^n guarantees that

$$\begin{aligned} &\limsup_{n \rightarrow \infty} \int_{\Omega} C_4 N^n(x, T) \, dx + \limsup_{n \rightarrow \infty} \int_0^T \int_{\Omega} C_1 N^n - (C_3 + C_2 I^n) I^n \, dx dt \\ &\geq \lim_{n \rightarrow \infty} \int_{\Omega} C_4 N^n(x, T) \, dx + \int_0^T \int_{\Omega} C_1 N^n - (C_3 + C_2 I^n) I^n \, dx dt \\ &= \sup_{I \in U} J(I). \end{aligned}$$

Therefore, $I^* \in U$ is an optimal control that maximizes the objective functional J . $\square$

Remark 2.4.1. *The results of Theorem 2.4 can be generalized to more general coefficients depending on (x, t) . Moreover, the results would also hold if Neumann boundary condition is considered.*

2.4.2 Derivation of the Optimality System

In this section we investigate the existence of solutions to the sensitivity and adjoint systems. These systems will help to characterize the optimal control by connecting the state system with the objective functional.

The Sensitivity System

We start off this part with the following theorem that shows the existence of solutions to the sensitivity PDE system. The sensitivity PDE system is simply a linearized version of our nonlinear PDE in system (2.6).

Theorem 2.5. *(Sensitivities) The mapping $I \in U \mapsto (N, R) \in V_1 \times V_2$ is differentiable in the following sense: for each control $I \in U$ and $k \in L^\infty(Q)$ with $I + \epsilon k \in U$ for all $\epsilon > 0$*

sufficiently small, then there exist $\Psi_1 \in V_1$ and $\Psi_2 \in V_2$ such that

$$\begin{aligned} \frac{N^\epsilon - N}{\epsilon} &\rightharpoonup \Psi_1 && \text{in } V_1 \\ \frac{R^\epsilon - R}{\epsilon} &\rightharpoonup \Psi_2 && \text{in } V_2 \end{aligned}$$

as $\epsilon \rightarrow 0$. Moreover, the sensitivities Ψ_1 and Ψ_2 satisfy the following PDE system:

$$\begin{aligned} (\Psi_1)_t - d\Delta\Psi_1 &= \alpha_1(\Psi_1 R + \Psi_2 N) - \mu\Psi_1 && \text{on } Q \\ (\Psi_2)_t &= k - \alpha_2(\Psi_1 R + \Psi_2 N) + p\mu\Psi_1 - q\Psi_2 && \text{on } Q \\ \Psi_1(x, t) &= 0 && \text{on } \partial\Omega \times (0, T) \\ \Psi_1(x, 0) &= 0 && \text{on } \Omega \\ \Psi_2(x, 0) &= 0 && \text{on } \Omega. \end{aligned} \tag{2.34}$$

Proof. Choose $k \in L^\infty(Q)$ and $I \in U$ such that $I^\epsilon = I + \epsilon k \in U$ for any small positive ϵ . Let (N^ϵ, R^ϵ) and (N, R) be the corresponding states for the controls I^ϵ and I . Consider the following difference quotients $\frac{N^\epsilon - N}{\epsilon}$ and $\frac{R^\epsilon - R}{\epsilon}$ and the equations satisfied by them with their respective boundary and initial conditions

$$\begin{aligned} \left(\frac{N^\epsilon - N}{\epsilon}\right)_t - d\Delta\left(\frac{N^\epsilon - N}{\epsilon}\right) &= \alpha_1 \frac{N^\epsilon R^\epsilon - NR}{\epsilon} - \mu \frac{N^\epsilon - N}{\epsilon} \\ \left(\frac{R^\epsilon - R}{\epsilon}\right)_t &= k - \alpha_2 \frac{N^\epsilon R^\epsilon - NR}{\epsilon} + p\mu \frac{N^\epsilon - N}{\epsilon} - q \frac{R^\epsilon - R}{\epsilon} \\ \frac{N^\epsilon(x, 0) - N(x, 0)}{\epsilon} &= 0 \\ \frac{R^\epsilon(x, 0) - R(x, 0)}{\epsilon} &= 0 \\ \frac{N^\epsilon - N}{\epsilon} &= 0 \quad \text{on } \partial\Omega \times (0, T). \end{aligned} \tag{2.35}$$

We proceed to show that the difference quotients are uniformly bounded in their corresponding spaces given ϵ small. Observe that the second equation can be written as

$$\left(\frac{R^\epsilon - R}{\epsilon}\right)_t = k + (p\mu - \alpha_2 R^\epsilon) \frac{N^\epsilon - N}{\epsilon} - (q + \alpha_2 N) \frac{R^\epsilon - R}{\epsilon}$$

and rearranging the terms

$$\left(\frac{R^\epsilon - R}{\epsilon}\right)_t + (q + \alpha_2 N) \frac{R^\epsilon - R}{\epsilon} = k + (p\mu - \alpha_2 R^\epsilon) \frac{N^\epsilon - N}{\epsilon}.$$

We can write the above ODE as

$$v'(x, t) + a(x, t)v(x, t) = k(x, t) + b(x, t)u(x, t)$$

where v and u represent the corresponding difference quotients and the function k , a and b are $L^\infty(Q)$ bounded. Solving the above ODE using integrating factor technique we obtain that

$$v(x, t) = e^{-\int_0^t a(x, s) ds} \int_0^t e^{\int_0^s a(x, \tau) d\tau} \left(k(x, s) + b(x, s)u(x, s) \right) ds.$$

It can be shown that the function $v(x, t)$ can be estimated as

$$v(x, t) \leq e^{CT} \left(CT + C \int_0^t u(x, s) ds \right)$$

where $C = \max\{\sup k, \sup a, \sup b\}$ is independent of ϵ . Thus, squaring both sides and integrating over Q_t

$$\begin{aligned} \int_{Q_t} v^2(x, t) dx dt &\leq |Q_t| e^{2CT} (CT)^2 + 2e^{2CT} C^2 T \int_{Q_t} u(x, s) dx ds \\ &\quad + e^{2CT} C^2 T \int_{\Omega} \left(\int_0^t u(x, s) ds \right)^2 dx \\ &\leq |Q_t| e^{2CT} C^2 T (C + 1) + e^{2CT} C^2 T |Q_t| \int_{Q_t} u^2(x, t) dx dt \\ &\quad + e^{2CT} C^2 T \int_{\Omega} \left(\int_0^t u(x, s) ds \right)^2 dx \end{aligned}$$

with $|Q_t|$ being the measure of Q_t and taking square roots

$$\begin{aligned} \|v\|_{L^2(Q_t)} &\leq \sqrt{|Q_t| T (C + 1)} e^{CT} C + e^{CT} C \sqrt{T |Q_t|} \|u\|_{L^2(Q_t)} + e^{CT} C \sqrt{T} \int_{Q_t} u(x, s) dx ds \\ &\leq \sqrt{|Q_t| T (C + 1)} e^{CT} C + e^{CT} C \sqrt{T |Q_t|} \|u\|_{L^2(Q_t)} + e^{CT} C \sqrt{|Q_t| T} \|u\|_{L^2(Q_t)} \\ &= \sqrt{|Q_t| T (C + 1)} e^{CT} C + 2e^{CT} C \sqrt{T |Q_t|} \|u\|_{L^2(Q_t)}. \end{aligned}$$

If we return to our initial difference quotients and since $|Q_t| \leq |Q|$ yields to the following inequality

$$\left\| \frac{R^\epsilon - R}{\epsilon} \right\|_{L^2(Q)} \leq C_1(T, |Q|, C) + C_2(T, |Q|, C) \left\| \frac{N^\epsilon - N}{\epsilon} \right\|_{L^2(Q)}. \quad (2.36)$$

where the constants C_1 and C_2 do not depend on our choice of ϵ .

Now, we multiply the first equation in system (2.35) by the test function $\frac{N^\epsilon - N}{\epsilon}$ and integrate over Q_t :

$$\begin{aligned} \frac{1}{2} \int_{\Omega} \left(\frac{N^\epsilon - N}{\epsilon} \right)^2 dx + d \int_{Q_t} \left| \nabla \left(\frac{N^\epsilon - N}{\epsilon} \right) \right|^2 dx ds &= \alpha_1 \int_{Q_t} \frac{N^\epsilon R^\epsilon - N R}{\epsilon} \frac{N^\epsilon - N}{\epsilon} dx ds \\ &\quad - \mu \int_{Q_t} \left(\frac{N^\epsilon - N}{\epsilon} \right)^2 dx ds \\ &= \alpha_1 \int_{Q_t} R^\epsilon \left(\frac{N^\epsilon - N}{\epsilon} \right)^2 dx ds \\ &\quad + \alpha_1 \int_{Q_t} N \frac{(N^\epsilon - N)(R^\epsilon - R)}{\epsilon^2} dx ds \\ &\quad - \mu \int_{Q_t} \left(\frac{N^\epsilon - N}{\epsilon} \right)^2 dx ds \\ &\leq \alpha_1 M \int_{Q_t} \left(\frac{N^\epsilon - N}{\epsilon} \right)^2 dx ds \\ &\quad + \alpha_1 M \int_{Q_t} \frac{(N^\epsilon - N)(R^\epsilon - R)}{\epsilon^2} dx ds \\ &\leq \left(\alpha_1 M + \frac{\alpha_1 M}{2} \right) \int_{Q_t} \left(\frac{N^\epsilon - N}{\epsilon} \right)^2 dx ds \\ &\quad + \frac{\alpha_1 M}{2} \int_{Q_t} \left(\frac{R^\epsilon - R}{\epsilon} \right)^2 dx ds. \end{aligned}$$

where $M = \sup\{N, R^\epsilon\}$ is a uniform bound by Theorem 2.1. Using our estimate in (2.36) in the above inequality it can be seen that

$$\begin{aligned} \frac{1}{2} \int_{\Omega} \left(\frac{N^\epsilon - N}{\epsilon} \right)^2 dx + d \int_{Q_t} \left| \nabla \left(\frac{N^\epsilon - N}{\epsilon} \right) \right|^2 dx ds \\ \leq \left(\alpha_1 M + \frac{\alpha_1 M}{2} + \frac{C_2 \alpha_1 M}{2} \right) \int_{Q_t} \left(\frac{N^\epsilon - N}{\epsilon} \right)^2 dx ds + \frac{C_1 \alpha_1 M}{2} \end{aligned} \quad (2.37)$$

Using similar techniques to those applied in Lemma 2.2 in with the inequality in (2.37) we can obtain a uniform bound for $\frac{N^\epsilon - N}{\epsilon}$ in $L^2(0, T; H_0^1(\Omega))$, that is

$$\left\| \frac{N^\epsilon - N}{\epsilon} \right\|_{L^2(0, T; H_0^1(\Omega))} \leq C_3$$

which also implies that $\frac{R^\epsilon - R}{\epsilon}$ is uniformly bounded in $L^2(Q)$, so

$$\left\| \frac{R^\epsilon - R}{\epsilon} \right\|_{L^2(Q)} \leq C_4$$

where C_3 and C_4 only depend on T , $|Q|$, C and M . Such bounds guarantee the existence of $\Psi_1 \in V_1$ and $\Psi_2 \in V_2$ with the corresponding convergence of the difference quotients, that is

$$\begin{aligned} \frac{N^\epsilon - N}{\epsilon} &\rightharpoonup \Psi_1 \text{ in } V_1 \\ \frac{R^\epsilon - R}{\epsilon} &\rightharpoonup \Psi_2 \text{ in } V_2. \end{aligned}$$

Similarly, using the techniques in Lemma 2.3 with the estimate in 2.2 it can be shown that $\left(\frac{N^\epsilon - N}{\epsilon} \right)_t$ is uniformly bounded in $L^2(0, T; H_0^1(\Omega)^*)$, hence

$$\left(\frac{N^\epsilon - N}{\epsilon} \right)_t \rightharpoonup (\Psi_1)_t \text{ in } L^2(0, T; H_0^1(\Omega)^*).$$

In the same way as in the proof of Theorem 2.4 we have that $\frac{N^\epsilon - N}{\epsilon}$ converges strongly in $L^2(Q)$, thus

$$\frac{N^\epsilon - N}{\epsilon} \rightarrow \Psi_1 \text{ in } L^2(Q).$$

Finally, we pass the limit as $\epsilon \rightarrow 0$ in system (2.35) and see that the sensitivity functions Ψ_1 and Ψ_2 solve system (2.34). $\square$

Theorem 2.5 guarantees the existence of the sensitivity system. We are now ready to show the existence and determine conditions of the adjoint system.

The Adjoint System

The sensitivities Ψ_1 and Ψ_2 solve a linearized version of the PDE system (2.6). Note also that the sensitivity PDE system (2.34) for Ψ_1 and Ψ_2 can be written in vector form as

$$\begin{aligned} L\Psi &= \begin{pmatrix} L_1\Psi_1 \\ L_2\Psi_2 \end{pmatrix} + M \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ k \end{pmatrix} \quad \text{on } Q \\ \Psi_1(x, 0) &= 0 \quad \text{on } \Omega \\ \Psi_2(x, 0) &= 0 \quad \text{on } \Omega \\ \Psi_1(x, t) &= 0 \quad \text{on } \partial\Omega \times (0, T) \end{aligned}$$

where

$$\begin{aligned} L_1\Psi_1 &= (\Psi_1)_t - d\Delta\Psi_1 \\ L_2\Psi_2 &= (\Psi_2)_t \end{aligned}$$

and

$$M = \begin{pmatrix} \mu - \alpha_1 R & -\alpha_1 N \\ \alpha_2 R - p\mu & q + \alpha_2 N \end{pmatrix}.$$

We are ready to find the adjoint operator L^* . For any $\vec{\lambda} = (\lambda_1, \lambda_2) \in V_1 \times V_2$, we need to show

$$\begin{aligned} \int_Q \vec{\lambda} L(\vec{\Psi}) \, dxdt &= \int_Q (\lambda_1, \lambda_2) \begin{pmatrix} L_1\Psi_1 \\ L_2\Psi_2 \end{pmatrix} \, dxdt = \int_Q (\Psi_1, \Psi_2) \begin{pmatrix} L_1^*\lambda_1 \\ L_2^*\lambda_2 \end{pmatrix} \, dxdt \\ &= \int_Q \vec{\Psi} L^*(\vec{\lambda}) \, dxdt \end{aligned} \tag{2.38}$$

in the corresponding weak sense. First, we formally start by multiplying λ_1 times the first component of $L(\vec{\Psi})$ and integrate over our domain Q . In other words, use λ_1 as a test function in the weak solution form of Ψ_1 :

$$\begin{aligned} \int_0^T \int_\Omega \lambda_1 L_1\Psi_1 + \lambda_1 (\Psi_1(\mu - \alpha_1 R) - \Psi_2\alpha_1 N) \, dxdt &= \int_0^T \int_\Omega L_1^*\lambda_1 \Psi_1 \\ &\quad + \lambda_1 (\Psi_1(\mu - \alpha_1 R) - \Psi_2\alpha_1 N) \, dxdt. \end{aligned}$$

Note that the L_1^* operator can be found using integration by parts and assuming the corresponding initial condition of Ψ_1 as well as boundary and transversality conditions for λ_1 ($\lambda_1(x, T) = C4$),

$$\begin{aligned} \int_0^T \int_{\Omega} \lambda_1 L_1 \Psi_1 \, dx dt &= \int_0^T \int_{\Omega} \lambda_1 ((\Psi_1)_t - d \nabla \cdot \nabla \Psi_1) \, dx dt \\ &= \int_{\Omega} \lambda_1(x, T) \Psi_1(x, T) \, dx + \int_0^T \int_{\Omega} (-(\lambda_1)_t - d \nabla \cdot \nabla \lambda_1) \Psi_1 \, dx dt \\ &= \int_{\Omega} C4 \Psi_1(x, T) \, dx + \int_0^T \int_{\Omega} \left(L_1^* \lambda_1 \right) \Psi_1 \, dx dt \end{aligned}$$

Second, we use λ_2 as a test function in the weak solution form of Ψ_2 , then

$$\begin{aligned} \int_0^T \int_{\Omega} \lambda_2 L_2 \Psi_2 + \lambda_2 (\Psi_1(\alpha_2 R - p\mu) + \Psi_2(q + \alpha_2 N)) \, dx dt &= \int_0^T \int_{\Omega} \left(L_2^* \lambda_2 \right) \Psi_2 \\ &\quad + \lambda_2 (\Psi_1(\alpha_2 R - p\mu) \\ &\quad + \Psi_2(q + \alpha_2 N)) \, dx dt. \end{aligned}$$

To determine L_2^* operator we use integration by parts one more time and the corresponding initial condition of Ψ_2 and transversality condition for λ_2 ($\lambda_2(x, T) = 0$),

$$\begin{aligned} \int_0^T \int_{\Omega} \lambda_2 L_2 \Psi_2 \, dx dt &= \int_0^T \int_{\Omega} \lambda_2 (\Psi_2)_t \, dx dt \\ &= \int_0^T \int_{\Omega} -(\lambda_2)_t \Psi_2 \, dx dt \\ &= \int_0^T \int_{\Omega} \left(L_2^* \lambda_2 \right) \Psi_2 \, dx dt \end{aligned}$$

The functions λ_1 and λ_2 are the adjoint variables and they will satisfy the following PDE system:

$$L^* \lambda = \begin{pmatrix} L_1^* \lambda_1 \\ L_2^* \lambda_2 \end{pmatrix} + M^T \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = \begin{pmatrix} C_1 \\ 0 \end{pmatrix} \quad \text{on } Q \quad (2.39)$$

with transversality conditions and boundary condition

$$\lambda_1(x, T) = C_4 \quad \text{on } \Omega$$

$$\begin{aligned}
\lambda_2(x, T) &= 0 && \text{on } \Omega \\
\lambda_1(x, t) &= 0 && \text{on } \partial\Omega \times (0, T)
\end{aligned}$$

where

$$\begin{aligned}
L_1^* \lambda_1 &= -(\lambda_1)_t - d\Delta \lambda_1 \\
L_2^* \lambda_2 &= -(\lambda_2)_t.
\end{aligned} \tag{2.40}$$

The right hand side of the adjoint equations for λ_1 and λ_2 are the corresponding derivatives of the integrand of the objective functional with respect to the states N and R respectively.

Consequently,

$$\frac{\partial \text{integrand of } J}{\partial N} = C_1 \quad \text{and} \quad \frac{\partial \text{integrand of } J}{\partial R} = 0.$$

Theorem 2.6. *Given an optimal control I^* and its corresponding state solutions (N^*, R^*) , there exist a weak solution $(\lambda_1, \lambda_2) \in V_1 \times V_2$ that satisfies the adjoint system (2.39). Moreover, the optimal control characterization is given by*

$$I^*(x, t) = \min \left\{ M_1, \max \left\{ 0, \frac{\lambda_2(x, t) - C_3}{2C_2} \right\} \right\} \tag{2.41}$$

for any $(x, t) \in Q$ and any positive constants C_2 and C_3 .

Proof. Let $I^* \in U$ be an optimal control and $(N^*, R^*) = (N(I^*), R(I^*))$ be its corresponding state weak solutions. Thus, the associated adjoint system to the optimal control is given by

$$\begin{aligned}
-(\lambda_1)_t - d\Delta \lambda_1 + (\mu - \alpha_1 R^*) \lambda_1 + (\alpha_2 R^* - p\mu) \lambda_2 &= C_1 && \text{on } Q \\
-(\lambda_2)_t - \alpha_1 N^* \lambda_1 + (q + \alpha_2 N^*) \lambda_2 &= 0 && \text{on } Q \\
\lambda_1(x, T) &= C_4 && \text{on } \Omega \\
\lambda_2(x, T) &= 0 && \text{on } \Omega \\
\lambda_1(x, t) &= 0 && \text{on } \partial\Omega \times (0, T).
\end{aligned} \tag{2.42}$$

Since the adjoint system (2.42) is linear with respect to the adjoint variables λ_1 and λ_2 , there exists weak solution $(\lambda_1, \lambda_2) \in V_1 \times V_2$ that satisfies system (2.42). In order to determine the

optimal control characterization, we start off by differentiating the map $I \mapsto J(I)$. Define $I^\epsilon = I^* + \epsilon k \in U$ with $(N^\epsilon, R^\epsilon) = (N(I^\epsilon), R(I^\epsilon))$ be its corresponding state variables. Observe that since I^* was chosen to be the optimal control, then the maximum objective functional is achieved at I^* such that

$$\begin{aligned} \frac{J(I^\epsilon) - J(I^*)}{\epsilon} &= \int_{\Omega} C_4 \frac{N^\epsilon(x, T) - N(x, T)}{\epsilon} dx \\ &\quad + \int_0^T \int_{\Omega} C_1 \frac{N^\epsilon - N}{\epsilon} - C_3 \frac{I^\epsilon - I^*}{\epsilon} - C_2 \frac{(I^\epsilon)^2 - (I^*)^2}{\epsilon} dx dt. \end{aligned}$$

Passing the limit as $\epsilon \rightarrow 0^+$,

$$\begin{aligned} 0 &\geq \lim_{\epsilon \rightarrow 0^+} \int_{\Omega} C_4 \frac{N^\epsilon(x, T) - N(x, T)}{\epsilon} dx \\ &\quad + \lim_{\epsilon \rightarrow 0^+} \int_0^T \int_{\Omega} C_1 \frac{N^\epsilon - N^*}{\epsilon} - C_3 \frac{I^\epsilon - I^*}{\epsilon} - C_2 \frac{(I^\epsilon - I^*)(I^\epsilon + I^*)}{\epsilon} dx dt \\ &= \int_{\Omega} C_4 \Psi_1(x, T) dx + \int_0^T \int_{\Omega} C_1 \Psi_1 - k(C_3 + 2C_2 I^*) dx dt \\ &= \int_{\Omega} C_4 \Psi_1(x, T) dx + \int_0^T \int_{\Omega} \begin{pmatrix} \Psi_1 & \Psi_2 \end{pmatrix} \begin{pmatrix} C_1 \\ 0 \end{pmatrix} - k(C_3 + 2C_2 I^*) dx dt \\ &= \int_{\Omega} C_4 \Psi_1(x, T) dx + \int_0^T \int_{\Omega} \begin{pmatrix} \Psi_1 & \Psi_2 \end{pmatrix} L^* \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} - k(C_3 + 2C_2 I^*) dx dt \\ &= \int_0^T \int_{\Omega} \begin{pmatrix} \lambda_1 & \lambda_2 \end{pmatrix} L \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} - k(C_3 + 2C_2 I^*) dx dt \\ &= \int_0^T \int_{\Omega} \begin{pmatrix} \lambda_1 & \lambda_2 \end{pmatrix} \begin{pmatrix} 0 \\ k \end{pmatrix} - k(C_3 + 2C_2 I^*) dx dt \\ &= \int_0^T \int_{\Omega} k(\lambda_2 - C_3 - 2C_2 I^*) dx dt. \end{aligned}$$

From the above calculations we can conclude that

$$0 \geq \int_0^T \int_{\Omega} k(\lambda_2 - C_3 - 2C_2 I^*) dx dt \quad (2.43)$$

In order to provide a full characterization of the optimal control pair I^* , we analyze more in depth inequality (2.43) through the following cases:

Case 1: Consider the set $U_1 = \{(x, t) \in Q \mid 0 < I^*(x, t) < M_1\}$. The variation function k can have any sign and it has compact support on U_1 . Then, we force $\lambda_2 - C_3 - 2C_2 I^* = 0$ for inequality (2.43) to hold. Thus, $I^*(x, t) = \frac{\lambda_2(x, t) - C_3}{2C_2}$ on U_1 .

Case 2: Consider the set $U_2 = \{(x, t) \in Q \mid I^*(x, t) = 0\}$. In this case the variation function satisfies $k \geq 0$ with compact support on U_2 . Then, we force $\lambda_2 - C_3 - 2C_2 I^* \leq 0$ for inequality (2.43) to hold. Thus, $\lambda_2(x, t) \leq C_3$ on U_2 .

Case 3: Consider the set $U_3 = \{(x, t) \in Q \mid I^*(x, t) = M_1\}$. In this case the variation function satisfies $k \leq 0$ with compact support on U_3 . Then, we force $\lambda_2 - C_3 - 2C_2 I^* \geq 0$ for inequality (2.43) to hold. Thus, $\frac{\lambda_2(x, t) - C_3}{2C_2} \geq M_1$ on U_3 .

Considering all the three cases above, we obtain that the optimal control characterization is

$$I^*(x, t) = \min \left\{ M_1, \max \left\{ 0, \frac{\lambda_2(x, t) - C_3}{2C_2} \right\} \right\} \quad (2.44)$$

for any $(x, t) \in Q$ and any positive constant C_2 and C_3 . $\square$

Remark 2.4.2. Notice that the differential equation for λ_2 in the adjoint system (2.42) is not defined at the spatial boundary. However, one can show that $\lambda_2 = 0$ at the boundary. One can assume that the λ_2 equation holds at the boundary $\partial\Omega \times (0, T]$, then it is easy to see that the equation reduces to

$$-(\lambda_2)_t + q\lambda_2 = 0.$$

Solving the above differential equation and using that $\lambda_2(x, T) = 0$ yields

$$\int_t^T \frac{d}{dt} \left[\lambda_2(x, t) e^{-qt} \right] dt = \lambda_2(x, T) e^{-qT} - \lambda_2(x, t) e^{-qt} = 0.$$

From here, we observe that $\lambda_2(x, t) = 0$ at the boundary.

Remark 2.4.3. By remark 2.4.2 we know that $\lambda_2 = 0$ at the spatial boundary. Using the optimal control characterization in (2.44), the optimal control must also be zero at the boundary.

In the following section we define the optimality system and derive conditions for the uniqueness of the optimal control problem.

The Optimality System

The optimality system for the resource allocation model is formed by the state equations in (2.6), the adjoint system (2.42) and the optimal control characterization in (2.44). The following theorem shows that the optimal control may be unique under certain conditions.

Theorem 2.7. *If $C_2 \neq 0$ and T is sufficiently small, then the optimal control of problem (2.6) is unique.*

Proof. Let (N, R) with (λ_1, λ_2) and $(\hat{N}, \hat{R})$ with $(\hat{\lambda}_1, \hat{\lambda}_2)$ be two solutions of the optimality system formed by systems (2.6) and (2.42). The corresponding optimal controls for both of the solutions are determined by

$$I(x, t) = \min \left\{ M_1, \max \left\{ 0, \frac{\lambda_2(x, t) - C_3}{2C_2} \right\} \right\} \text{ and } \hat{I}(x, t) = \min \left\{ M_1, \max \left\{ 0, \frac{\hat{\lambda}_2(x, t) - C_3}{2C_2} \right\} \right\}.$$

Consider the following change of functions:

$$\begin{aligned} w &= e^{-\lambda t} N, & z &= e^{-\lambda t} R, & p_1 &= e^{\lambda t} \lambda_1, & p_2 &= e^{\lambda t} \lambda_2, \\ \hat{w} &= e^{-\lambda t} \hat{N}, & \hat{z} &= e^{-\lambda t} \hat{R}, & \hat{p}_1 &= e^{\lambda t} \hat{\lambda}_1, & \hat{p}_2 &= e^{\lambda t} \hat{\lambda}_2. \end{aligned}$$

Subsequently, consider the differences $w - \hat{w}$, $z - \hat{z}$, $p_1 - \hat{p}_1$, $p_2 - \hat{p}_2$ with their associated PDE problems:

$$\begin{aligned} (w - \hat{w})_t - d\Delta(w - \hat{w}) + \lambda(w - \hat{w}) &= \alpha_1 e^{\lambda t} (wz - \hat{w}\hat{z}) - \mu(w - \hat{w}) && \text{on } Q \\ (z - \hat{z})_t + \lambda(z - \hat{z}) &= (I - \hat{I})e^{-\lambda t} - \alpha_2 e^{\lambda t} (wz - \hat{w}\hat{z}) \\ &\quad + p\mu(w - \hat{w}) - q(z - \hat{z}) && \text{on } Q \\ (w - \hat{w})(x, 0) &= 0 && \text{on } \Omega \\ (z - \hat{z})(x, 0) &= 0 && \text{on } \Omega \\ (w - \hat{w})(x, t) &= 0 && \text{on } \partial\Omega \times [0, T] \end{aligned}$$

and

$$\begin{aligned}
& -(p_1 - \hat{p}_1)_t - d\Delta(p_1 - \hat{p}_1) + (\lambda + \mu)(p_1 - \hat{p}_1) - \alpha_1 e^{\lambda t}(zp_1 - \hat{z}\hat{p}_1) \\
& \quad + \alpha_2 e^{\lambda t}(zp_2 - \hat{z}\hat{p}_2) - p\mu(p_2 - \hat{p}_2) = C_1 e^{\lambda t} \quad \text{on } Q \\
& -(p_2 - \hat{p}_2)_t + (\lambda + q)(p_2 - \hat{p}_2) - \alpha_1 e^{\lambda t}(wp_1 - \hat{w}\hat{p}_1) \\
& \quad + \alpha_2 e^{\lambda t}(wp_2 - \hat{w}\hat{p}_2) = 0 \quad \text{on } Q \\
& (p_1 - \hat{p}_1)(x, T) = 0 \quad \text{on } \Omega \\
& (p_2 - \hat{p}_2)(x, T) = 0 \quad \text{on } \Omega \\
& (p_1 - \hat{p}_1)(x, t) = 0 \quad \text{on } \partial\Omega \times (0, T).
\end{aligned}$$

We multiply the difference quotient PDEs stated above by appropriately test functions and integrate over $Q = \Omega \times (0, T)$ such that

$$\begin{aligned}
& \frac{1}{2} \int_{\Omega} (w - \hat{w})^2(x, T) \, dx + d \int_Q |\nabla(w - \hat{w})|^2 \, dxds \\
& \quad + (\lambda + \mu) \int_Q (w - \hat{w})^2 \, dxds = \alpha_1 \int_Q e^{\lambda s} (wz - \hat{w}\hat{z})(w - \hat{w}) \, dxds \\
& \frac{1}{2} \int_{\Omega} (z - \hat{z})^2(x, T) \, dx + (\lambda + q) \int_Q (z - \hat{z})^2 \, dxds = \int_Q e^{\lambda s} (I - \hat{I})(z - \hat{z}) \, dxds \\
& \quad - \alpha_2 \int_Q e^{\lambda s} (wz - \hat{w}\hat{z})(z - \hat{z}) \, dxds \\
& \quad + p\mu \int_Q (w - \hat{w})(z - \hat{z}) \, dxds
\end{aligned} \tag{2.45}$$

$$\begin{aligned}
& \frac{1}{2} \int_{\Omega} (p_1 - \hat{p}_1)^2(x, 0) \, dx + d \int_Q |\nabla(p_1 - \hat{p}_1)|^2 \, dxds \\
& \quad + (\lambda + \mu) \int_Q (p_1 - \hat{p}_1)^2 \, dxds = C_1 \int_Q e^{\lambda s} (p_1 - \hat{p}_1) \, dxds \\
& \quad + \alpha_1 \int_Q e^{\lambda s} (zp_1 - \hat{z}\hat{p}_1)(p_1 - \hat{p}_1) \, dxds \\
& \quad - \alpha_2 \int_Q e^{\lambda s} (zp_2 - \hat{z}\hat{p}_2)(p_1 - \hat{p}_1) \, dxds \\
& \quad + p\mu \int_Q (p_2 - \hat{p}_2)(p_1 - \hat{p}_1) \, dxds \\
& \frac{1}{2} \int_{\Omega} (p_2 - \hat{p}_2)^2(x, 0) \, dx + (\lambda + q) \int_Q (p_2 - \hat{p}_2)^2 \, dxds = \alpha_1 \int_Q e^{\lambda s} (wp_1 - \hat{w}\hat{p}_1)(p_2 - \hat{p}_2) \, dxds \\
& \quad - \alpha_2 \int_Q e^{\lambda s} (wp_2 - \hat{w}\hat{p}_2)(p_2 - \hat{p}_2) \, dxds
\end{aligned} \tag{2.46}$$

We proceed to estimate the right hand side of the 4 equations in (2.45) and (2.46). We start off by estimating

$$\begin{aligned}
\left| \int_Q e^{-\lambda s} (I - \hat{I})(z - \hat{z}) \, dx ds \right| &\leq \int_Q |(I - \hat{I})(z - \hat{z})| \, dx ds \\
&= \int_Q \left| \min \left\{ M_1, \max \left\{ 0, \frac{\lambda_2 - C_3}{2C_2} \right\} \right\} \right. \\
&\quad \left. - \min \left\{ M_1, \max \left\{ 0, \frac{\hat{\lambda}_2 - C_3}{2C_2} \right\} \right\} \right| |z - \hat{z}| \, dx ds \\
&\leq \int_Q \left| \frac{\lambda_2(x, s) - \hat{\lambda}_2(x, s)}{2C_2} \right| |z - \hat{z}| \, dx ds \\
&= \frac{1}{2C_2} \int_Q e^{-\lambda s} |p_2(x, t) - \hat{p}_2(x, t)| |z - \hat{z}| \, dx ds \\
&\leq \frac{1}{4C_2} \left(\int_Q (p_2 - \hat{p}_2)^2 \, dx ds + \int_Q (z - \hat{z})^2 \, dx ds \right) \\
&\leq \bar{C} \left(\int_Q (z - \hat{z})^2 \, dx ds + \int_Q (w - \hat{w})^2 \, dx ds \right. \\
&\quad \left. + \int_Q (p_1 - \hat{p}_1)^2 \, dx ds + \int_Q (p_2 - \hat{p}_2)^2 \, dx ds \right)
\end{aligned}$$

where $\bar{C} = \frac{1}{4C_2}$. Note also that

$$\begin{aligned}
\int_Q e^{\lambda s} (wz - \hat{w}\hat{z})(w - \hat{w}) \, dx ds &\leq e^{\lambda T} \int_Q w(w - \hat{w})(z - \hat{z}) + \hat{z}(w - \hat{w})^2 \, dx ds \\
&\leq e^{2\lambda T} M \int_Q (w - \hat{w})(z - \hat{z}) + (w - \hat{w})^2 \, dx ds \\
&\leq e^{2\lambda T} M \left(\int_Q (z - \hat{z})^2 \, dx ds + \frac{3}{2} \int_Q (w - \hat{w})^2 \, dx ds \right) \quad (2.47) \\
&\leq Ce^{2\lambda T} \left(\int_Q (z - \hat{z})^2 \, dx ds + \int_Q (w - \hat{w})^2 \, dx ds \right. \\
&\quad \left. + \int_Q (p_1 - \hat{p}_1)^2 \, dx ds + \int_Q (p_2 - \hat{p}_2)^2 \, dx ds \right)
\end{aligned}$$

where C is a constant depending on the final time T , $|Q|$, bounds over the parameter space as well as L^∞ bounds of the state and adjoint solutions. Hence, adding up the estimates for the four integrals in (2.45) and (2.46) combined with similar estimate techniques as (2.47),

we can see that

$$\begin{aligned}
& \frac{1}{2} \int_{\Omega} (w - \hat{w})^2(x, T) \, dx + d \int_Q |\nabla(w - \hat{w})|^2 \, dx ds + \mu \int_Q (w - \hat{w})^2 \, dx ds \\
& \quad + \frac{1}{2} \int_{\Omega} (z - \hat{z})^2(x, T) \, dx + q \int_Q (z - \hat{z})^2 \, dx ds \\
& \quad + \frac{1}{2} \int_{\Omega} (p_1 - \hat{p}_1)^2(x, 0) + d \int_Q |\nabla(p_1 - \hat{p}_1)|^2 \, dx ds \\
& \quad + \mu \int_Q (p_1 - \hat{p}_1)^2 \, dx ds + \frac{1}{2} \int_{\Omega} (p_2 - \hat{p}_2)^2(x, 0) + q \int_Q (p_2 - \hat{p}_2)^2 \, dx ds \\
& (\lambda - \bar{C} - Ce^{2\lambda T}) \left(\int_Q (z - \hat{z})^2 \, dx ds + \int_Q (w - \hat{w})^2 \, dx ds + \int_Q (p_1 - \hat{p}_1)^2 \, dx ds \right. \\
& \quad \left. + \int_Q (p_2 - \hat{p}_2)^2 \, dx ds \right) \leq 0
\end{aligned} \tag{2.48}$$

Choosing $\lambda > \bar{C} + C$ and then T sufficiently small such that $\lambda - \bar{C} - Ce^{2\lambda T} > 0$, we must have that $w = \hat{w}$, $z = \hat{z}$, $p_1 = \hat{p}_1$ and $p_2 = \hat{p}_2$. Thus, $N = \hat{N}$, $R = \hat{R}$, $\lambda_1 = \hat{\lambda}_1$ and $\lambda_2 = \hat{\lambda}_2$. Since the optimal control depends only on the adjoint $\lambda_2 = \hat{\lambda}_2$, then we must have that $I = \hat{I}$. $\square$

Remark 2.4.4. *Under some minor modifications in the theorems above, but using the same techniques, it can be shown that the optimality system is also unique under zero Neumann boundary condition.*

2.4.3 Existence of an Optimal Diffusion Rate

The diffusion rate controls the movement that the population has to spread and find its resource. The next theorem guarantees the existence of an optimal diffusion rate that maximizes the objective functional at the optimal control and states. By showing the existence of this diffusion rate, we can identify which populations are expected to maximize the goal better than others by looking at the rate they are moving. Later in Subsection 2.7.3, we will numerically illustrate the existence of an intermediate diffusion rate for this maximization problem when the population is exposed to favorable and unfavorable habitats with Dirichlet boundary conditions.

Theorem 2.8. *There exist $d^* \in [d_{\min}, d_{\max}]$ and corresponding optimal control $I^*(d^*) \in U$ with corresponding states (N^*, R^*) such that*

$$J_{d^*}(I^*(d^*)) = \sup_{d \in [d_{\min}, d_{\max}]} \left\{ \sup_{I \in U} J_d(I) \right\}$$

where

$$J_d(I) = \int_{\Omega} C_4 N(x, T) dx + \int_0^T \int_{\Omega} C_1 N - (C_3 + C_2 I) I dx dt.$$

Proof. Observe that I is uniformly bounded in $L^\infty(Q)$. Also, N and R are uniformly bounded in $L^\infty(Q)$ by Theorem 2.1. For any $d \in [d_{\min}, d_{\max}]$, it can be seen that

$$\begin{aligned} \sup_{I \in U} J_d(I) &= \sup_{I \in U} \int_{\Omega} C_4 N(x, T) dx + \sup_{I \in U} \int_0^T \int_{\Omega} C_1 N - (C_3 + C_2 I) I dx dt \\ &\leq \sup_{I \in U} \int_{\Omega} C_4 N(x, T) dx + \sup_{I \in U} \int_0^T \int_{\Omega} C_1 N dx dt \\ &\leq (C_4 + C_1 T) |\Omega| M e^{\lambda T} \\ &\leq (C_4 + C_1 T) |\Omega| M e^{\lambda T}. \end{aligned}$$

where $\|N\|_{L^\infty(Q)} \leq M e^{\lambda T}$. Moreover, from the above inequality yields

$$\sup_{d \in [d_{\min}, d_{\max}]} \left\{ \sup_{I \in U} J_d(I) \right\} \leq (C_4 + C_1 T) |\Omega| M e^{\lambda T} < \infty.$$

By Theorem 2.4 we can guarantee that for any given $d \in [d_{\min}, d_{\max}]$ there exist an optimal control $I^*(d) \in U$ such that

$$J_d(I^*(d)) = \sup_{I \in U} J_d(I)$$

and by the uniform bound on J , there exist a maximizing sequence

$(I^*(d^m), d^m) \in U_d = U \times [d_{\min}, d_{\max}]$ such that

$$\lim_{m \rightarrow \infty} J_{d^m}(I^*(d^m)) = \sup_d J_d(I^*(d)) = \sup_d \left\{ \sup_I J_d(I) \right\}.$$

Using Theorem 2.1, we can guarantee the existence of a sequence of state solutions given $(I^*(d^m), d^m) \in U_d$

$$(N^m, R^m) = (N(I^*(d^m), d^m), R(I^*(d^m), d^m))$$

for every m . Note that $\{I^*(d^m)\}_{m \in \mathbb{N}}$ represents a sequence of optimal controls with corresponding diffusing rate d^m .

The next step is to determine uniform bounds for $\|N^m\|_{L^2(0,T;H_0^1(\Omega))}$, $\|N_t^m\|_{L^2(0,T;H_0^1(\Omega)^*)}$ and $\|R^m\|_{L^2(Q)}$ for all n and m . Since N^m is a weak solution of problem (2.8), we can apply Lemmas 2.2 and 2.3 to obtain uniform bounds for $\|N^m\|_{L^2(0,T;H_0^1(\Omega))}$ and $\|N_t^m\|_{L^2(0,T;H_0^1(\Omega)^*)}$. Similarly, we can use remark 2.3.2 (since R^m is a weak solution of problem (2.8)) to obtain an uniform bound for $\|R^m\|_{L^2(Q)}$.

Due to $\|N^m\|_{L^2(0,T;H_0^1(\Omega))}$, $\|N_t^m\|_{L^2(0,T;H_0^1(\Omega)^*)}$ and $\|R^m\|_{L^2(Q)}$ are uniformly bounded independently of m , $I^*(d^m) \in L^\infty(Q)$ and $d^m \in [d_{\min}, d_{\max}]$, there exist subsequences N^m , R^m and $I^*(d^m)$ such that

$$\begin{aligned} N^m &\rightharpoonup N^* \text{ weakly in } L^2(0, T; H_0^1(\Omega)) \\ N_t^m &\rightharpoonup N_t^* \text{ weakly in } L^2(0, T; H_0^1(\Omega)^*) \\ R^m &\rightharpoonup R^* \text{ weakly in } L^2(Q) \\ I^*(d^m) &\rightharpoonup I^*(d^*) \text{ weakly in } L^2(Q) \\ d^m &\rightarrow d^* \end{aligned}$$

One must show next that N^* and R^* are the corresponding state solutions associated with the optimal control (I^*, d^*) where I^* represents the optimal control corresponding to the optimal diffusion rate d^* . The weak formulation of system (2.8) satisfied by N^m and R^m with a test function Φ is given by

$$\begin{aligned} \int_0^T \langle N_t^m, \Phi \rangle dt + d^m \int_0^T \int_\Omega \nabla N^m \cdot \nabla \Phi \, dx dt &= \int_0^T \int_\Omega \alpha_1 N^m(x, t) R^m(x, t) \Phi(x, t) \\ &\quad - \mu N(x, t) \Phi(x, t) \, dx dt \\ R^m(x, t) - R(x, 0) &= \int_0^t I^*(d^m)(x, s) - \alpha_2 N^m(x, s) R^m(x, s) \\ &\quad + p\mu N^m(x, s) - qR^m(x, s) \, ds. \end{aligned} \tag{2.49}$$

We require stronger convergence results in system (2.33) in order to pass the limit. A compactness result of Simon in [45] guarantees that

$$N^m \rightarrow N^* \text{ strongly in } L^2(Q)$$

Observe that from the weak convergences, we have that

$$\lim_{m \rightarrow \infty} \int_0^T \langle N_t^m, \Phi \rangle dt = \int_0^T \langle N_t^*, \Phi \rangle dt$$

$$\lim_{m \rightarrow \infty} d^m \int_0^T \int_{\Omega} \nabla N^m \cdot \nabla \Phi \, dx dt = d^* \int_0^T \int_{\Omega} \nabla N^* \cdot \nabla \Phi \, dx dt$$

and using the strong convergence of N^m and weak convergence of R^m we can see that

$$\begin{aligned} & \left| \int_0^T \int_{\Omega} \alpha_1 \left(N^m(x, t) R^m(x, t) - N^*(x, t) R^*(x, t) \right) \Phi(x, t) \, dx dt \right| \\ & \leq \int_0^T \int_{\Omega} \alpha_1 \left| N^m(x, t) - N^*(x, t) \right| R^m(x, t) \Phi(x, t) \, dx dt \\ & + \alpha_1 \left| \int_0^T \int_{\Omega} \left(R^m(x, t) - R^*(x, t) \right) N^*(x, t) \Phi(x, t) \, dx dt \right| \\ & \leq \alpha_1 C \|\Phi\|_{L^2(Q)} \|N^m - N^*\|_{L^2(Q)} + \alpha_1 \left| \int_0^T \int_{\Omega} \left(R^m(x, t) - R^*(x, t) \right) N^*(x, t) \Phi(x, t) \, dx dt \right| \\ & \rightarrow 0 \text{ as } m \rightarrow \infty. \end{aligned}$$

Note that $N^* \Phi \in L^2(Q)$ since $N^* \in L^\infty(Q)$. Now, we can pass the limit as $m \rightarrow \infty$ in (2.49) and obtain that $(N^*, R^*) = (N(I^*, d^*), R(I^*, d^*))$. Finally, by the strong convergence of the sequence N^m and since the function

$$I \mapsto \int_0^T \int_{\Omega} (C_3 + C_2 I) I \, dx dt$$

is weakly lower semi-continuous in $L^2(Q)$ [20], we have that

$$\begin{aligned} \int_0^T \int_{\Omega} (C_3 + C_2 I^*(d^*)) I^*(d^*) \, dx dt & \leq \liminf_{m \rightarrow \infty} \int_0^T \int_{\Omega} C_3 I^*(d^m) \, dx dt \\ & + \liminf_{m \rightarrow \infty} \int_0^T \int_{\Omega} C_2 (I^*(d^m))^2 \, dx dt \\ & \leq \liminf_{m \rightarrow \infty} \int_0^T \int_{\Omega} (C_3 + C_2 I^*(d^m)) I^*(d^m) \, dx dt \end{aligned}$$

which implies that

$$\begin{aligned}
-\int_0^T \int_{\Omega} (C_3 + C_2 I^*(d^*)) I^*(d^*) \, dx dt &\geq -\liminf_{m \rightarrow \infty} \int_0^T \int_{\Omega} C_3 I^*(d^m) \, dx dt \\
&\quad - \liminf_{m \rightarrow \infty} \int_0^T \int_{\Omega} C_2 (I^*(d^m))^2 \, dx dt \\
&= \limsup_{m \rightarrow \infty} \int_0^T \int_{\Omega} -C_3 I^*(d^m) \, dx dt \\
&\quad + \limsup_{m \rightarrow \infty} \int_0^T \int_{\Omega} -C_2 (I^*(d^m))^2 \, dx dt \\
&\geq \limsup_{m \rightarrow \infty} \int_0^T \int_{\Omega} -(C_3 + C_2 I^*(d^m)) I^*(d^m) \, dx dt
\end{aligned}$$

Thus,

$$\begin{aligned}
J_{d^*}(I^*) &= \int_{\Omega} C_4 N^*(x, T) \, dx + \int_0^T \int_{\Omega} C_1 N^* - (C_3 + C_2 I^*) I^* \, dx dt \\
&\geq \limsup_{m \rightarrow \infty} \int_{\Omega} C_4 N^m(x, T) \, dx + \limsup_{m \rightarrow \infty} \int_0^T \int_{\Omega} C_1 N^m - (C_3 + C_2 I_m^n) I_m^n \, dx dt,
\end{aligned}$$

but our choice of the maximizing sequence $(I^*(d^m), d^m)$ guarantees that

$$\begin{aligned}
&\limsup_{m \rightarrow \infty} \int_{\Omega} C_4 N^m(x, T) \, dx + \limsup_{m \rightarrow \infty} \int_0^T \int_{\Omega} C_1 N^m - (C_3 + C_2 I^*(d^m)) I^*(d^m) \, dx dt \\
&\geq \lim_{m \rightarrow \infty} \int_{\Omega} C_4 N^m(x, T) \, dx + \int_0^T \int_{\Omega} C_1 N^m - (C_3 + C_2 I^*(d^m)) I^*(d^m) \, dx dt \\
&= \sup_{d \in [d_{\min}, d_{\max}]} \left\{ \sup_{I \in U} J_d(I) \right\}.
\end{aligned}$$

Therefore, $(I^*, d^*) \in U_d$ is an optimal control that maximizes the objective functional J_d . $\square$

2.5 Resource Allocation Model with Diffusion of Resource

In this section we extend our original resource-population model in (2.6) by allowing the resource to diffuse. Consider the following resource allocation model with diffusing

population and resource for a given ecosystem:

$$\begin{aligned}
N_t - d_1 \Delta N &= \alpha_1 N R - \mu N && \text{on } Q \\
R_t - d_2 \Delta R &= I(x, t) - \alpha_2 N R + p\mu N - qR && \text{on } Q \\
N(x, 0) &= N_0(x) && \text{on } \Omega \\
R(x, 0) &= R_0(x) && \text{on } \bar{\Omega} \\
N(x, t) &= 0 && \text{on } \partial\Omega \times [0, T] \\
R(x, t) &= 0 && \text{on } \partial\Omega \times [0, T]
\end{aligned} \tag{2.50}$$

We assign d_1 and d_2 to be the diffusion coefficients for the population and resource. We make this assumption since there's no reason to believe that both N and R should spread out at the same rate. All other parameter definitions remained the same as explained in Section 2.2. Another difference from the previous model is the Dirichlet boundary condition imposed on R .

We are unable to use the weak formulation in (2.8) due to the resource is allowed to diffuse. Hence, the functions $N, R \in L^2((0, T), H_0^1(\Omega)) \cap L^\infty(Q)$ and $N_t, R_t \in L^2((0, T), H_0^1(\Omega)^*)$ are said to be weak solutions of problem (2.50) if for any test functions

$$\Phi_1, \Phi_2 \in L^2((0, T), H_0^1(\Omega)) \cap L^\infty(Q)$$

$$\begin{aligned}
\int_0^T \langle N_t, \Phi_1 \rangle dt + d_1 \int_0^T \int_\Omega \nabla N \cdot \nabla \Phi_1 \, dx dt &= \int_0^T \int_\Omega \alpha_1 N(x, t) R(x, t) \Phi_1(x, t) \\
&\quad - \mu N(x, t) \Phi_1(x, t) \, dx dt \\
\int_0^T \langle R_t, \Phi_2 \rangle dt + d_2 \int_0^T \int_\Omega \nabla R \cdot \nabla \Phi_2 \, dx dt &= \int_0^T \int_\Omega I(x, t) \Phi_2 - \alpha_2 N(x, t) R(x, t) \Phi_2 \\
&\quad + p\mu N(x, t) \Phi_2 - qR(x, t) \Phi_2 \, dx dt
\end{aligned} \tag{2.51}$$

with initial and boundary conditions

$$\begin{aligned}
N(x, 0) &= N_0(x) && \text{on } \Omega \\
R(x, 0) &= R_0(x) && \text{on } \Omega \\
N(x, t) &= 0 && \text{on } \partial\Omega \times [0, T] \\
R(x, t) &= 0 && \text{on } \partial\Omega \times [0, T].
\end{aligned} \tag{2.52}$$

Similarly to what we did in Section 2.3, one can show the existence of state solutions and *a priori* estimates for system (2.50). However, in this section we will skip this part and instead we will assume all necessary convergence results to derive necessary conditions for solution of the optimal control problem. The control problem consists in maximizing the objective functional described in Section 2.4, that is

$$\sup_{I \in U} J(I) \quad \text{where } J(I) = \int_{\Omega} C_4 N(x, T) dx + \int_0^T \int_{\Omega} C_1 N - (C_3 + C_2 I) I dx dt$$

subject to the state system (2.50) with corresponding initial and boundary conditions.

Given two admissible controls I and $I^\epsilon = I + \epsilon k$ with corresponding state variables (N, R) and (N^ϵ, R^ϵ) , one can show that the sensitivity equations Ψ_1 and Ψ_2 satisfy

$$\begin{aligned} L\Psi &= \begin{pmatrix} L_1 \Psi_1 \\ L_2 \Psi_2 \end{pmatrix} + M \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ k \end{pmatrix} \quad \text{on } Q \\ \Psi_1(x, t) &= 0 \quad \text{on } \partial\Omega \times (0, T) \\ \Psi_2(x, t) &= 0 \quad \text{on } \partial\Omega \times (0, T) \\ \Psi_1(x, 0) &= 0 \quad \text{on } \Omega \\ \Psi_2(x, 0) &= 0 \quad \text{on } \Omega \end{aligned}$$

where

$$\begin{aligned} L_1 \Psi_1 &= (\Psi_1)_t - d_1 \Delta \Psi_1 \\ L_2 \Psi_2 &= (\Psi_2)_t - d_2 \Delta \Psi_2 \end{aligned}$$

and

$$M = \begin{pmatrix} \mu - \alpha_1 R & -\alpha_1 N \\ \alpha_2 R - p\mu & q + \alpha_2 N \end{pmatrix}.$$

Moreover, the functions λ_1 and λ_2 are the adjoint variables and they define the following PDE system:

$$\begin{aligned}
L^*\lambda &= \begin{pmatrix} L_1^*\lambda_1 \\ L_2^*\lambda_2 \end{pmatrix} + M^T \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = \begin{pmatrix} C_1 \\ 0 \end{pmatrix} \quad \text{on } Q \\
\lambda_1(x, t) &= 0 \quad \text{on } \partial\Omega \times (0, T) \\
\lambda_2(x, t) &= 0 \quad \text{on } \partial\Omega \times (0, T) \\
\lambda_1(x, T) &= C_4 \quad \text{on } \Omega \\
\lambda_2(x, T) &= 0 \quad \text{on } \Omega
\end{aligned} \tag{2.53}$$

where

$$\begin{aligned}
L_1^*\lambda_1 &= -(\lambda_1)_t - d_1\Delta\lambda_1 \\
L_2^*\lambda_2 &= -(\lambda_2)_t - d_2\Delta\lambda_2.
\end{aligned} \tag{2.54}$$

Recall that the right hand side of the adjoint equations corresponds to the derivatives of the integrand of the objective functional with respect to the states N and R respectively.

Assume I^* is an optimal control and define $I^\epsilon = I^* + \epsilon k$ to be another admissible control.

Differentiating the map $I \mapsto J(I)$ one can see that

$$\begin{aligned}
\frac{J(I^\epsilon) - J(I^*)}{\epsilon} &= \int_{\Omega} C_4 \frac{N^\epsilon(x, T) - N(x, T)}{\epsilon} dx \\
&\quad + \int_0^T \int_{\Omega} C_1 \frac{N^\epsilon - N}{\epsilon} - C_3 \frac{I^\epsilon - I^*}{\epsilon} - C_2 \frac{(I^\epsilon)^2 - (I^*)^2}{\epsilon} dx dt.
\end{aligned}$$

Passing the limit as $\epsilon \rightarrow 0^+$,

$$\begin{aligned}
0 &\geq \lim_{\epsilon \rightarrow 0^+} \int_{\Omega} C_4 \frac{N^\epsilon(x, T) - N(x, T)}{\epsilon} dx \\
&\quad + \lim_{\epsilon \rightarrow 0^+} \int_0^T \int_{\Omega} C_1 \frac{N^\epsilon - N^*}{\epsilon} - C_3 \frac{I^\epsilon - I^*}{\epsilon} - C_2 \frac{(I^\epsilon - I^*)(I^\epsilon + I^*)}{\epsilon} dx dt \\
&= \int_{\Omega} C_4 \Psi_1(x, T) dx + \int_0^T \int_{\Omega} C_1 \Psi_1 - k(C_3 + 2C_2 I^*) dx dt \\
&= \int_{\Omega} C_4 \Psi_1(x, T) dx + \int_0^T \int_{\Omega} \begin{pmatrix} \Psi_1 & \Psi_2 \end{pmatrix} \begin{pmatrix} C_1 \\ 0 \end{pmatrix} - k(C_3 + 2C_2 I^*) dx dt
\end{aligned}$$

$$\begin{aligned}
&= \int_{\Omega} C_4 \Psi_1(x, T) dx + \int_0^T \int_{\Omega} \begin{pmatrix} \Psi_1 & \Psi_2 \end{pmatrix} L^* \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} - k(C_3 + 2C_2 I^*) dx dt \\
&= \int_0^T \int_{\Omega} \begin{pmatrix} \lambda_1 & \lambda_2 \end{pmatrix} L \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} - k(C_3 + 2C_2 I^*) dx dt \\
&= \int_0^T \int_{\Omega} \begin{pmatrix} \lambda_1 & \lambda_2 \end{pmatrix} \begin{pmatrix} 0 \\ k \end{pmatrix} - k(C_3 + 2C_2 I^*) dx dt \\
&= \int_0^T \int_{\Omega} k(\lambda_2 - C_3 - 2C_2 I^*) dx dt.
\end{aligned}$$

From the above calculations and taking into account the bounds for any admissible control, the characterization of the optimal control is given by

$$I^*(x, t) = \min \left\{ M_1, \max \left\{ 0, \frac{\lambda_2(x, t) - C_3}{2C_2} \right\} \right\}. \quad (2.55)$$

2.6 Numerical Simulations without Optimal Control

Throughout this section we perform some numerical simulations of the model (2.6) with a fixed source $I(x, t)$, to understand its dynamics under some simplified assumptions. Assume $\mu = 0$, $q = 0$, $p = 0$ and $Q = [0, 1] \times [0, 1]$. These assumptions on the parameters mean that natural death in the population, natural resource decay and contribution from population death to the resource do not occur. The resulting system is given by

$$\begin{aligned}
N_t - d\Delta N &= \alpha_1 NR && \text{on } Q \\
R_t &= I(x, t) - \alpha_2 NR && \text{on } Q \\
N(x, 0) &= N_0(x) && \text{on } [0, 1] \\
R(x, 0) &= R_0(x) && \text{on } [0, 1] \\
N(x, t) &= 0 && \text{on } \{0, 1\} \times [0, 1].
\end{aligned} \quad (2.56)$$

A uniform grid of $[0, 1]$ with grid spacing $h = 0.01$ was used to solve system (2.56) using explicit finite difference method. The numerical scheme satisfied the corresponding CFL-type condition for time step size to guarantee the stability and convergence of the method [12].

Figure 2.1 depicts a set of initial conditions in absence of input amount of resource, $I(x, t) = 0$. In addition, it is assumed that the initial population size is always higher than the initial amount of resource over the entire domain.

To understand the effect of varying the diffusion rate, we illustrate the state system with initial conditions in Figure 2.1, $\alpha_1 = \alpha_2 = 0.4$ and three different levels of diffusion rate d . Recall that α_1 represents the conversion rate of resource into population growth and α_2 is the rate of resource uptake by the population. Figure 2.2 top shows a population that is spreading out quickly under high level of diffusion rate ($d = 1$). In this case the population hits the inhospitable boundaries too soon and eventually dies out. Nevertheless, in Figure 2.2 middle and bottom, the population is spreading under lower levels of diffusion rate, $d = 0.1$ and $d = 0.01$ respectively. In Figure 2.2 middle, it can be observed that the population is slowly decreasing due to it is approaching to inhospitable boundaries. Moreover, in Figure 2.2 bottom, the population is able to grow when it is further away from the hostile boundaries. On the other hand, we also observe that under a high diffusion rate the resource mostly remains the same over the entire domain due to low population size compared to lower diffusion rates where lower resource levels occur near the final time.

We now explore the case when the resource has access to a fixed input rate of resource that depends only on space, $I(x, t) = I(x)$. The set of initial conditions as well as the spatial resource rate are depicted in Figure 2.3. By looking at the green and blue curves, one can see that the initial population is exposed to low and high levels of resource on different parts of the domain.

In Figure 2.4, we analyze the dynamics of a population under high, medium and low diffusion rates with initial conditions depicted in Figure 2.3, $\alpha_1 = 1$ and $\alpha_2 = 0.4$. At the top of Figure 2.4, the population size becomes very low in a short period of time since high diffusion rate leads the population to hit the inhospitable boundaries very quickly. In contrast to high level of diffusion rate, the population is able to survive when diffusion rates

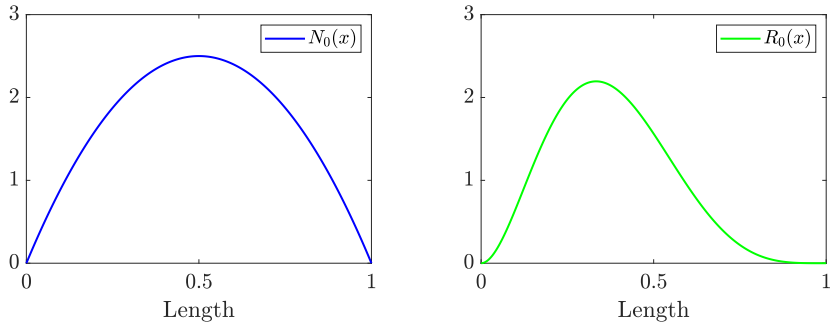


Figure 2.1: Initial conditions without input amount of resource for Figure 2.2.

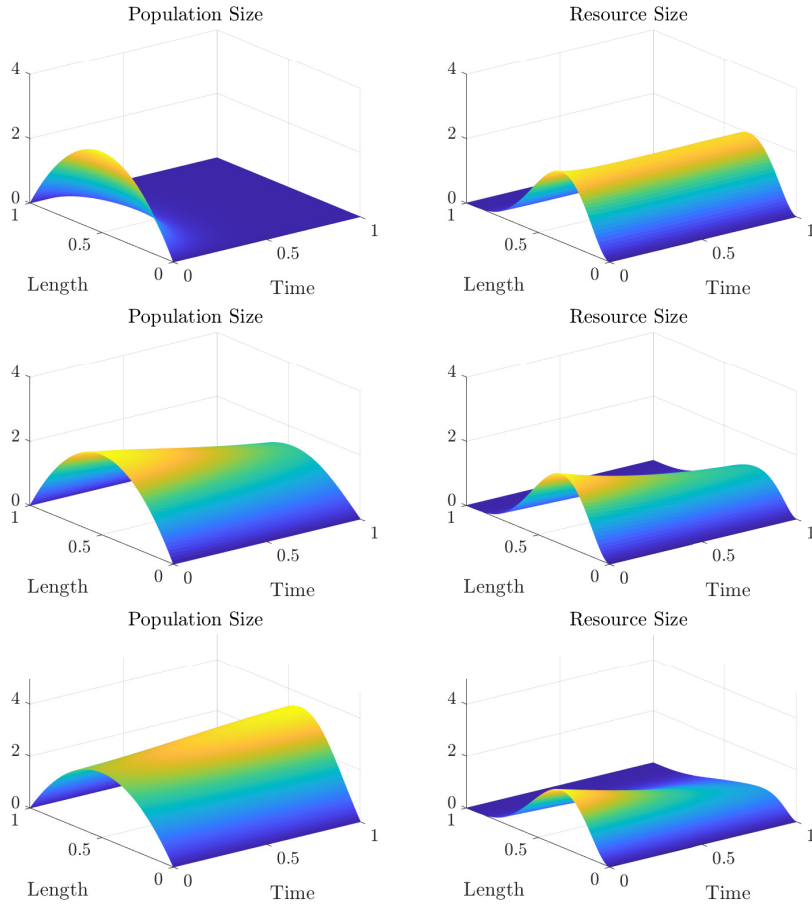


Figure 2.2: On the left hand side the population size distribution is represented while on the right hand side is the corresponding resource level. Three levels of the diffusion rate are used subject to initial conditions in Figure 2.1 with $\alpha_1 = \alpha_2 = 0.4$ and $I = 0$. The top, middle and bottom scenarios correspond to high, medium and low diffusion rates for $d = 1$, $d = 0.1$ and $d = 0.01$ respectively.

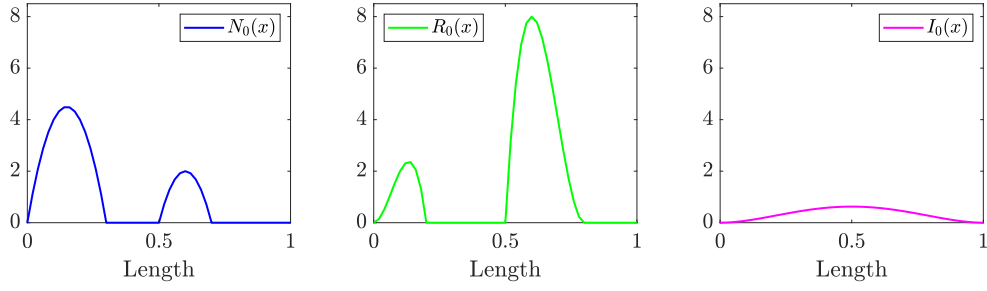


Figure 2.3: Initial conditions with added source for Figure 2.4.

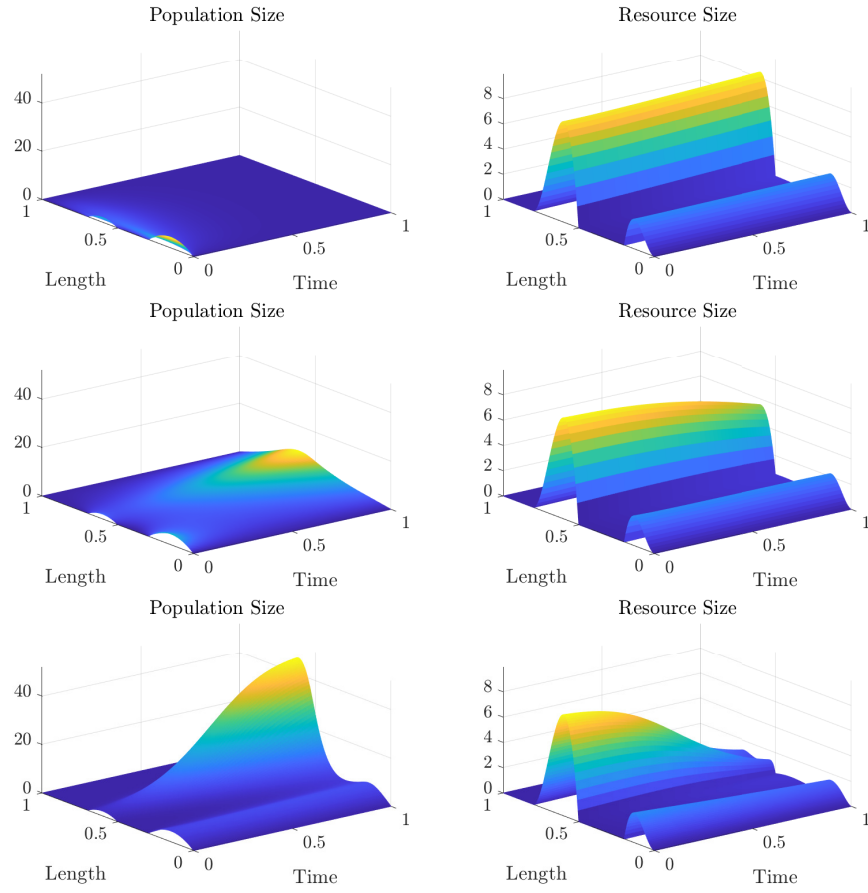


Figure 2.4: On the left hand side the population size distribution is represented while on the right hand side its corresponding resource level with $I = I_0(x)$. Three levels of the diffusion rate are used subject to initial conditions in Figure 2.3 with $\alpha_1 = 1$ and $\alpha_2 = 0.4$. The top, middle and bottom scenarios correspond to high, medium and low diffusion rates for $d = 1$, $d = 0.1$ and $d = 0.01$ respectively.

are medium or low. In this case, a population with a low diffusion rate is more likely to obtain a higher population size than a population with a medium diffusion rate. Moreover, we can observe that under a high diffusion rate the resource levels remain almost constant across time due to population has rapidly reached very low density levels and thus, no resource uptake is produced. However, when the population has medium and low diffusion rates the amount of resource seems to decrease closer to the final time in some parts of the domain. Thus, areas with high level of population are leading the resource to low densities and the input rate of resource is not enough to compensate that resource loss. Perhaps, higher levels of source could help maintain higher levels of the resource for a longer time when diffusion rates are low or medium.

2.7 Numerical Simulations with Optimal Control

The focus of the next numerical simulation subsections is to illustrate the dynamics of the resource allocation system when some parameters, thresholds, boundary conditions and spatial domains are changed. We develop Subsection 2.7.1 to understand the impact produced by the critical resource threshold, R_c , on the population size when considering different initial amount of resources in absence and presence of optimal control. We calculate the total population abundance at the final time for each example to compare with the initial total population size and measure whether the population has grown or shrunk. In Subsection 2.7.2, we explore the resource allocation model under two different values of the resource conversion rate, α_3 . In addition, we also investigate the relationship between α_3 and R_c as well as how the total population abundance and the objective functional values behave as a function of R_c . We dedicate Subsection 2.7.3 to analyze some of the effects produced by the diffusion parameter, d , to the ecosystem model. Here we numerically show the existence of an intermediate diffusion rate for the population that maximizes the objective functional and validates the results of Theorem 2.8. For the three previous subsections, we always assume that the initial spatial distributions of the population and its resource are known. However, in order to obtain more realistic set of initial conditions for N and R , in Subsection 2.7.4, we allow the population and resource interact for some time and then use the population and

resource sizes at the final time as new initial conditions. The new initial conditions are used to run simulations in presence of optimal control and compute the population abundance. In Subsection 2.7.5, we illustrate some numerical scenarios of the model when the population can have Neumann (favorable) or Dirichlet (unfavorable) boundary conditions. Furthermore, we report the objective functional and total population abundance values to compare both type of boundary conditions. In the last numerical Subsection 2.7.6, we present two examples of the resource allocation model in presence of control when Ω is a squared domain instead of an interval as considered in all the previous subsections.

Before we illustrate several numerical examples of the optimal control problem associated with the resource allocation model, we explain the idea behind solving the optimality system, (2.6), (2.42) and (2.44), numerically:

1. Explicit Finite Difference method will be used to approximate N_t , R_t , N_{xx} and ΔN .
2. The Forward-Backward Sweep method for PDEs will be used to solve the optimality systems and the convergence results for this algorithm can be found in [23]. The steps of this iterative method are summarized below.
 - Make an initial guess for the optimal control I over your domain $\Omega \times [0, T]$.
 - Use the initial and boundary conditions with the state equations and the value for I , to solve for N and R forward in time and space subject to the PDE in the optimality system.
 - Use the transversality and boundary conditions and the values for I , N and R to solve the adjoint system λ_1 and λ_2 backwards in time and space subject to the PDE in the optimality system.
 - Obtain the new control I by substituting the new N , R , λ_1 and λ_2 into the optimal control characterization. Form the control for the next iteration as a convex combination of old and new control.
 - Check that the values for the states and control from the last and current iterations satisfy a convergence criteria. If the iterations are close enough, return the outputs of current iteration. Otherwise return to the second bullet.

2.7.1 A Critical Threshold for Population Growth

In this section we explore some numerical scenarios to illustrate the dynamics of the population with respect to the relationship between R_0 and the critical resource threshold when $R > R_c$, $R = R_c$ and $R < R_c$ under a specific level of diffusion without and with optimal control (I^*). Here $R_c = \frac{\alpha_1}{\mu}$ is a critical value of the resource that can determine when the total population size can grow or shrink. In Section 2.3, we showed that when the resource function is below the R_c critical threshold, then the total population size is expected to decrease over time regardless the value of the diffusion rate. However, when the resource function exceeds this threshold and the population diffuses at a low or medium rate, the dynamic of the total population size is less predictable. We have used the parameters in Table 2.1 to illustrate the numerical simulations in Figure 2.5 in presence of Dirichlet boundary condition for the population and in absence of control. Moreover, for these parameters, $R_c = 0.33$ and the total population abundance at the initial time is given by

$$\int_0^1 N(x, 0) dx = 1.67.$$

In Figure 2.5, we illustrate the impact produced by the critical resource value R_c on the state solutions in absence of control when the initial resource size is lower, equal or higher than R_c near the middle of the habitat. The initial population density is assumed the same for all three cases with a higher population density near the middle of the habitat and lower population density close to the inhospitable boundaries. All the green curves are the population and resource densities at the final time. In Table 2.2, we report the total population size at the final time for each case. As expected, due to the lack of external source almost all resource at the final time has already been consumed by the population. Thus, in the case without control as time goes on, we expect the total population size to approach to zero regardless how high the initial resource is from R_c since the population eventually runs low on resource and it is diffusing toward the hostile boundaries.

Using the state system (2.6) and objective functional (2.44), we illustrate the scenario when the optimal control rate of the resource, I^* , is available in the model to examine the impact produced by the critical threshold R_c on the total population size. Table 2.3

Table 2.1: Parameters used for Table 2.2 and Figure 2.5.

Parameter	α_1	μ	α_2	p	q	d	L	T
Baseline	0.3	0.1	0.3	0	0.01	0.001	1	10

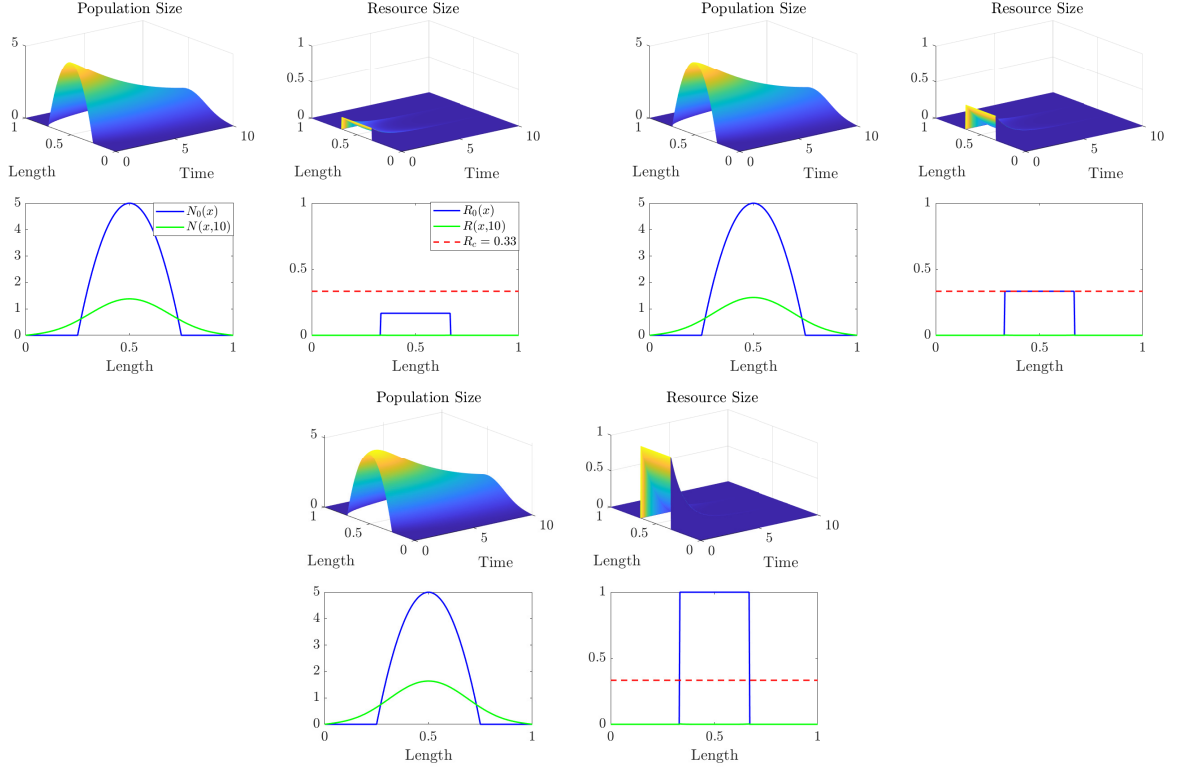


Figure 2.5: Population size and resource allocation in absence of control given that $R_0(x) < R_c$ (two at the upper left), $R_0(x) = R_c$ (two at the upper right) and $R_0(x) > R_c$ (two at the bottom). In this case $R_c = 0.33$ and $d = 0.001$.

Table 2.2: Population abundance at the final time without optimal control given the initial condition for $R_0(x)$ was smaller, equal and bigger than $R_c = 0.33$ in the middle of the habitat.

Cases	$\int_0^1 N(x, 10) dx$
$R_0(x) < R_c$	0.63
$R_0(x) = R_c$	0.65
$R_0(x) > R_c$	0.74

Table 2.3: Parameters used for Table 2.4 and Figure 2.6.

Parameter	α_1	μ	α_2	p	q	C_1	C_2	C_3	C_4	d	M_1	L	T
Baseline	0.3	0.1	0.3	0	0.01	30	50	0	1	0.001	0.3	1	10

shows the parameter values used for Figure 2.6. The weight parameters, C_i for $i = 1, 2, 3, 4$, represent the importance of maximizing or minimizing each of the four quantities on the objective functional. Figure 2.6 shows the dynamics of the population and resource sizes as well the optimal control when the initial resource size is bigger, equal or smaller than R_c near the middle of the habitat. In Table 2.4, we report the total population size at the final for each case. Unlike Figure 2.5, where the resource densities at the final time were very low, in this case we observe that the resource densities at the final time have the same nonzero distribution regardless the initial condition for the resource. The resource distribution at the final time indicates low resource concentration near the middle of the habitat and two resource peaks closer to the hostile boundaries. The areas with low resource at the final time have a higher population density due to consumption of resource by the population while the areas with high resource density near the boundaries have low population density since the population is expected to die near these areas. In this particular example, we observe that there are high concentrations of resource near the hostile boundaries because as the population with high density in the middle of the habitat spreads out towards the edges, they can find enough resource to maintain the population size, but as the population approaches to the boundaries it quickly dies out. As noticed in Table 2.4, the total population size at the final time grows for each case from an initial total population size of 1.66.

In Figure 2.7, we want to illustrate the impact caused by the resource threshold in the size of a population without and with access to an external resource rate when the initial resource near the middle of the habitat always exceeds R_c and the peak of the initial population size is much lower than the last two previous examples. In this case the initial total population size is equal to 0.08. The parameters for this simulations were taken as in Table 2.3 with the exception that the upper bound for the control was lowered to $M_1 = 0.15$. The total population size at the final time for both cases was higher as shown in Table 2.5. In this case, the resource density near the middle of the habitat was mostly above the resource threshold because of high level of population density on these areas. However, near areas close to the boundary the resource was mostly below the critical threshold since the population is expected to die near the boundary. Thus, in presence of optimal control, when the initial

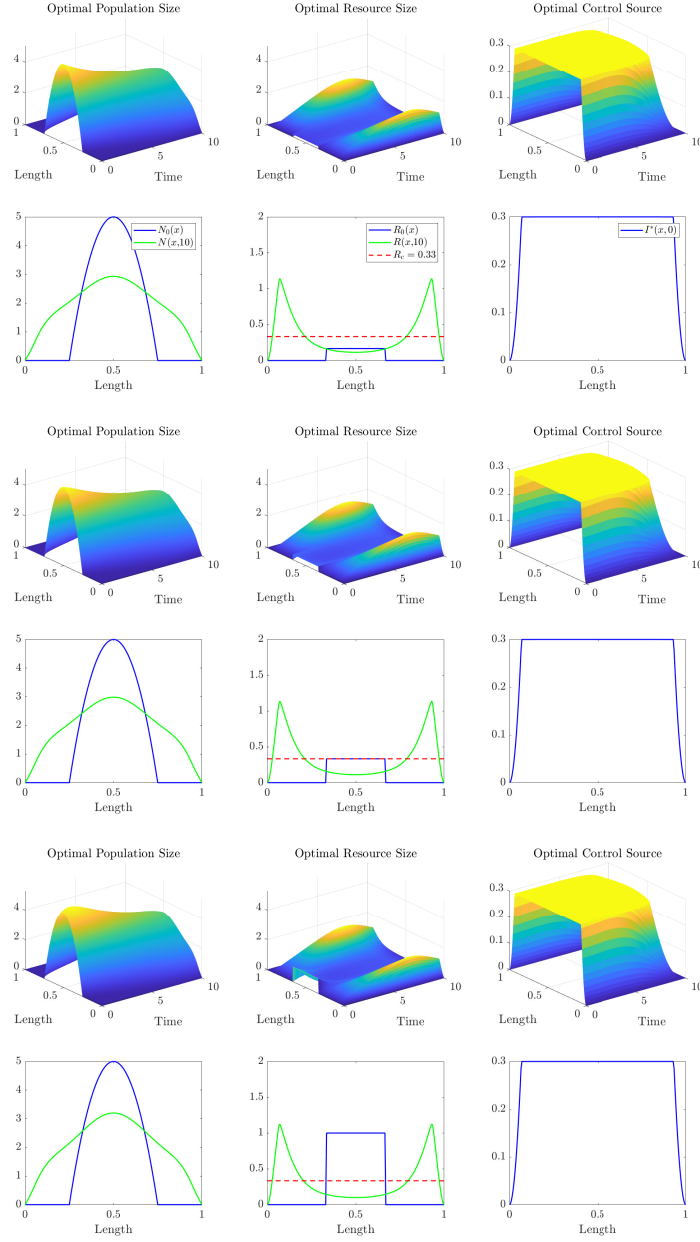


Figure 2.6: Population and resource sizes in presence of the optimal control given that $R_0(x) < R_c$ (two at the top), $R_0(x) = R_c$ (two at the middle) and $R_0(x) > R_c$ (two at the bottom). The blue and green curves represent states at the initial and final time. In this case $R_c = 0.33$.

Table 2.4: Population abundance at the final time with optimal control given the initial condition for $R_0(x)$ was smaller, equal and bigger than $R_c = 0.33$.

Cases	$\int_0^1 N(x, 10) dx$
$R_0(x) < R_c$	1.91
$R_0(x) = R_c$	1.93
$R_0(x) > R_c$	2.03

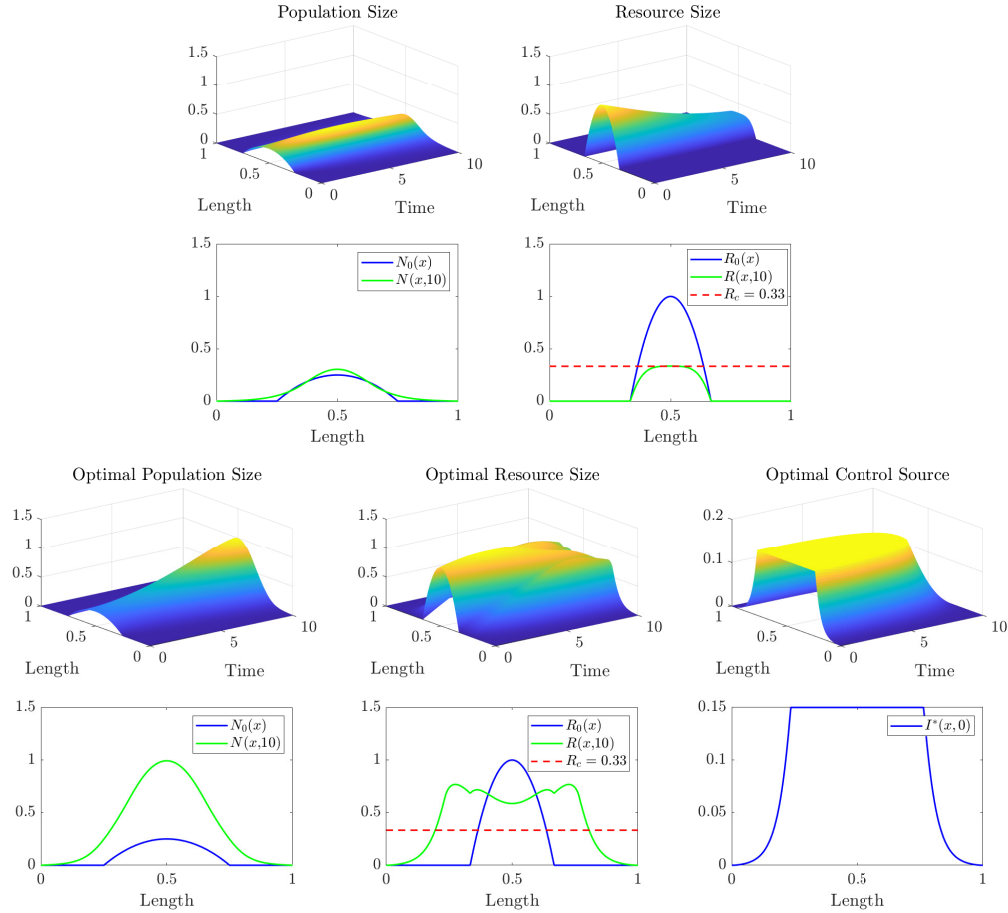


Figure 2.7: Population and resource sizes in absence (top) and presence (bottom) of optimal control given that $R_0(x)$ takes values above and below R_c as x varies. In this case $R_c = 0.33$.

Table 2.5: Population abundance at the final time without and with optimal control given the initial condition for $R_0(x)$ was above and below than $R_c = 0.33$.

Cases	$\int_0^1 N(x, 10) dx$
No control	0.11
With Control	0.37

population size is small relative to the initial resource size, we can expect the total population size to increase over time as long as the diffusion rate is small.

2.7.2 The Effect of the Resource Conversion Rate

The parameter α_3 ($\alpha_1 = \alpha_3 \alpha_2$) represents the rate at which the resource uptake by the population is transferred into population growth. In this subsection we are interested in examining the influence on the population size of this parameter when $\alpha_3 = 1$ and $\alpha_3 = 0.7$ while other parameters in the model are fixed. Thus, the baseline parameters for the next numerical simulations are illustrated in Table 2.6.

For all the simulation the diffusion rate was fixed at the intermediate level $d = 0.01$ and the set of admissible controls is

$$U = \left\{ I \in L^\infty(Q) \mid 0 \leq I(x, t) \leq 1, \text{ a.e. } (x, t) \in Q \right\}.$$

Here the weight parameters choices represent that we equally care about the importance of maximizing the total population abundance over the entire domain ($C_1 = 1$) and at the final time ($C_4 = 1$) as well as minimizing the amount of square of the input resource across the habitat ($C_2 = 1$), but not linear input resource ($C_3 = 0$). However, if we would have chosen $C_4 = 0$, this would mean that it is not important to maximize the total abundance of the population at the final time. Note that our weight parameter choices here for C_1 and C_2 are different from the examples with optimal control in Subsection 2.7.1 were $C_1 = 30$ and $C_2 = 50$.

In Figure 2.8 we display two numerical simulations of the optimal control problem when the initial abundance of population and resource are both distributed heterogeneously along the habitat. Note also that initial distribution of population and resource are far from the hostile boundaries. A clear observation is that there is a higher abundance of population when the conversion of resource into population growth is $\alpha_3 = 1$ instead of $\alpha_3 = 0.7$, especially near the final time. In both cases, the amount of resource close to $t = 5$ have been consumed more by the population. This make sense, since as population abundance increases, the population requires a higher resource uptake to maintain its size. It is worth

Table 2.6: Baseline parameters for tables and figures in Section 2.7.2.

Parameter	μ	α_2	p	q	C_1	C_2	C_3	C_4	M_1	L	T
Baseline	0.1	0.4	0.5	0.01	1	1	0	1	1	1	10

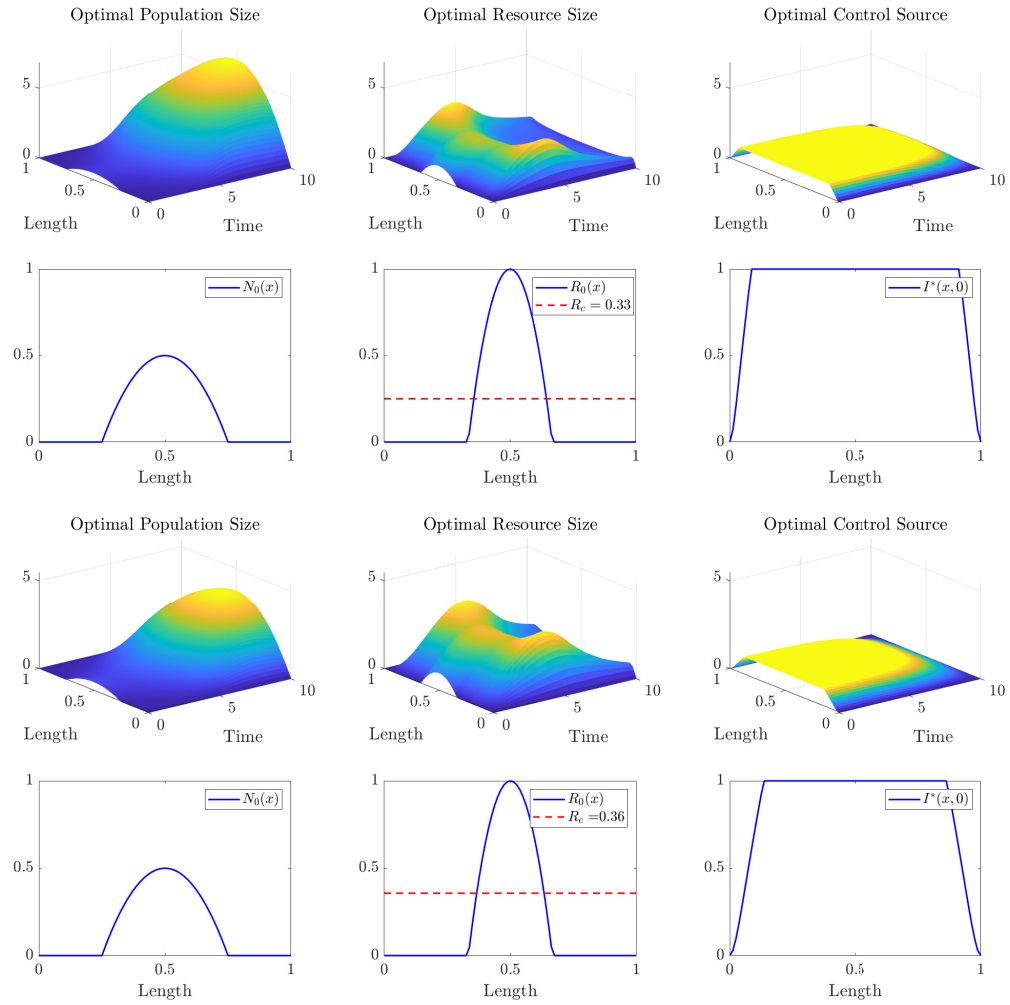


Figure 2.8: Distribution of population, resource and optimal control when the conversion of resource into population growth is $\alpha_3 = 1$ (first two rows at the top) and $\alpha_3 = 0.7$ (last two rows). The initial population and resource densities are both allocated heterogeneously.

mentioning also that the optimal input rate of resource implicitly affects the distribution of resource in space since throughout time there have been resources allocated in areas where they were not initially. This is explained by the implementation of the optimal control in areas that initially were unoccupied by resources. Such dynamics allows the population to spread and grow in areas away from the inhospitable boundaries. We calculate the objective functional J with the parameters in Table 2.6 and obtain that $J = 20.3$ for $\alpha_3 = 1$ and $J = 8.4$ for $\alpha_3 = 0.7$. Our objective functional values allow us to validate that when the conversion rate of resource into population growth is higher, then the total abundance of the population at the final time are expected to be higher, as seen with 4.13 for $\alpha_3 = 1$ and 2.52 when $\alpha_3 = 0.7$.

Similar observations to those made for Figure 2.8 can be made to Figure 2.9. The main difference consists in how the initial condition for the resource was chosen. In Figure 2.9 we display two numerical simulations of the optimal control problem when the initial population abundance is distributed heterogeneously along the habitat while the initial amount of resource is assumed to be constant in the middle part of the habitat and zero near the boundary. Even though in this simulation we allocate higher resource abundance near the middle of the habitat than in the previous example, the population abundance at the final time when $\alpha_3 = 1, 0.7$ was 4.13 and 2.52 respectively. These are the same values we obtained in Figure 2.8.

Despite choosing different favorable initial spatial arrangements for the population and resource abundance, the total population abundance at the final time was always higher when the conversion of resource into population growth was higher as well. In the next Subsection 2.7.3, we explore a more extreme circumstance when the initial spatial arrangement for the population is unfavorable, that is, the resource is located far away from the initial location of the population. In this case we will expect the diffusion rate to play a key role in increasing the population abundance.

Back to the critical threshold under this subsection with the resource conversion rate, the main objective of the following numerical simulations is to illustrate the impact that the critical threshold has on the objective functional as well as the population abundance due to changing α_3 affects the value of R_c . We start off by considering the parameters in Table 2.6

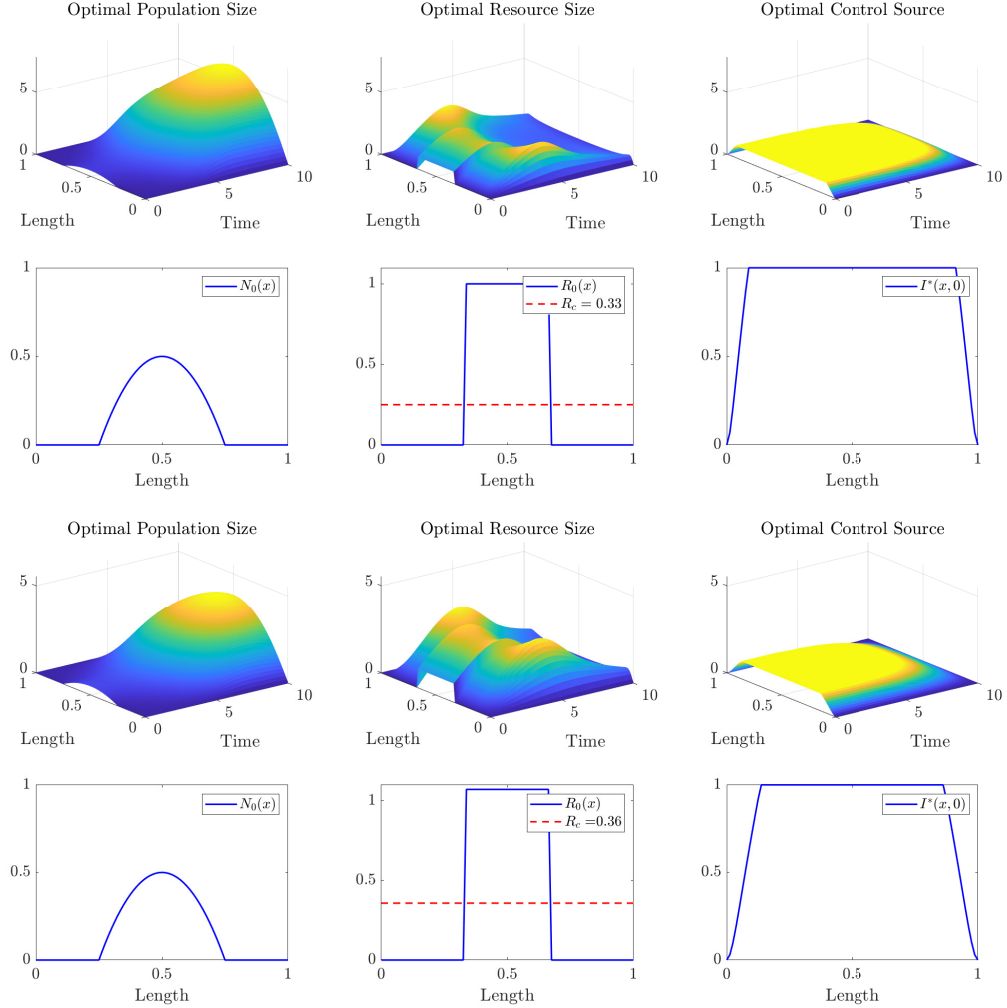


Figure 2.9: Distribution of population, resource and optimal control when the conversion of resource into population growth is $\alpha_3 = 1$ (first two rows at the top) and $\alpha_3 = 0.7$ (last two rows). The initial population is allocated heterogeneously while the initial resource is constant near the middle of the habitat and zero near the boundary.

and the initial conditions in Figure 2.10. Moreover, we let R_c be a function of α_3 such that

$$R_c(\alpha_3) = \frac{\mu}{\alpha_1} = \frac{\mu}{\alpha_2 \alpha_3}.$$

In particular, for this example

$$R_c(\alpha_3) = \frac{0.1}{0.4\alpha_3} = \frac{1}{4\alpha_3}$$

with $\alpha_3 \in [0.1, 1]$. In general, α_3 takes on any values between 0 and 1. For values of α_3 close to 0, it represents that low population growth is produced by the uptake of resource. On the other side, when α_3 is near 1, it means that most of the resource uptake by the population transfers into population growth. Thus, since R_c gets really large as α_3 approaches to zero, the lower bound for α_3 is fixed at 0.1 instead of 0. Ecologically, this means that very high level of resource size would be needed along the habitat to increase the population size when α_3 is near its lower bound.

The initial conditions in Figure 2.10 show high levels of population size near the middle of the habitat, but very low near the boundaries. The initial amount of resource is homogeneously distributed along the habitat and it is set at 1 since R_c takes values between 0.25 and 2.5. These values can be easily computed based on our bounds for α_3 .

In Figure 2.11, we display the total population abundance at the initial and final time as a function of R_c when no control, $I_{\min} = 0$, optimal control, I^* , and constant control at the highest level, $I_{\max} = 1$, are implemented. The vertical line represents the initial amount of resource and the dashed line is initial total abundance of the population.

In Figure 2.12, we display the objective functional as a function of R_c corresponding to no control, optimal control and constant control at the highest level. Something to highlight from this figure is that as R_c is closer to 0.25, the cost of using optimal control approaches to the cost of using constant control at the highest level. This means that the total population abundance can be maintained with the amount of resource above 0.25 and low values of diffusion. This situation can be guaranteed as long as constant control at the highest level is added to the resource. However, the situation gets reversed when R_c is near 2.5, in that

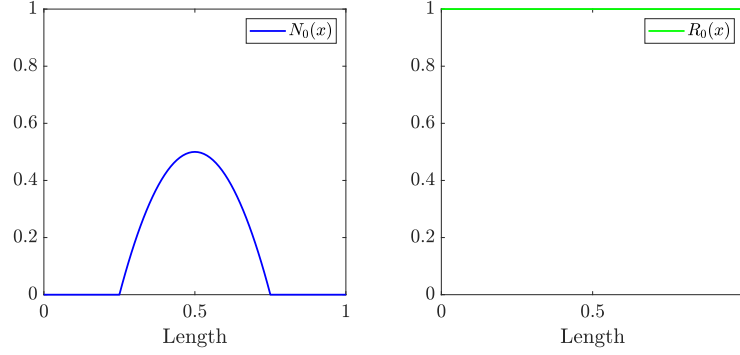


Figure 2.10: Initial conditions used for Figures 2.11 and 2.12.

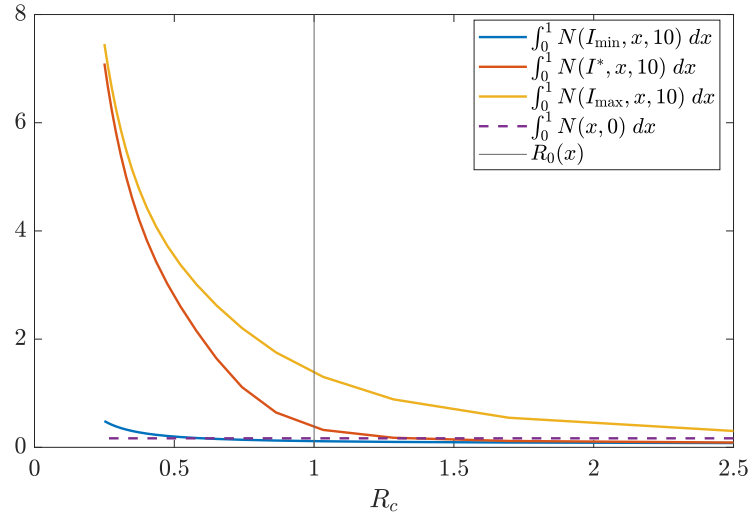


Figure 2.11: Total population abundance at the initial and final time on the vertical axis as a function of the resource threshold $R_c = \frac{1}{4\alpha_3}$ when no control, optimal control, and constant control at the highest level are implemented. To illustrate this example, we used parameter values in Table 2.6 and the initial conditions in Figure 2.10. Recall that $I_{\min} = 0$ and $I_{\max} = 1$ are the lower and upper bounds for all admissible controls.

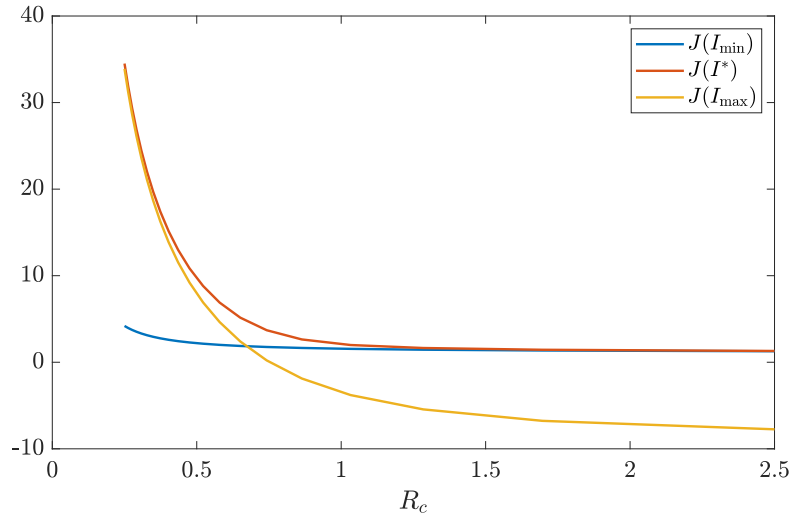


Figure 2.12: Objective functional on the vertical axis as a function of the resource threshold $R_c = \frac{1}{4\alpha_3}$ when no control, optimal control, and control at the highest level are implemented. To illustrate this example, we used parameter values in Table 2.6 and the initial conditions in Figure 2.10. Recall that $I_{\min} = 0$ and $I_{\max} = 1$ are the lower and upper bounds for all admissible controls.

case, the J values of using optimal control or with no control are almost the same. In this situation, the total population size at the final time would be close to zero since the resource uptake by the population and adding control at the highest level are not enough to increase the resource levels above 2.5. Thus, the J values corresponding to the optimal control approach to the J values corresponding to no control as the resource threshold gets closer to 2.5.

2.7.3 The Impact of Different Levels of Diffusion Rate

One parameter that can clearly change the dynamics of the optimal control problem in (2.32) is the diffusion coefficient, d . In Subsection 2.7.2, we studied the effects of the resource conversion rate into population growth, α_3 , while other parameters were fixed. We observed that as α_3 increased or decreased, it was expected that objective functional and the population abundance at the final time would increase or decrease as well. Unlike the conversion rate α_3 , the dynamics of the diffusion coefficient d may require more analysis to be understood. In this section, we have prepared some numerical scenarios to analyze the impact of d on the objective functional $J_d(I(d))$. Moreover, for each example, we numerically approximate d^* such that

$$J_{d^*}(I^*(d^*)) = \sup_{d \in [d_{\min}, d_{\max}]} \left\{ \sup_{I \in U} J_d(I) \right\}$$

to validate the theoretical results in Section 2.4.3. One key question we also want to address in this section is whether low diffusion rates are more advantageous than high diffusion rates for the population. Also, how do the initial spatial arrangements of population and resource contribute to answer our previous question? The baseline parameters used for simulations in this section are shown in Table 2.7.

To begin answering these questions, we initially allocate the population far away from its resource as an extreme scenario. The idea of this simulation is to test whether or not fast diffusion in the population could be beneficial since resource is far away. This situation where the population has an initial unfavorable habitat is described on Figure 2.13.

Table 2.7: Baseline parameters for Tables 2.8-2.10 and Figures 2.13-2.18.

Parameter	α_1	μ	α_2	p	q	C_1	C_2	C_3	C_4	M_1	L	T
Baseline	0.3	0.1	0.3	0.4	0.01	1	1	0	1	1	1	10

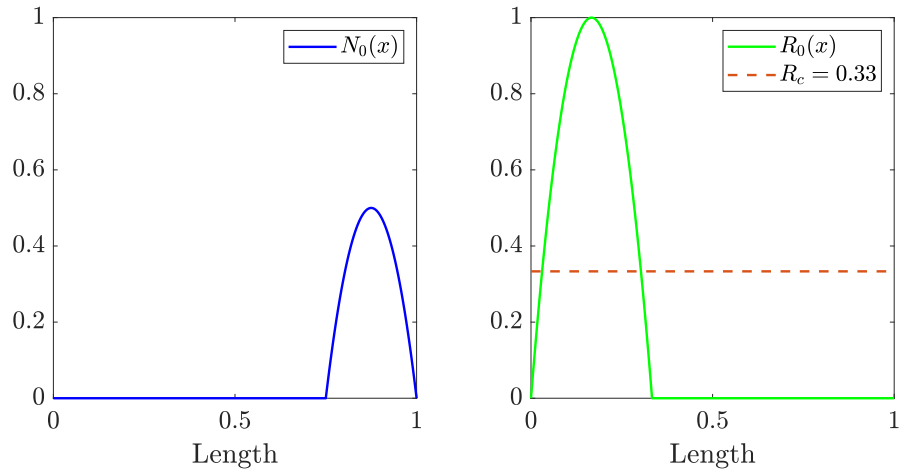


Figure 2.13: Initial conditions for Table 2.8 and Figures 2.14- 2.15.

We have created Table 2.8 taking into account the initial conditions displayed on Figure 2.13 and the baseline parameters in Table 2.7. Table 2.8 contains 10 different diffusion rates in decreasing order with their corresponding values for the objective functional

$$J_d(I^*) = C_4 \int_0^1 N^*(x, 10) dx + \int_0^{10} \int_0^1 C_1 N^*(x, t) - C_2 I^{*2}(x, t) dx dt$$

as well as the total population abundance at the final time ($T = 10$), that is

$$\int_0^1 N^*(x, 10) dx.$$

The idea is to use the objective functional and the population abundance as a metric to determine if there is a d where the population abundance is higher than any other. With this in mind, it can be observed that the diffusion rates ranging from $0.01 - 0.003$ have an increasing payoff J while diffusion rates ranging from $0.003 - 0.0001$ have a decreasing payoff J . Hence, there is an intermediate diffusion rate where the objective functional was maximized. Furthermore, there was also an intermediate diffusion rate where the total population abundance at the final time was maximized. Note that the diffusion rates that maximizes $J_d(I^*)$ and $\int_0^1 N^*(x, 10) dx$ are not the same. This can be seen more easily from Figure 2.14 where we have depicted the graphs of $J_d(I^*)$ and the total population abundance at the final time both as a function of d . Around 200 values of d between $0.0001 - 0.01$ were used to create Figure 2.14. Thus, we had to numerically solve the optimality system around 200 times to obtain the values for J and the total population abundance at the final time.

We compare the application of the optimal control against no control ($I = 0$) and constant control at the highest level ($I = 1$) to measure the importance that the optimal control has in improving the ecological system compared to two constant controls. We do this by computing the J value of using each control strategy when a population diffuses at a rate of $d = 0.004$ (see Table 2.9). Note that we chose the diffusion rate, 0.004 , that provides the highest J_d value in Table 2.8. Not surprisingly, the J value corresponding to the optimal control strategy was much higher than the cost of using no control. Nonetheless, the J value of applying constant control at the highest level was only 6% less compared with the J value of using optimal control. Note that this extreme scenario where population and resource are in opposite locations as well as a not very high cost of using the control ($C_2 = 1$ and $C_3 = 0$)

Table 2.8: Ten levels of diffusion rates in decreasing order along with their corresponding objective functional values and population sizes at the final time using initial conditions in Figure 2.13.

d	$J_d(I^*)$	$\int_0^1 N^*(x, 10) dx$
0.01	13.68	4.5094
0.008	14.74	4.8345
0.006	15.79	5.2318
0.004	16.62	5.7542
0.002	15.85	6.3835
0.001	12.94	4.9957
0.0008	12.28	4.5399
0.0006	11.60	4.1305
0.0004	10.81	3.6768
0.0002	9.78	3.0922
0.0001	9.06	2.6845

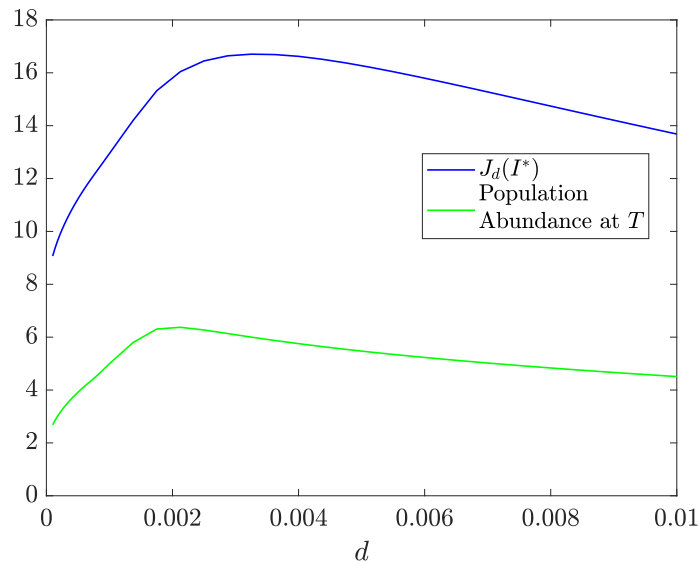


Figure 2.14: Objective functional and total population abundance at the final time as a function of the diffusion rate with unfavorable habitat for the population.

Table 2.9: Comparing the objective functional values of implementing optimal control strategy with no control ($I = 0$) and when control is constant at the highest level ($I = 1$). We choose the diffusion rate with the highest J_d value from Table 2.8, that is, $d = 0.004$.

$J_d(I^*)$	$J_d(0)$	$J_d(1)$	$\frac{J_d(I^*)}{J_d(1)}$
16.62	0.3	15.59	1.0661

might lead the J value of using optimal control or constant control to be very similar. The next examples will illustrate some of the reasons why the J value difference between using optimal control and constant control at the highest level remain so close.

Continuing with the same example where the population and resource are located on opposite sites of the habitat as shown in Figure 2.13, in Figure 2.15, we display the dynamics of the population with its resource and optimal control at three different diffusion rates, $d = 0.01$ (high), $d = 0.004$ (medium) and $d = 0.0001$ (low). At first sight, the dynamics of the population under high and medium diffusion rates were significantly similar. On the other hand, the population dynamics under low diffusion rate was different than high and medium rates. The slowest population was not able to occupy those areas where resource had been allocated initially due to low diffusion rate. It can also be observed that under low diffusion, $d = 0.001$, no control was implemented at the other side of the habitat where population was absent. Thus, the population diffusing faster ($d = 0.01$) was able to spread and grow with a higher population abundance than the population diffusing slower.

In our next numerical scenario, we investigate the case when the initial location of the population is close to its resource and far enough from the inhospitable boundaries. Basically, the population is not forced to travel or wait for the optimal control effects to obtain its energy through the resource. This situation is represented with the initial conditions for N and R in Figure 2.16. Here, we want to examine a more favorable case for the population to compare against the previous extreme initial spatial arrangement.

We have created Table 2.10 and Figure 2.17 (with 100 d values from 0.0001 to 0.01) using the initial conditions in Figure 2.16 and the baseline parameters in Table 2.7. Moreover, Table 2.10 is constructed as Table 2.8, consisting of 7 diffusion rates with their corresponding objective functional and total population abundance at the final time. Further, Figure 2.17 displays the objective functional and total population abundance as a function of the diffusion rate. In this case the total population size at the final time is maximized when $d = 0.001$ and the objective functional is maximized near $d = 0.0004$ of using optimal control was higher than the cost in absence of control. One observation from Figure 2.17 is that there are two different diffusion rates where either the objective functional or the total population

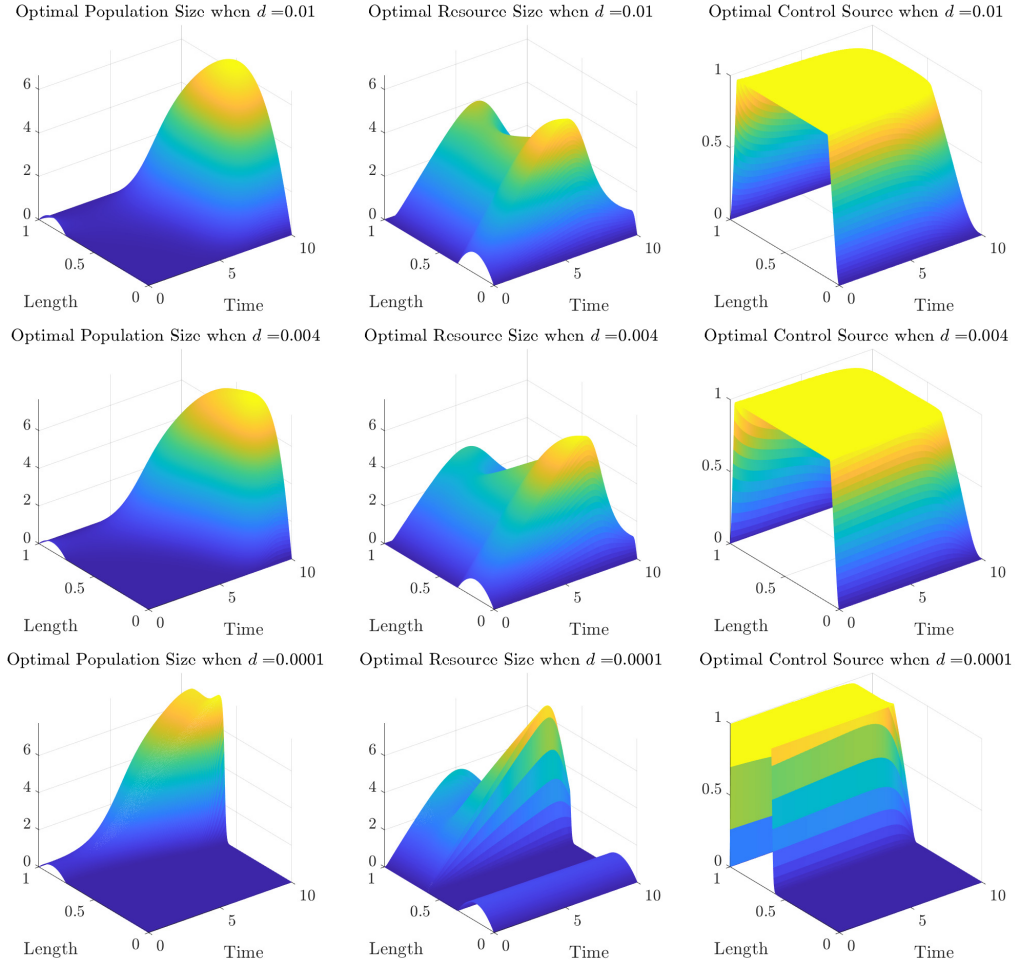


Figure 2.15: Population, resource and optimal control dynamics in space and time for three different diffusion rates, $d = 0.01$ (top), $d = 0.004$ (middle) and $d = 0.0001$ (bottom) under unfavorable initial habitat for the population depicted in Figure 2.13.

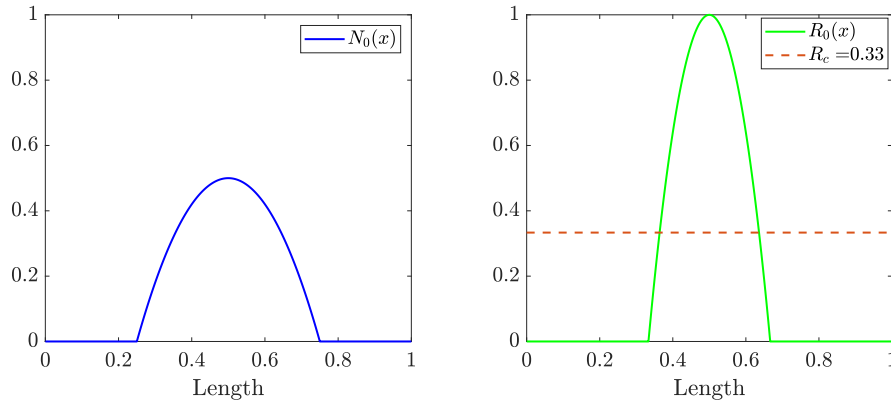


Figure 2.16: Initial conditions for Table 2.10 and Figures 2.17-2.18.

Table 2.10: Seven levels of diffusion rates in decreasing order along with their corresponding objective functional and population size values at the final time using initial conditions in Figure 2.16.

d	$J_d(I^*)$	$\int_0^1 N^*(x, 10) dx$
0.01	17.64	4.1329
0.004	22.75	5.4045
0.001	25.52	6.6538
0.0008	25.51	6.8067
0.0004	24.73	7.2149
0.0002	22.64	6.9113
0.0001	20.75	5.9269

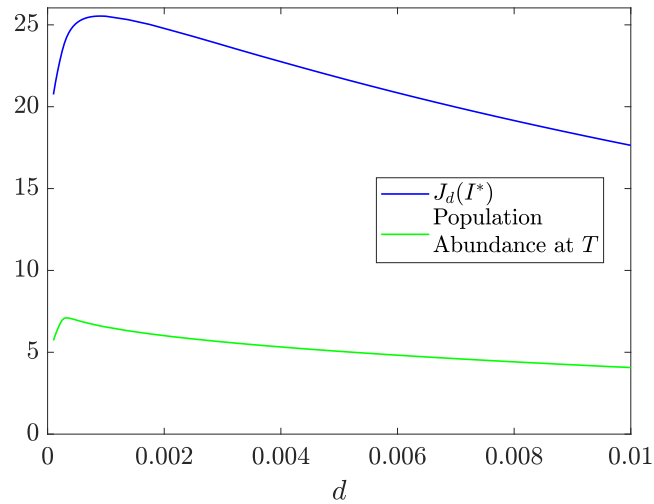


Figure 2.17: Objective functional and total population abundance at the final time as a function of diffusion rate with favorable habitat for the population.

abundance are maximized. Notice that one might be mistaken in assuming that there is only one diffusion rate that can maximize both $J(I^*)$ and $\int_0^1 N(x, 10) dx$.

Dependence on the cost coefficients is important, we have constructed Table 2.11 to compare the cost of using different control strategies as in Table 2.9. As expected, the objective functional at the optimal control was higher than any other control, but it was only 2% better than the cost when constant control at the highest level was used. One can see that despite of more advantageous initial conditions, the cost of using optimal control and constant control when $I = 1$ are still very similar as we discussed on Table 2.9. Consequently, we can say that regardless our choice for the initial conditions, but due to a the low cost relative to the use of control, it means almost the same to implement optimal control as it is to implement constant control at the highest level.

We illustrate the dynamics of the population with its resource and optimal control for three diffusion rates in Figure 2.18 using the initial conditions on Figure 2.16. It can be seen that at the final time when $d = 0.01$ and $d = 0.001$ the population size is higher compared to any previous time while the resource is at the lowest level. Nonetheless, when low diffusion, $d = 0.0001$, the population is mostly concentrated in the middle of the habitat where the resource is low since it has been consumed by the population. But the resource level near the boundaries are high due to the population is spreading slowly and it can grow near areas close to the hostile boundaries. The application of the optimal control seem to have a similar dynamics for each of the diffusion rates.

Although the last two numerical examples in Figures 2.15 and 2.18 the value of the objective functional at the optimal control and control at the upper bound were very similar, that is not always the case. In the following scenario we show a case when there is a significant difference between the J values of I^* and $I = I_{\max}$. The goal is set to maximize the total abundance of the population at the final time and minimize the cost of implementing the control

$$J_d(I^*) = C_4 \int_0^1 N(x, 10) dx - C_2 \int_0^{10} \int_0^1 I^{*2}(x, t) dx dt.$$

The parameters to be considered are given in Table 2.12 and the initial conditions are displayed on Figure 2.19. Unlike the parameters in Table 2.7, this time our parameter

Table 2.11: Comparing the objective functional values of implementing optimal control strategy, no control and when control is constant at the highest level. We choose the diffusion rate with the highest J_d value from Table 2.10, that is, $d = 0.001$.

$J_d(I^*)$	$J_d(0)$	$J_d(1)$	$\frac{J_d(I^*)}{J_d(1)}$
25.52	2.06	24.79	1.0293

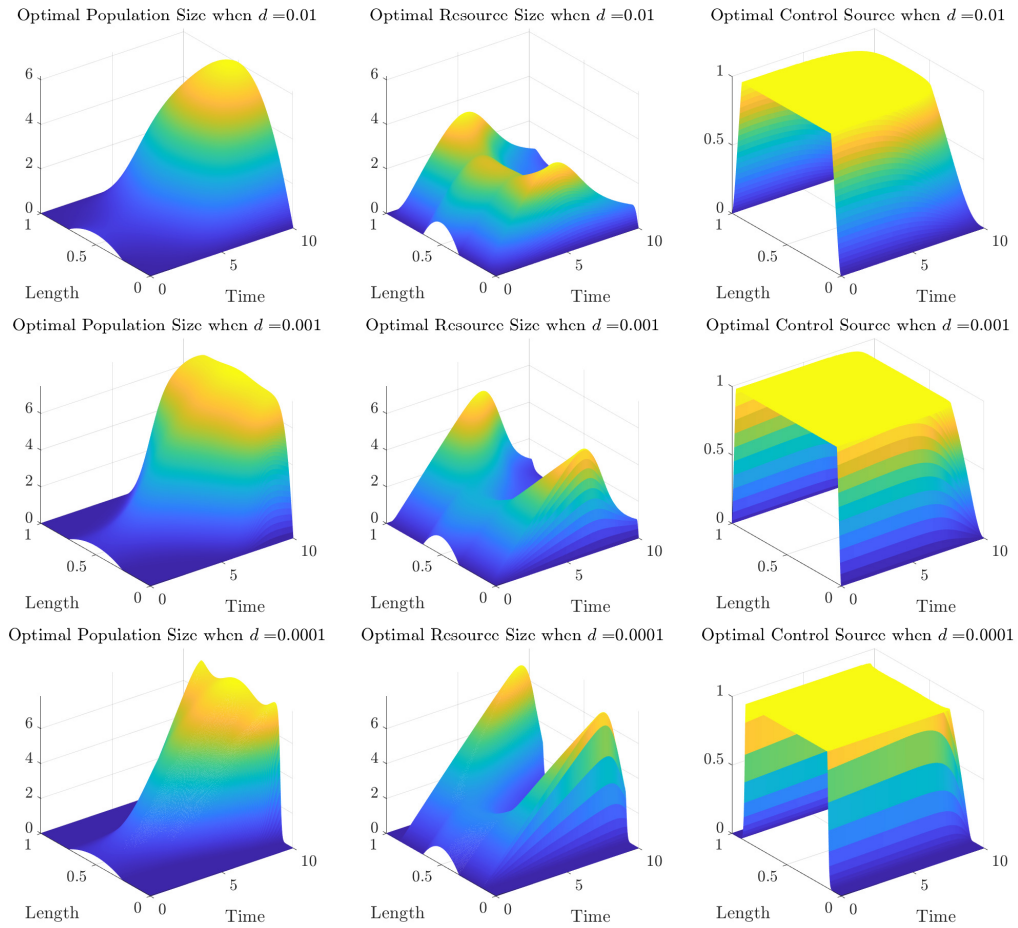


Figure 2.18: Population, resource and optimal control dynamics in space and time for three different diffusion rates, $d = 0.01$ (top), $d = 0.001$ (middle) and $d = 0.0001$ (bottom) under favorable initial habitat for the population depicted in Figure 2.16.

Table 2.12: Baseline parameters for Table 2.13 and Figure 2.19-2.21.

Parameter	α_1	μ	α_2	p	q	C_1	C_2	C_3	C_4	M_1	L	T
Baseline	0.3	0.1	0.3	0	0.01	0	100	0	50	0.2	1	20

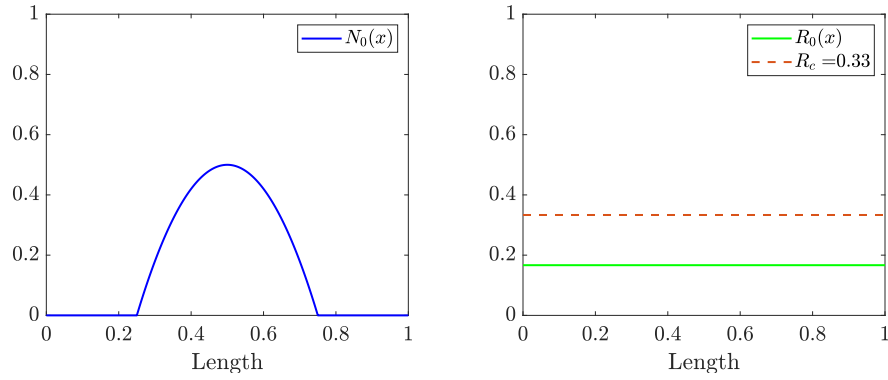


Figure 2.19: Initial conditions for Table 2.13 and Figures 2.20-2.21.

choices represent an ecosystem where the death of the population doesn't contribute to the resource growth since $p = 0$. Our choices for the weight parameters reflect a high relative importance to maximize the population abundance at the final since $C_4 = 50$ while the cost relative to minimize the optimal control is high due to $C_2 = 100$. Note that in this example because of $C_1 = 0$, it is not important to maximize the population size between $(0, T)$. The upper bound for the optimal control has also been reduced to 0.2 from 1 as it was considered for the previous two examples. Later we will see that due to our new weight parameter choices and new upper bound for all admissible controls the J values corresponding to the optimal control and when $I = 0.2$ are significantly different unlike the previous two scenarios where their J values were very similar.

The initial conditions on Figure 2.19 represent a high population size at the middle of the habitat while the resource size are homogeneous along the habitat and below the R_c level. Moreover, we know from Section 2.7.1 that despite of how fast or slow the population diffuses, the population is unable to increase its size anywhere due to low levels of resource. Thus, the implementation of a control is of great importance to improve the resource and subsequently allow for population growth. The time period was also extended from 10 to 20.

In Table 2.13, we have a sample of diffusion values with corresponding objective functional values used to create Figure 2.20. As you can observe in Figure 2.20, there is a small d^* that maximizes the objective functional at the optimal control.

In order to assess the implementation of the optimal control to other admissible controls, we choose to compare their objective functional values as it is shown in Table 2.14. We choose a population able to diffuse at rate of $d = 0.002$ to perform these comparisons. One can clearly see that the value of J at the optimal control was much higher than the objective functional value corresponding to no control or constant control at $I = 0.2$. By computing the ratio between the objective functional of the optimal control and the constant control, we notice that the J value of using optimal control is almost 68% higher than when constant control was used. This difference in the J value is really significant since the two previous examples the J values were very similar (only 6% and 2% better, look at Tables 2.9 and 2.11). Therefore, by considering the two high costs relative to increase the population size at the

Table 2.13: Seven levels of diffusion rates in decreasing order along with their corresponding objective functional and population size at the final time using unfavorable initial conditions in Figure 2.19.

d	$J_d(I^*)$	$\int_0^1 N^*(x, 20) dx$
0.01	4.48	0.46
0.006	11.05	0.77
0.002	20.97	1.12
0.001	25.80	1.31
0.0006	28.97	1.43
0.0002	33.15	1.68
0.0001	28.77	1.45

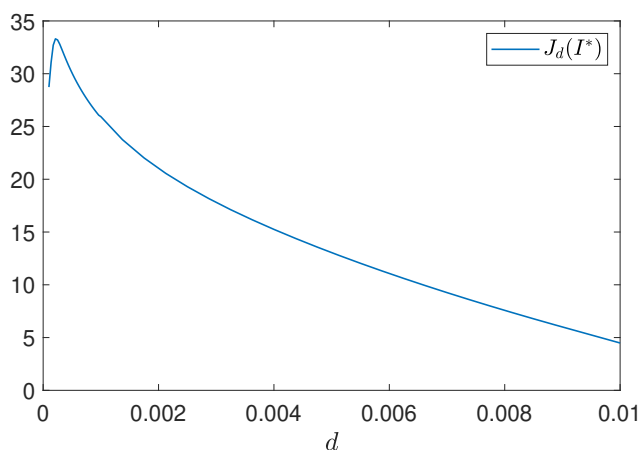


Figure 2.20: Objective functional as a function of the diffusion rate with unfavorable initial habitat for the population.

Table 2.14: Comparing the objective functional values of implementing optimal control strategy, no control ($I = 0$) and when control is constant at the highest level ($I = 0.2$). We choose the diffusion rate with the highest J_d value from Table 2.13, that is, $d = 0.0002$.

$J_d(I^*)$	$J_d(0)$	$J_d(0.2)$	$\frac{J_d(I^*)}{J_d(0.2)}$
33.15	1.85	19.65	1.6870

final time (C_4) and the use of control (C_2), we could observe a significant difference between the cost of using optimal control instead of simply applying a constant control at the highest level.

One can notice that the dynamics of the population and resource regardless of slow or fast diffusion are very different near the final time. In Figure 2.21 we display the dynamics of two populations diffusing at two different rates ($d = 0.004$ and $d = 0.0002$) along with their resource and optimal control using the initial conditions in Figure 2.19. This occurs since the goal is to maximize the population size at the final time as much as we can. Thus, this justifies the low population densities in the beginning for both cases. To explain some of the effects that these populations have near the final time, observe that when population diffuses at a rate of $d = 0.004$, it hits the inhospitable boundaries sooner than the population that diffuses slower. For this reason, you can see that the optimal control when $d = 0.004$ is more important near the middle of the habitat as the population approaches to the final time. But when $d = 0.0002$ more optimal control is needed near the boundaries as the population is expected to spread slowly allowing it to grow away from its initial location.

Returning to our original question, does the population that diffuses slower have more abundance than those moving faster? Based on our numerical scenarios, it depends. Our numerical results have been able to detect an 'intermediate' optimal diffusion rate that maximizes the population size (see Figures 2.14 and 2.17). Similar findings like this have been discussed and proven for other reaction diffusion equations in [32, 58, 13, 7]. In our selections of initial spatial arrangement of the population being unfavorable (see Figure 2.13) or favorable (see Figure 2.16), they showed similar numerical results between the diffusion rate and its population size. Here, we only focused on values of d close to the optimal d^* to show that large values of d do not always decrease the population abundance. More precisely, we varied the value of d between 0.0001 and 0.01 to represent the slow and fast spread of the population. Nevertheless, we explored the impact of the diffusion rate as d becomes smaller. When the population diffuses very slowly, we found out that the population abundance levels off due to the lack of resource to sustain a higher population abundance. Although, we did not show any examples when the population diffuses faster, we expect the population abundance to decline to zero as it would hit the hostile boundaries too quickly.

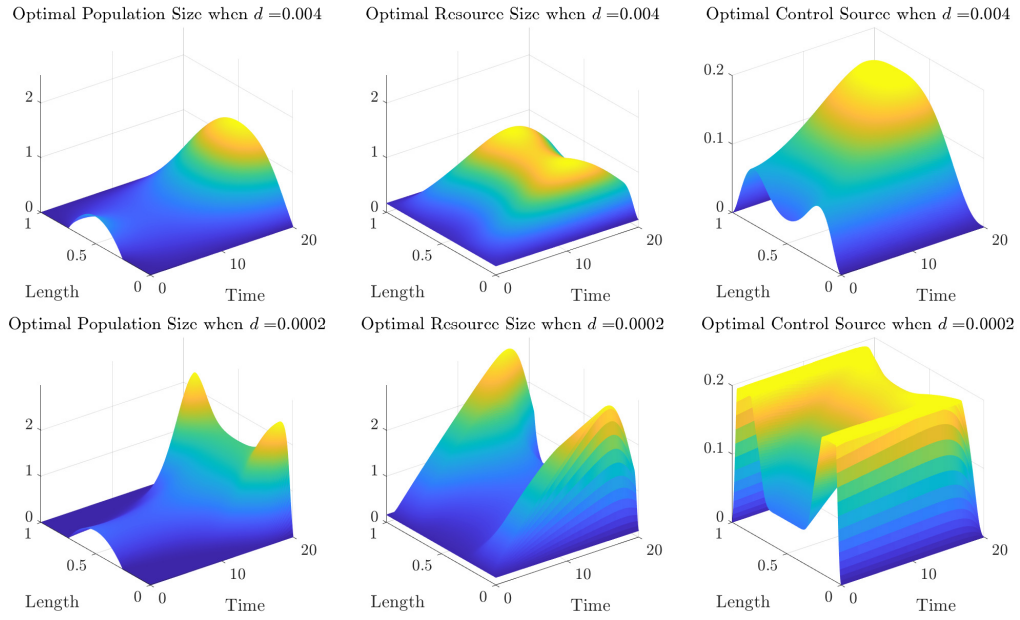


Figure 2.21: Population, resource and optimal control dynamics in space and time for two different diffusion rates, $d = 0.004$ (top) and $d = 0.0002$ (bottom) under unfavorable initial habitat for the population depicted in Figure 2.19.

Therefore, we could investigate whether other boundary conditions for the population can have the same impact as the hostile boundaries as we change the diffusion rate.

2.7.4 Optimal Resource Rate at a Later Time

So far, based on our previous numerical scenarios the initial amount of resource ($R_0(x)$) has always been assumed to be heterogeneously or homogeneously distributed along the habitat. Those initial conditions do not necessarily reflect the dynamics of the system with specific set of parameters. If we revisit the numerical examples in Subsection 2.7.2, it can be hard to know how to estimate the amount of initial resource for the population to grow. Assuming a mistaken initial distribution of resource can lead to wrong conclusions about the total population abundance. In this subsection, we investigate the scenario when the initial amount of resource along the entire habitat is equal or larger than the critical value, R_c . We let the population interact with its resource in absence of optimal control and once the resource-population dynamic has occurred for long enough, we use the population and resource spatial distributions at the final time to start a new resource-population dynamic in presence of optimal control. By allowing the interaction of population-resource without control, we can obtain a more realistic representation of the ecosystem before introducing the optimal control. The baseline parameters used for the following numerical simulations are shown in Table 2.15.

In the previous Subsections 2.7.2 and 2.7.3, the upper bound for all admissible controls have been chosen to be 1, but in this subsection we lower the upper bound to 0.1. By decreasing the upper bound, we are simply reducing the highest rate at which the optimal control can be applied. Notice that the choices of $p = 0$ and $q = 0$ represent that there is almost no contribution to the resource from the death of the population and natural resource decay is negligible. While we have chosen these parameters to be 0 in the model, in reality this means that the contributions from p and q to the resource are negligible within the ecosystem due to a short time period.

In the first numerical example we allow the population to interact with its resource when the initial amount of resource is equal to the critical resource value ($R_0(x) = R_c = 0.33$ for all $x \in [0, 1]$) and there is an initial high population density near the middle of the habitat

Table 2.15: Parameters used for Table and Figure in this section.

Parameter	α_1	μ	α_2	p	q	C_1	C_2	C_3	C_4	d	M_1	L	T
Baseline	0.3	0.1	0.3	0	0	10	1	0	10	0.001	0.1	1	40

as shown in Figure 2.22. Looking at the population-resource dynamic in Figure 2.23, as time goes on, the population quickly consumes the resource near the middle of the habitat and as it moves towards the boundary. Note that the resource at the edges are not affected throughout time since the population dies at the boundary due to the inhospitable boundary conditions. Next, we want to use the spatial distributions of population and resource at the final time as our new initial conditions as illustrated in Figure 2.24. Now, we let the population and resource start with this new set of initial conditions and in presence of optimal control. The dynamics of the population, resource and optimal control is given in Figure 2.25. One can see that due to initial low levels of resource, the population does not reflect a significant change in size after time $t = 20$. The optimal input rate of resource was at the highest level at all times along the habitat. At the beginning the optimal control help the resource to increase its size above the critical resource level to provide enough resource for population growth. And from time $t = 20$ to the final time $T = 40$, the optimal control is needed to help sustain the resource level such that the population can have enough resource to maintain its size. For this simulation, the population abundance increased from 0.01 at the initial time to 0.87 at the final time. In our next numerical simulation, we explore the scenario when the initial amount of resource is a constant three times larger than the resource threshold. The initial conditions for N and R are given in Figure 2.26. The dynamics of the population and resource sizes in Figure 2.27 show that the population is expected to increase its size in areas closer to the edges by $t = 20$, but since most of the resource has been consumed by then, the population size gets lower as it approaches the final time. The initial conditions in Figure 2.28 are the spatial distribution of population and resource at the final time of the previous simulation. Moreover, in Figure 2.29, we illustrate the dynamics of N and R when control is available. By looking at Figure 2.29, we observe that the dynamics of these three functions are very similar to those in Figure 2.25. Thus, the interpretation of the population, resource and optimal control follows similarly. For this case, the total population abundance at the final time is 0.84 and the initial population abundance was 0.05.

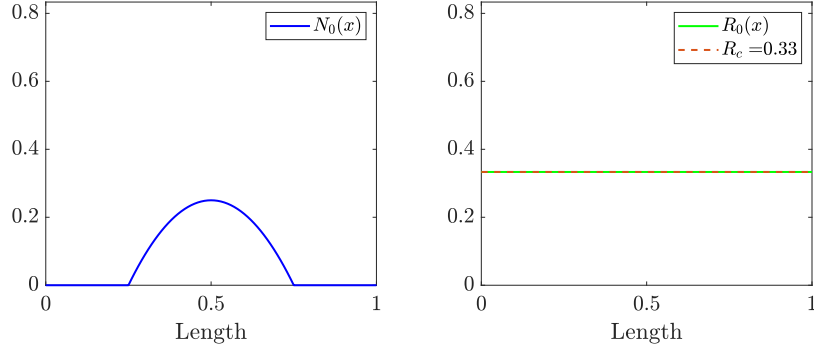


Figure 2.22: Initial conditions when $R_0(x) = R_c = 0.33$.

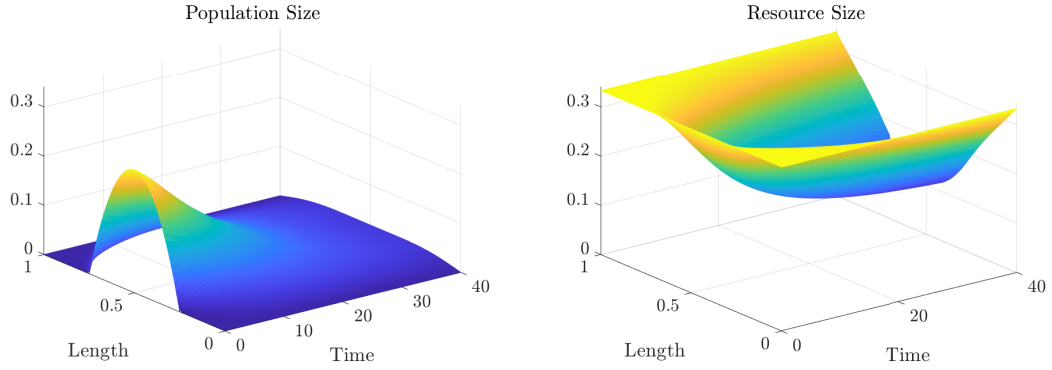


Figure 2.23: Population and resource dynamics in absence of optimal control using initial conditions on Figure 2.22. The parameter values are shown in Table 2.15.

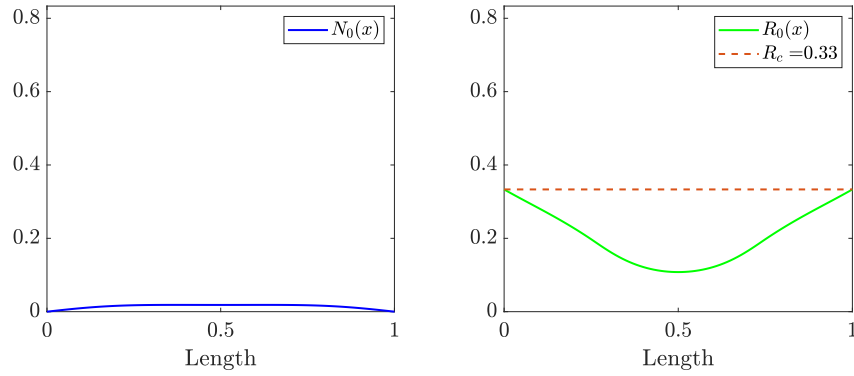


Figure 2.24: Initial conditions here are the final time distributions for population and resource in Figure 2.23, denoted by $R_0(x) = R_1(x, 40)$ and $N_0(x) = N_1(x, 40)$.

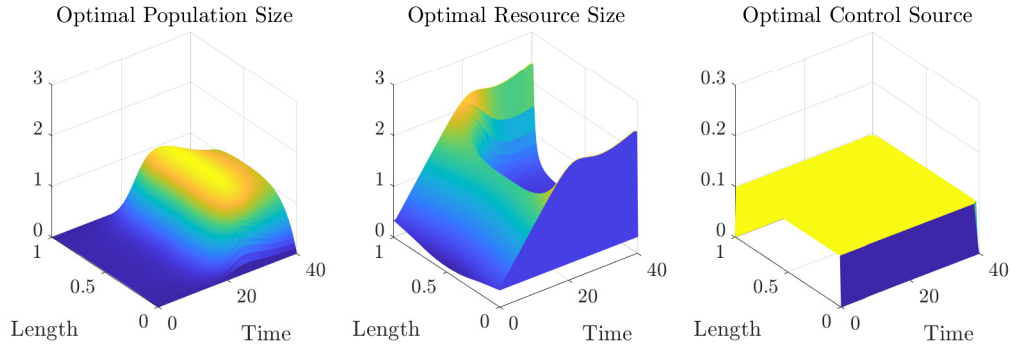


Figure 2.25: Dynamics of the population, resource and optimal control using initial conditions from Figure 2.24. The parameter values are shown in Table 2.15.

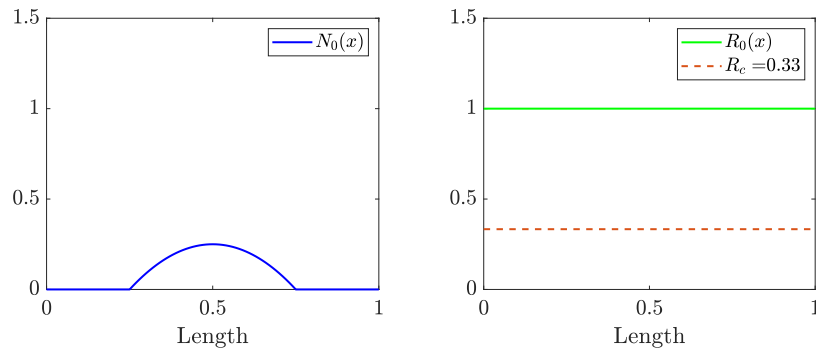


Figure 2.26: Initial conditions when $R_0(x) = 1 > R_c = 0.33$ for Figure 2.27.

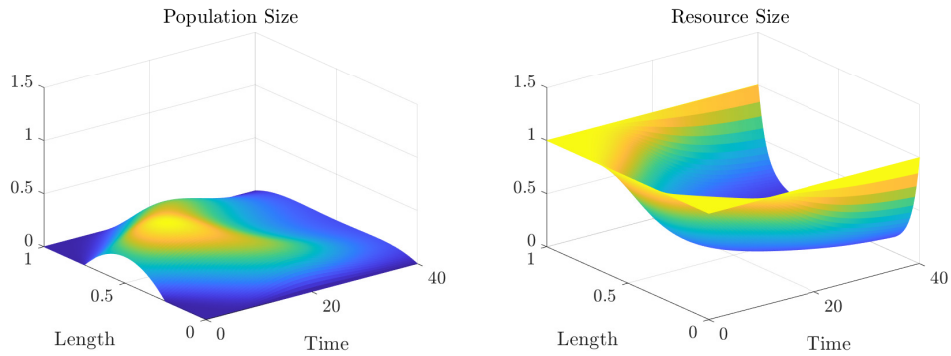


Figure 2.27: Population and resource dynamics in absence of optimal control using initial conditions on Figure 2.26. The parameter values are shown in Table 2.15.

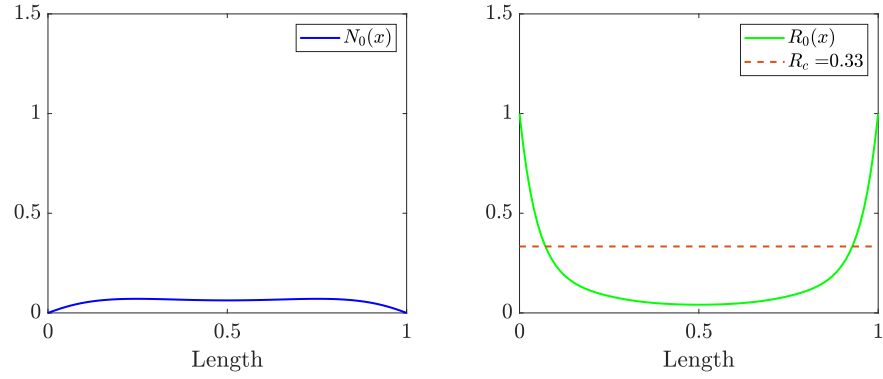


Figure 2.28: Initial conditions here are the final time distributions for population and resource in Figure 2.27, denoted by $R_0(x) = R_1(x, 40)$ and $N_0(x) = N_1(x, 40)$.

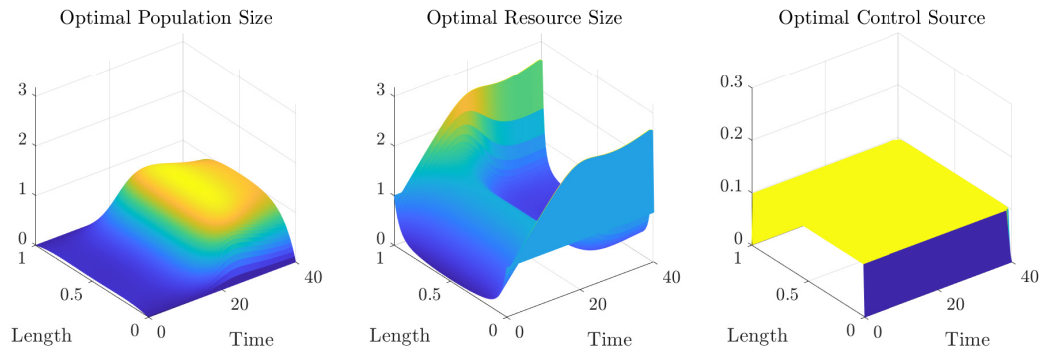


Figure 2.29: Dynamic of the population, resource and optimal control using initial conditions on Figure 2.28. The parameter values are shown in Table 2.15.

2.7.5 Neumann Boundary Condition

Up to this point, most of the numerical simulations have been under hostile boundary conditions. In this section we want to perform numerical simulations considering Neumann boundary conditions

$$N_x(x, t) = 0 \text{ on } \{0, L\},$$

meaning no flux for the population. Our no flux boundary condition represents a more suitable environment where emigration by the population does not occur (in this context, the habitat is more advantageous for the population since the diffusion of the population toward the boundaries doesn't reduce the population size directly). Some factors that can diminish the population size are the natural death rate and the lack of resource. In this case we assume that the resource ODE holds at the boundary as mentioned in Remark 2.2.1. The parameters in Table 2.16 are used to illustrate some numerical simulations in this section unless something else is specified. The main point of these numerical examples is to compare the dynamics of the population and its resource under favorable (Neumann) and unfavorable (Dirichlet) boundary conditions.

For our first numerical scenario in Figure 2.31 we want to illustrate the dynamics of N and R in absence of control when Dirichlet and Neumann boundary conditions are used. The initial conditions for N and R are in Figure 2.30 where the initial resource is constant everywhere. It can be seen in Figure 2.31 that in the absence of optimal control, the population and resource dynamics are different when Neumann (top row) or Dirichlet (bottom row) boundary conditions are considered. In the case when no flux boundary condition is used, the population abundance has always higher levels at any time compared to Dirichlet boundary condition. Thus, no flux boundary conditions will produce a more suitable habitat for the population under any initial resource distribution. Note that the dynamics of resource despite of our boundary conditions seem to be very similar except at the boundaries. The difference in dynamics are due to resource uptake by the population is allowed at the boundaries when no flux boundary condition is considered instead of Dirichlet. The slow decay observed in the resource graph when Dirichlet boundary conditions are

Table 2.16: Parameters used for numerical simulation in Section 2.7.5.

Parameter	α_1	μ	α_2	p	q	C_1	C_2	C_3	C_4	d	M_1	L	T
Baseline	0.3	0.1	0.3	0.4	0.01	1	100	0	1	0.001	0.1	1	40

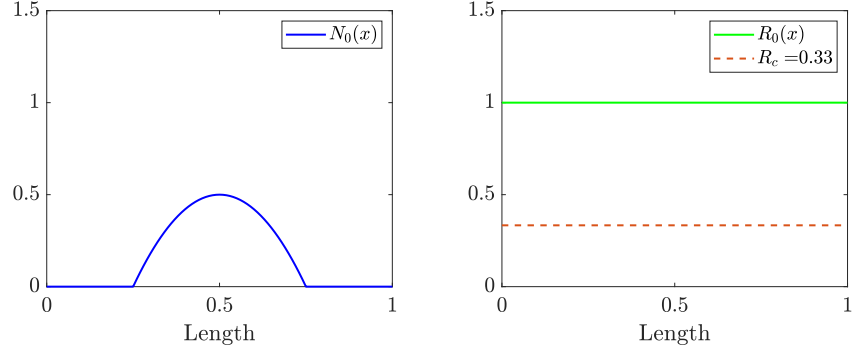


Figure 2.30: Initial conditions for Figure 2.31.

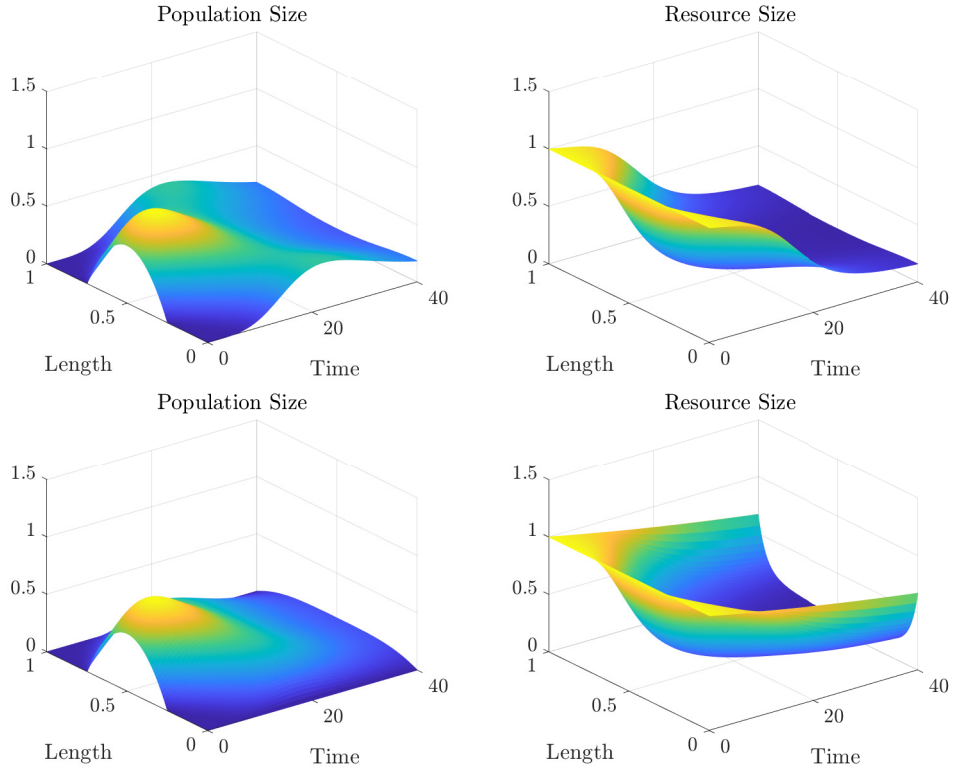


Figure 2.31: Population and resource dynamics in absence of optimal control using initial conditions on Figure 2.30. Top row shows no flux boundary condition while bottom row displays zero Dirichlet boundary condition.

considered is not due to resource uptake by the population since population dies at the boundary, but natural resource decay instead.

The next numerical simulations depicted in Figure 2.32 show the dynamic of N and R under the implementation of optimal control using the initial conditions on Figure 2.30. From here, we can highlight that in presence of optimal control the population size near the middle of the habitat is expected to increase regardless of what type of boundary condition are used. However, when no flux boundary conditions are used in presence of control, it helps the population to maintain its high size level near the boundaries as well. When Dirichlet boundary conditions are used, the optimal control pulls the population up by allocating more resource near the boundaries, but the effect of hostile boundary is too strong making it harder for the population to survive. For this reason, there are high amounts of resource allocated near the boundaries when Dirichlet boundary conditions are implemented. The total initial abundance of the population was 0.16. Furthermore, we compute the objective functional

$$J(I^*) = \int_0^1 N(x, 40) dx + \int_0^{40} \int_0^1 N(x, t) - 100I^{*2}(x, t) dx dt$$

for both types of boundary conditions. In the case of Neumann boundary conditions, the J -value was 51.11 and the total population abundance at the final was 1.6. For Dirichlet boundary conditions, the J -value was 22.6 and the final population size was 0.66. As expected, the population had higher abundance when no flux boundary conditions were used instead of Dirichlet. However, the population under harsh boundary conditions significantly increase its size at the end (since it jumped from 0.16 to 0.66) due to the implementation of the optimal control.

With our next next numerical scenario we want to explore the impact caused by both types of boundary conditions to the size of the population when the initial amount of resource is below the resource threshold. So, Figure 2.33 illustrates the initial spatial arrangement for the population and resource. As you can see from Figure 2.34, the total population abundance at the final time for both type of boundary conditions was much larger than its initial total population size. The implementation of the optimal control was at the highest level with Neumann boundary conditions rather than Dirichlet. This is caused by the effect

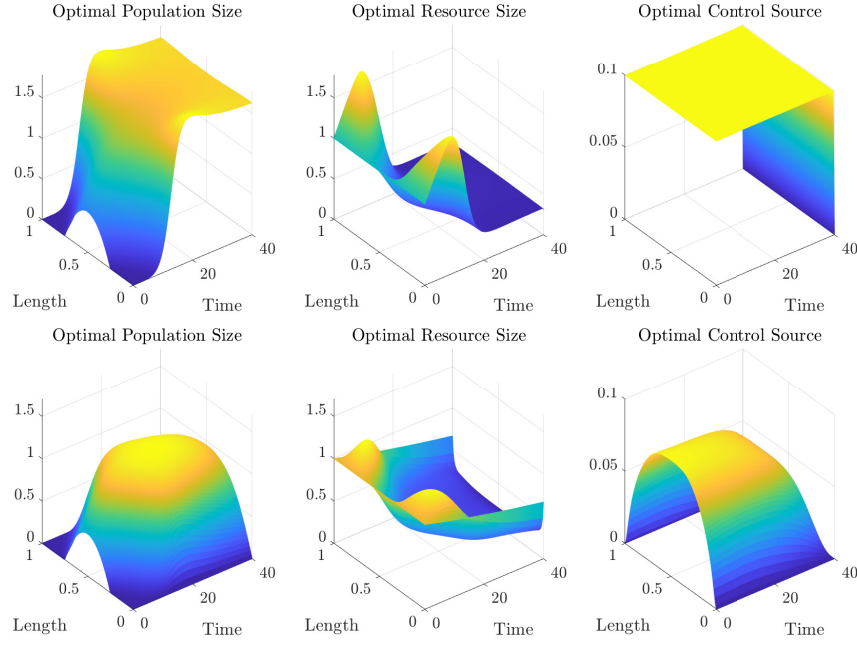


Figure 2.32: Population and resource dynamics in presence of optimal control using initial conditions on Figure 2.30. Top row shows no flux boundary condition while bottom row displays zero Dirichlet boundary condition. Note the vertical axis is scaled different for the optimal control.

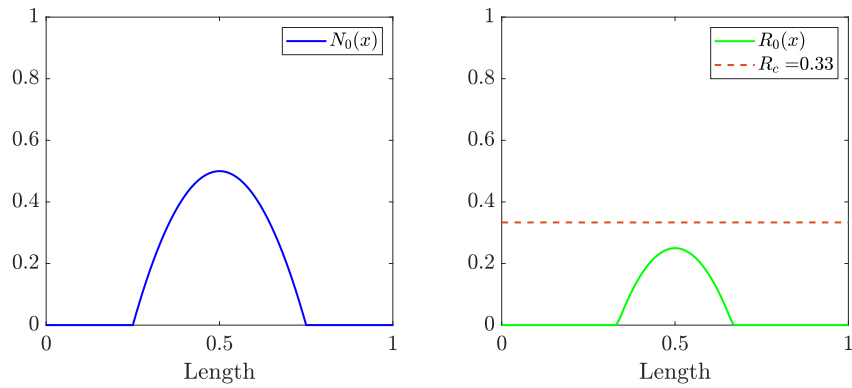


Figure 2.33: Initial conditions for N and R with R_0 always below R_c for Figure 2.34.

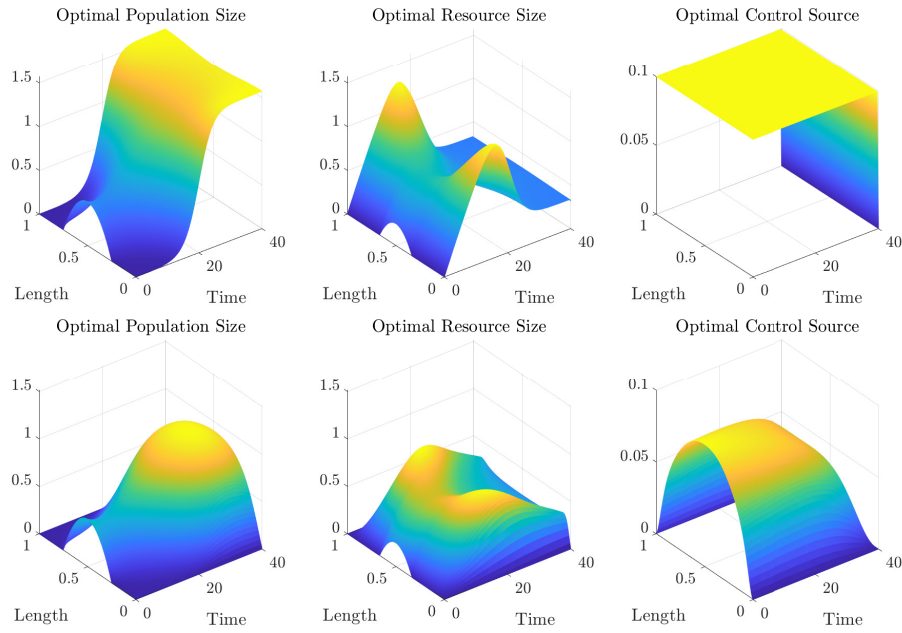


Figure 2.34: Population and resource dynamics in presence of optimal control using initial conditions on Figure 2.33. Top row shows no flux boundary condition while bottom row displays zero Dirichlet boundary condition. Note the vertical axis is scaled different for the optimal control.

of favorable boundary conditions in the population that allows the resource to grow near the boundary. Contrary to the case with hostile boundary conditions where the resource level near the boundary are low. The total population abundance at the initial time was the same as in the previous numerical scenario, that is 0.16 (since we kept the same $N_0(x)$). The value of the objective functional was higher for Neumann boundary condition rather than Dirichlet. Moreover, the values for the population abundance at the final time under no flux and Dirichlet boundary conditions were 1.54 and 0.65, respectively. The latter two numbers are relatively close to those found in the previous numerical scenario (in Figure 2.32) where the initial resource level was higher than R_c . Therefore, for these two numerical examples, regardless of choosing the initial resource levels above or below the resource threshold, with the help of the optimal control, the populations with favorable or unfavorable habitats had the same abundance at the final time.

As a fourth numerical example of more favorable boundary conditions, we assume the population has Neumann boundary conditions to interact with its resource in absence of optimal control from 0 to 40. After that, we use the the spatial distributions for N and R at the final time as initial conditions to run the model in presence of optimal control from 0 to 40 again. This method illustrates a more realistic choice of the initial condition for N and R as we discussed in Subsection 2.7.4. However, in the latter subsection, we identified possible initial distributions for N and R when the population had a hostile habitat at the boundaries. To illustrate this idea with favorable boundary conditions, we use the initial conditions for N and R on Figure 2.30. The dynamics in absence of control using this set of initial conditions under Neumann boundary conditions is shown at the top row in Figure 2.31. Thus, we take the final size distribution for the population and resource at the end as new initial conditions (this is shown at the top of Figure 2.35). The dynamics of the population and resource from 0 to 40 in presence of control is illustrated at the bottom row of Figure 2.35. With these numerical simulations we have a more accurate representation of the size distribution of a population with its resource under favorable edges and the optimal resource. In this case the population abundance at the initial and final times were 0.15 and 1.53. Hence, as we found in the previous two examples, the population size at the final grew nearly 10 times to its original size.

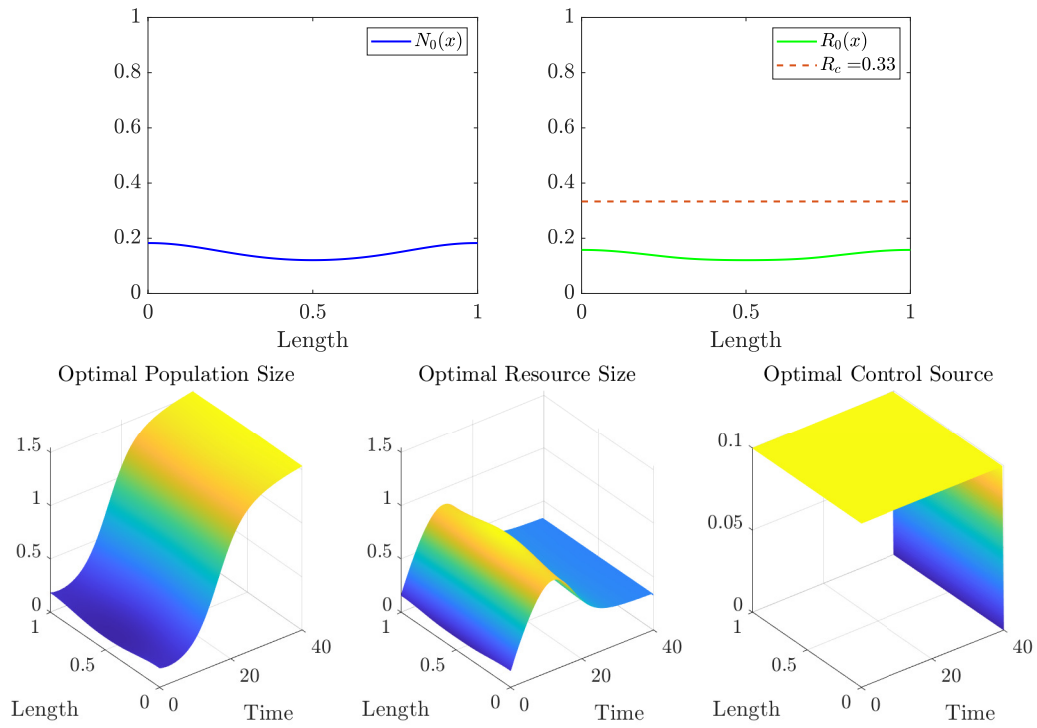


Figure 2.35: Initial conditions for N and R are at the top. Dynamics of population and resource in presence of optimal control with no flux boundary conditions are at the bottom.

2.7.6 Domain in Two Spatial Dimensions

Up to this point, among all the numerical examples that we have shown and discussed, the space domain Ω has been always a subset of $\mathbb{R}$. More precisely, we have chosen $\Omega = [0, 1]$. However, our resource allocation model can be applied to any smooth domain $\Omega \subset \mathbb{R}^n$. In this section, we want to illustrate two numerical simulations of our resource allocation model when $\Omega \subset \mathbb{R}^2$ has a square shape. Thus, for the next two numerical examples $\Omega = [0, 2]^2$ and the time interval is $[0, 1]$. Numerically, we use a uniform grid for Ω with grid spacing of $h = 0.02$. The diffusion rate d was taken as $d = 0.01$. Hence, a uniform grid for the time interval $[0, 1]$ with grid spacing of $s = \frac{h^2}{4d} = 0.01$ was used. Note that any value higher than $s = 0.01$ can make the numerical method to fail or not converge due to the CFL-condition is not satisfied.

For both simulations we assume the parameter values in Table 2.17 and Dirichlet boundary conditions for the population. Recall that the resource ODE holds at the boundary, thus no boundary conditions are required for the resource. With our choice for the parameters we assume that the population has a higher natural death rate than any of the previous examples and the resource has no natural resource decay rate or contribution by the death of the population. Moreover, the choice for the weight parameters C_1 and C_4 represent the importance of maximizing the abundance of the population at all times.

The idea of the first numerical scenario is to test how fast the population moves from areas with high population density to areas rich in resource where the population is absent. Figure 2.36 contains five heat maps of the population, resource and optimal control at different times starting at 0 and ending at 1. The first heat map when $t = 0$ represents the initial conditions for the population and resource in presence of control. As you can notice, the population only occupies the lower half of the habitat with high density near the middle and low density near the boundary. On the other hand, the resource are allocated along the entire habitat such that the highest density is concentrated in the middle of the habitat and it gets lower as it approaches the boundary. As time goes on, one can observe how the population quickly moves to areas on the upper half plane, but its size is getting lower by the population that dies at the boundary. In order to accomplish this results, the optimal

Table 2.17: Parameters used for numerical simulations in Section 2.7.6.

Parameter	α_1	μ	α_2	p	q	C_1	C_2	C_3	C_4	d	L	T
Baseline	0.4	1	0.4	0	0	50	1	0	50	0.01	2	1

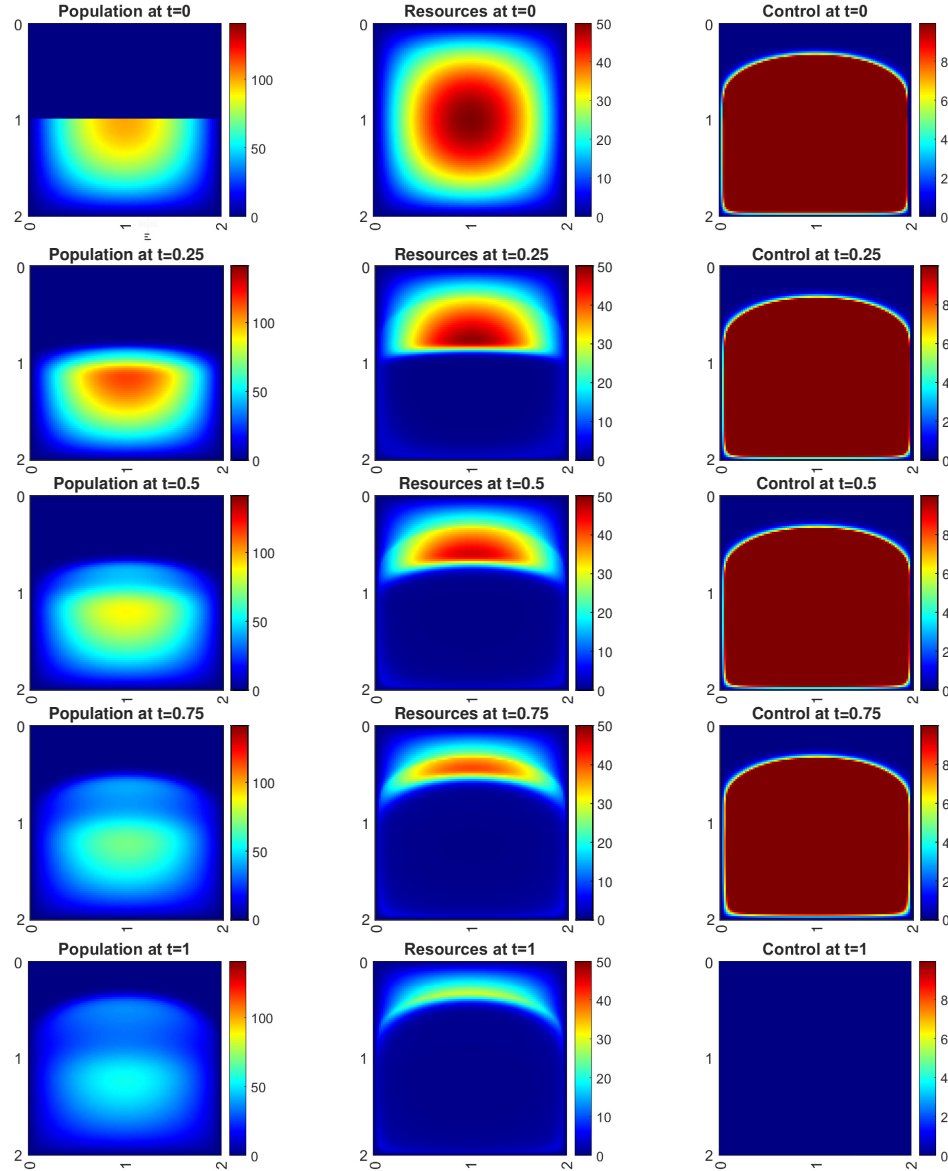


Figure 2.36: Heat maps to illustrate the dynamics of a population diffusing to areas with resource but no population. The upper bound for the controls was $M_1 = 10$.

control was used almost at the highest level in all the area except in small regions near the boundary and at the top.

The next example in Figure 2.37 illustrates the dynamics of a population and its resource when the implementation of the optimal control starts at a later time. More precisely, during the first half we let the system run in absence of control and after half time we incorporate the optimal control until the final time. We want to explore this case to have a more realistic initial condition for N and R as we discussed for the 1D case in Subsection 2.7.4. We start with a population that has low density in most of the habitat, but fortunately there are a lot of resource in middle for the population to grow. As we approach $t = 0.5$, we notice that the population has consumed most of the resource and it has improved its size significantly compared to its original size as reflected on the color bar. Once the optimal control is introduced to the system, we see a high allocation of the control in areas where the population has mostly consumed the resource. By the final time, we see that the resource were almost completely gone and the population size shrunk further. Perhaps if we allocate more time to run this simulation one could see a recovery for the resource since the optimal control would have longer time to make effect as we saw in the three examples in Subsection 2.7.4. Unfortunately, we skip this approach here since running 2D simulations for longer time intervals is computationally expensive.

2.8 Conclusion and Future Work

In this chapter we have proposed a resource allocation model to measure the impact that a diffusing population has within a heterogeneous or homogeneous habitat and in the presence of resource with dynamics in space and time. This ecological model consists of one nonlinear reaction diffusion equation to model the population growth and one nonlinear ordinary differential equation to study the rate of change of the resource. To enhance the resource, we allowed the possibility for the resource to be enhanced from outside the system by adding the function $I(x, t)$ that represents an input rate of resource (which later we consider as the control). To obtain theoretical results throughout this chapter, we assumed Dirichlet boundary conditions on the population and that the ODE for the resource holds at the

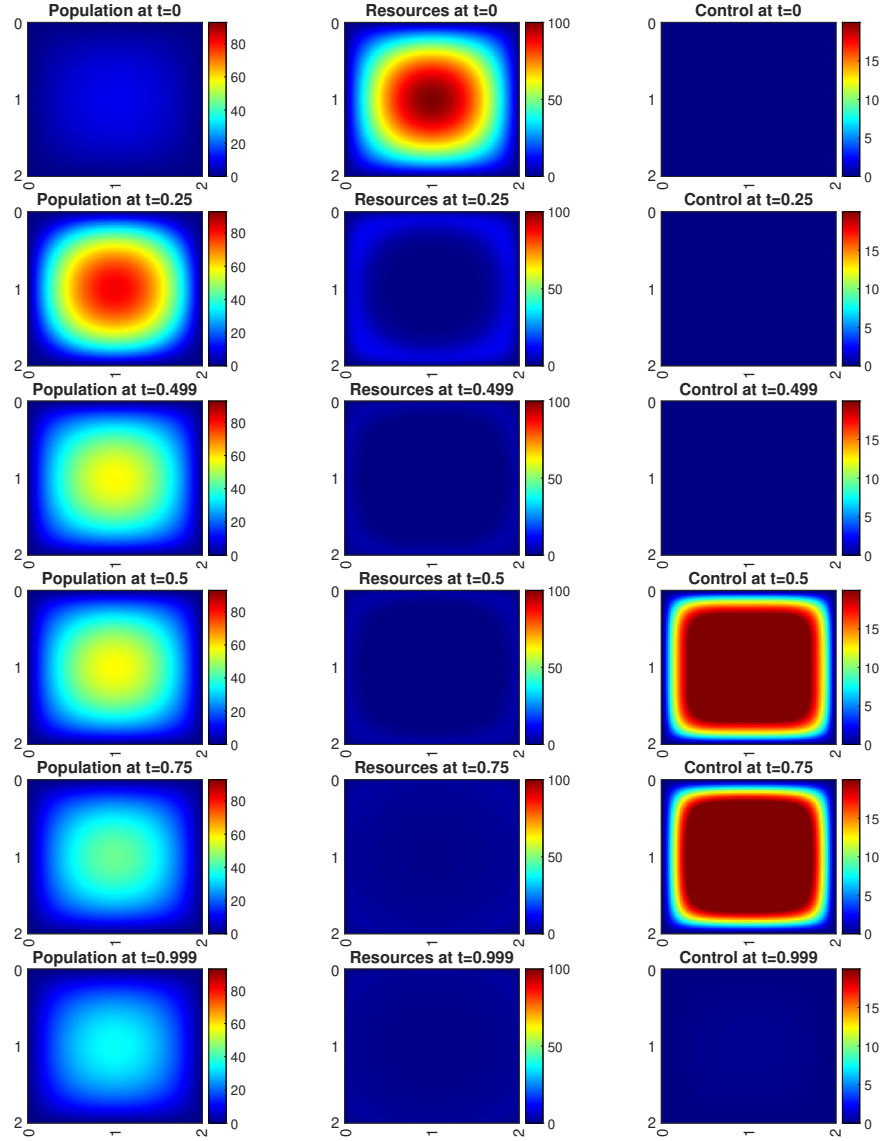


Figure 2.37: Heat maps to illustrate the use of optimal control starting at time $t = 0.5$. The upper bound for the control was $M_1 = 20$.

boundary. Our theoretical findings are also valid with Neumann boundary conditions. To analyze the resource allocation model, we provided its weak formulation, and Theorem 2.1 showed the existence of state solutions N and R in their corresponding weak solution space since the model may not have solutions in a classical sense. Moreover, we found a resource critical threshold, $R_c = \frac{\mu}{\alpha_1}$, as the ratio of natural population decay (μ) and the conversion of resource into population growth (α_1) to determine conditions for when the total population size is expected to shrink. If the resource level is below this critical level, then the population abundance is expected to decrease as time goes by. However, when the resource is above the critical threshold, the population is not guaranteed to grow in size unless the diffusion rate is low. In addition to formulating a resource allocation model, we also formulated an associated optimal control problem. The goal of the optimization problem was to maximize the total population abundance over time and minimize the cost associated with the optimal input rate of resource. Theorem 2.4 showed the existence of an optimal control by showing the existence of a maximizing sequence of admissible controls with corresponding sequence of state solutions. Subsequently, we derived the optimality system by proving the existence of solutions to the sensitivity equations in Theorem 2.5 and the existence of solutions to the adjoint equations associated with each state variable with a characterization of the optimal control in Theorem 2.6. Theorem 2.7 provided some conditions to show uniqueness of the optimal control problem. Furthermore, Theorem 2.8 proved the existence of an optimal diffusion rate that maximizes the objective functional at the optimal I^* subject to our model. Even though it was not the main focus of this chapter, we also considered an optimal control problem when the resource is able to diffuse as well.

Contributing to the understanding of the ecosystem model with a diffusing population and its dynamical resource, we performed several numerical simulations of the resource allocation model in the absence and presence of control to validate our theoretical findings. We implemented the Forward-Backward Sweep method to solve the optimality system. Within the numerical examples with optimal control, we validated the strength that the critical resource threshold has in diminishing the population size. We were also able to show numerically the existence of an intermediate diffusion rate that will maximize the objective functional. In doing this, we found that a different optimal diffusion rate than the one we

just mentioned maximizes the total population abundance at the final time. Further, we tested the scenario when the population and resource interact for some time and the optimal control is incorporated at a later time. For most of the numerical scenarios considered in this chapter, we used Dirichlet boundary conditions, however we dedicated a small part of the numerical simulation section with control to discuss some examples when the population was exposed to Neumann boundary conditions. We also illustrated two numerical examples when the spatial domain of the population was a square instead of a line. Although, we assumed in most of the numerical examples that the linear weight parameter C_3 was zero, in the future we could investigate more examples when C_3 values are nonzero.

As a future extension of this work, one can try to understand the dynamics of the resource allocation model without the spatial component and propose a simpler optimal control problem. By doing so, one can formulate the following optimization problem

$$\sup_{I \in U} J(I) \text{ where } J(I) = C_4 N(T) + \int_0^T C_1 N(t) - (C_3 + C_2 I(t)) I(t) dt$$

subject to

$$\begin{aligned} N_t &= \alpha_1 N R - \mu N && \text{on } (0, T) \\ R_t &= I(t) - \alpha_2 N R + p\mu N - qR && \text{on } (0, T) \\ N(0) &= N_0 \\ R(0) &= R_0 \end{aligned}$$

where

$$U = \left\{ I \in L^\infty((0, T)) \mid 0 \leq I(t) \leq M_1 \text{ and } \int_0^T I(t) dt = A \right\}.$$

Note that in this case all admissible controls are assumed to have an integral constraint. This constraint represents that only a fixed amount of input resource can be used from start to finish.

Another extension of this work is to incorporate more complex boundary conditions on the ecosystem model and integral constraints for all admissible controls. One could consider a Robin boundary condition on the population instead of simply Dirichlet or Neumann boundary conditions as we showed throughout this chapter. Thus, one of the maximization

problems to analyze would given by

$$\sup_{I \in U} J(I) \quad \text{where } J(I) = \int_{\Omega} C_4 N(x, T) \, dx + \int_0^T \int_{\Omega} C_1 N - (C_3 + C_2 I) I \, dx dt$$

subject to the ecosystem model

$$\begin{aligned} N_t - d\Delta N &= \alpha_1 N R - \mu N && \text{on } Q \\ R_t &= I(x, t) - \alpha_2 N R + p\mu N - qR && \text{on } Q \\ N(x, 0) &= N_0(x) && \text{on } \Omega \\ R(x, 0) &= R_0(x) && \text{on } \Omega \\ aN(x, t) + b \frac{\partial N(x, t)}{\partial \boldsymbol{\eta}} &= g(N) && \text{on } \partial\Omega \times [0, T]. \end{aligned}$$

In the problem above a and b represent the coefficients modifying the population density and rate of change of the population. Moreover, $\boldsymbol{\eta}$ is the outward unit normal vector along the boundary of Ω and $g(N)$ describes the density of the population along the boundary. A further discussion on the importance of boundary conditions affecting different species growth can be found in [18].

Chapter 3

Optimal Control Applied to a Zika Virus Epidemic

3.1 Introduction

Zika virus (ZIKV) is the first known vector borne disease that can be transmitted by the bite of a female mosquito as well as through direct contact between humans. The virus was first isolated in 1947 from the serum of a febrile rhesus monkey by intracerebral infection of mice [15]. The monkey served as sentinel animal for the surveillance of yellow fever virus (YFV) in the Zika forest in Uganda [15]. Nine months after, ZIKV was isolated again in the same region from mosquitoes of the species *Aedes africanus* [15]. The new virus was differentiated from known viruses such as YFV or Dengue virus by using defined antisera in neutralization tests. The virus was named after its place of first detection in the Zika forest.

ZIKV is transmitted to people primarily through the bite of an infected *Aedes* species mosquito and secondarily by direct contact from human to human. *Aedes* mosquitoes also spread dengue and chikungunya viruses. At this time there have been no reports of other animals becoming sick with ZIKV or of being able to spread ZIKV to people or other animals. The risk of catching ZIKV comes from the possibility of causing severe brain defects. If a woman is infected during pregnancy the virus can cause the baby to be born with microcephaly (babie's head smaller than expected) or even miscarriages. There have

also been reports of an increase of Guillain-Barré syndrome (rare neurological disorder where the immune system damages the nerves) cases in areas affected with the virus [10].

ZIKV can be passed through sexual contact from a person who has the virus to his or her sex partners [1, 35]. Such exposure includes sex without a condom with a person who traveled to or lives in an area with ZIKV even if the person does not have symptoms at the moment of contact. ZIKV can be transmitted from an infectious individual before their symptoms start, while they have symptoms, and after their symptoms end. It may also be passed by a person who has been infected with the virus, but never develops symptoms. Studies are underway to find out how long ZIKV stays in the semen and vaginal fluids of people who have the virus, and how long it can be transmitted to sex partners [1]. However, current research shows that ZIKV can remain in semen longer than in other body fluids, including vaginal fluids, urine, and blood [1].

Since ZIKV can be transmitted by mosquito bites or sexual contact, it is necessary to know how to control both methods of transmission to prevent severe brain damage the virus can cause in people. In this work, we provide alternatives control measures to prevent and control the spread of ZIKV based on issued guidance preventions in affected regions published by the national public health institutes of The United States.

According to the Centers for Disease Control and Prevention (CDC), there are practical ways to prevent ZIKV by avoiding vectorial transmission: that is, mosquitoes should be eliminated and mosquito bites prevented. In order to control mosquitoes outside a home, standing water where mosquitoes could lay eggs should be removed and any items that hold water like tires, buckets, planters, flowerpot or other trash containers should be emptied and scrubbed. Since mosquitoes can lay eggs near water, storage containers (buckets, cisterns) should also be covered. Different methods could be used to kill mosquitoes inside and outside homes. Outdoor insect spray could be used to kill mosquitoes outside homes, in areas where they rest. Windows and door screens are recommended to control mosquitoes inside homes. The use of commercial indoor insect spray would work immediately to kill mosquitoes and treat areas where they're resting. On the other hand, the use of insect repellents would help people avoid be bitten by mosquitoes, for example throughout the night.

The most effective control measure of direct (sexual) transmission is abstinence. However, prophylactics, such as condoms, should be used for sexually active individuals. Using female or male condoms might protect an individual during sex and reduce the chances of getting ZIKV from sexual contacts. To be effective, condoms should be used from start to finish, every time during a sexual contact. Not sharing sex toys can also prevent the risk of getting ZIKV from sex partners.

In particular, an effective and safe vaccine against ZIKV could help to prevent the terrible side effects such as microcephaly in babies and Guillain-Barré syndrome in adults. Since the 2015-2016 ZIKV epidemic, much effort has been devoted to produce a safe and cost-effective ZIKV vaccine [41, 48, 52]. There are several ZIKV vaccine candidates at different pre-clinical and clinical stages, but no candidate has been approved yet for mass distribution [48, 52, 55] (See Table 3.1). Without doubt, vaccines have been proven to be the most effective way to prevent infectious diseases.

This chapter is intended to expand the mathematical model of a ZIKV epidemic proposed in Valega-Mackenzie and Ríos-Soto [50] and capture the dynamics of a ZIKV disease transmission with three different optimal control strategies. Three time-dependent controls in a system of ordinary differential equations (ODEs) are implemented, one for mosquito-human contact by adequately informing about the use of mosquito repellents to prevent mosquito bites, another for the human-human sexual contacts by advertising campaigns informing about the use of condoms and a vaccination rate to measure how long a vaccination campaign should last to decrease the number of people infected with ZIKV at the lowest cost. Thus, our objective is to examine the impact of three time-varying controls in order to diminish a ZIKV epidemic by reducing the number of infected individuals (both humans and mosquitoes) while the implementation costs are minimized.

In order to understand the burden within ZIKV endemic regions, several mathematical epidemic models of mosquito-borne disease have been implemented with control and prevention strategies [4, 34, 22, 38, 44]. For instance, Bonyah et al. [4] used an ODE model of for the transmission of ZIKV in the absence of vaccination with optimal control strategies such as treatment, prevention and insecticide. Their numerical results showed the best way to eliminate disease transmission is by implementing all three controls at the same time.

Table 3.1: ZIKV vaccine candidates. Vaccines are to be administered by injection into the arm [36].

Type	Developer
A DNA-based vaccine	NIAID's Vaccine Research Center
A purified inactivated Zika vaccine	Walter Reed Army Institute of Research
Live attenuated Zika vaccine	NIAID's Laboratory of Viral Diseases
Investigational mRNA vaccines	NIAID

Miyaoka et al. [34] developed a reaction-diffusion epidemic model of ZIKV with vaccination using data from a region in Brazil. Their control variable was the vaccination rate which could be varied in space and time. Sasmal et al. [44] developed and fitted five different ODE models to data from World Health Organization (WHO) of the ZIKV outbreak in Colombia. They inferred the parameters and selected the most appropriate model that could adjust to the data. In addition, they performed mathematical analysis of the models and tested how different the routes of transmission are if the human population is stratified by gender and assuming only a portion of them have sexual contact. Okyere et al. [38] studied an ODE ZIKV model with five different controls including vaccination. They found that each of the optimal control strategies had a positive effect in reducing the number of infected individuals when compared with the model without controls.

This chapter is organized as follows: in Section 3.2, we propose the optimal control model of ZIKV spread under vaccination; in Section 3.3, we describe the six different scenarios to prevent the disease spread and formulate the associated optimal control problem. In Section 3.4 we explain data collected from ZIKV outbreaks in Colombia and Puerto Rico while in Section 3.5, we explain the numerical scheme to find fitted parameters. Sections 3.6 and 3.7 provide numerical simulations and results corresponding to each country and Section 3.8 concludes our work and provides a discussion.

3.2 Optimal Control Problem with Time-Dependent Vaccination Rate

In this chapter we propose the following non-autonomous, non-linear ODE model to capture the dynamics of a ZIKV epidemic:

$$\begin{aligned}
S'(t) &= \mu N(t) - \beta S(t) \frac{I_v(t)}{N_v(t)} (1 - u_2(t)) - \alpha S(t) \frac{I(t)}{N(t)} (1 - u_1(t)) - \phi(t) f S(t) \\
&\quad + \omega V(t) - \mu S(t), \\
V'(t) &= \phi(t) f S(t) - \omega V(t) - \mu V(t), \\
E'(t) &= \beta S(t) \frac{I_v(t)}{N_v(t)} (1 - u_2(t)) + \alpha S(t) \frac{I(t)}{N(t)} (1 - u_1(t)) - (\kappa + \mu) E(t) \\
I'(t) &= \kappa E(t) - (\gamma + \mu) I(t), \\
R'(t) &= \gamma I(t) - \mu R(t), \\
S'_v(t) &= \mu_v N_v(t) - \mu_v S_v(t) - \beta_v S_v(t) \frac{I(t)}{N(t)}, \\
E'_v(t) &= \beta_v S_v(t) \frac{I(t)}{N(t)} - (\mu_v + \eta) E_v(t), \\
I'_v(t) &= \eta E_v(t) - \mu_v I_v(t)
\end{aligned} \tag{3.1}$$

subject to corresponding initial conditions for each state equation. The total human population at time t , denoted by $N(t)$, is stratified into the state populations of susceptible $S(t)$, vaccinated $V(t)$, exposed $E(t)$, infected $I(t)$, and recovered $R(t)$ humans. Likewise, the total population of mosquito at time t , denoted by $N_v(t)$, is divided into the states of susceptible $S_v(t)$, exposed $E_v(t)$, and infected $I_v(t)$ mosquitoes. Thus, $N(t) = S(t) + V(t) + E(t) + I(t) + R(t)$ and $N_v(t) = S_v(t) + E_v(t) + I_v(t)$. In model (3.1), $N'(t) = 0$ and $N'_v(t) = 0$, therefore the total human and mosquito population remain constant for all time, that is $N(t) = N$ and $N_v(t) = N_v$. Figure 3.1 shows a flow chart of the model dynamics.

The parameter μ represents the birth and death rate of humans with μ_v similarly for mosquitoes. Susceptible humans are vaccinated at a rate ϕ with vaccine efficacy f , (where $0 < f \leq 1$). It is also assumed vaccines might not provide permanent immunity, hence ω represents a waning rate of the vaccine. That is, people who get vaccinated would become susceptible again at a rate ω . Note that vaccinated individuals are fully protected against ZIKV unless their immunity has waned. The contact rate β represents the rate at which a susceptible human becomes infected through the bites of infectious mosquitoes. The transmission rate from human to human is given by the parameter α while κ is the rate

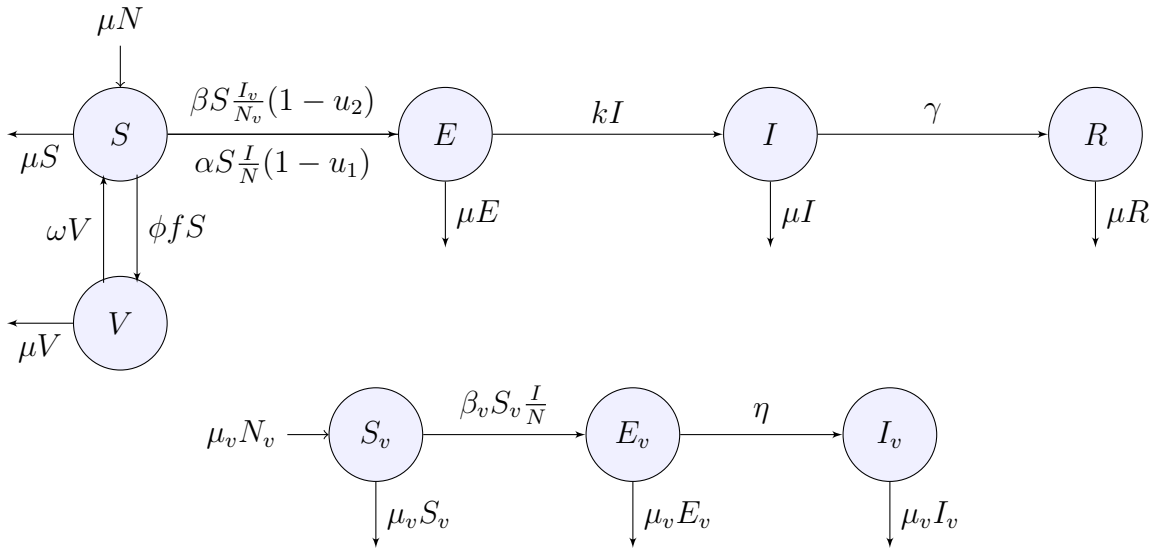


Figure 3.1: ZIKV vaccination model flow chart.

at which exposed humans become infectious. Infected humans recover from ZIKV at a rate of γ . Moreover, β_v is the transmission rate of susceptible mosquitoes becoming infected after biting an infected human, while exposed mosquitoes become infectious at a rate η . The definitions of the parameters are summarized in Table 3.2.

Within the human population, the direct transmission rate α may be reduced by a factor of $1 - u_1(t)$, where the control $u_1(t)$ represents the effort to inform humans about the use of prophylactics, such as condoms to prevent more people getting infected with ZIKV by sexual contacts. One way to address this strategy might be using different condom advertisement campaigns such as Internet, television and billboards in zones where ZIKV is more prevalent. On the other hand, the force of infection due to the vector transmission rate β may also be reduced by a factor of $1 - u_2(t)$, where the control $u_2(t)$ measures the level of informing the public about personal protection techniques to eliminate mosquito-human contact by increasing the use of repellent or mosquito nets. Thus, $u_2(t)$ represents the effort to advertise maintenance preventive actions by humans such as mosquito nets or insect repellents to avoid mosquito bites. In this chapter, we investigate the case when the vaccination rate ϕ is a time dependent function. It is assumed that the vaccine is not always effective ($f \neq 1$), and the immunity of the vaccine wanes at a rate ω (when $\omega = 0$ the vaccine provide permanent immunity) against ZIKV infection.

In the next section we investigate the existence and uniqueness of solution of model (3.1).

3.2.1 Existence, Uniqueness and Non-negativity of Solutions

In this section we show results given on the existence, uniqueness and non-negativity of solutions of the ZIKV vaccination model (3.1) provided a positive initial condition vector. Consider the following autonomous initial value problem

$$\begin{aligned} \frac{d\vec{y}}{dt} &= \vec{g}(t, \vec{y}(t)) \\ \vec{y}(t_0) &= \vec{y}_0 \end{aligned} \tag{3.2}$$

Table 3.2: Parameter description of model (3.1).

Parameter	Definition	Units
μ	Human birth and death rate	week ⁻¹
β	Transmission rate from vector to human	week ⁻¹
α	Transmission rate from human to human	week ⁻¹
κ	Transition rate from exposed to infected humans	week ⁻¹
ϕ	Vaccination control rate of susceptible humans	week ⁻¹
f	Vaccine efficacy	dimensionless
ω	Imperfect vaccination rate	week ⁻¹
γ	Recovery rate	week ⁻¹
μ_v	Mosquito birth and death rate	week ⁻¹
β_v	Transmission rate from human to vector	week ⁻¹
η	Extrinsic incubation rate	week ⁻¹
u_1	Human-human control	dimensionless
u_2	Mosquito-human control	dimensionless

where $(t, \vec{y}) \in [0, \infty) \times \mathbb{R}^n$ and $\vec{g} : C \rightarrow \mathbb{R}^n$ with C an open subset of $[0, \infty) \times \mathbb{R}^n$. Let Q be a rectangular region such that

$$Q = Q((t_0, \vec{y}_0), a, b) = \{(t, \vec{y}) : |t - t_0| \leq a \text{ and } \|\vec{y} - \vec{y}_0\| \leq b\} \quad (3.3)$$

with a and b positive numbers. The next theorem has been taken from [33] and it shows the existence and uniqueness for the initial value problem in (3.2).

Theorem 3.1. (From [33]) *The initial value problem (3.2) has a solution if for some $Q \subset C$ centered about $(t_0, \vec{y}_0)$ the function $\vec{g}$ satisfies the following three conditions:*

- (i) *the restriction of $\vec{g}$ to Q is continuous in $\vec{y}$ for fixed t ,*
- (ii) *the restriction of $\vec{g}$ to Q is measurable in t for fixed $\vec{y}$,*
- (iii) *there exists a Lebesgue integrable function $m : [t_0 - a, t_0 + a] \rightarrow [0, \infty]$ such that*

$$\|\vec{g}(t, \vec{y})\| \leq m(t), \quad (t, \vec{y}) \in Q.$$

Remark 3.2.1. *Theorem 3.1 is known as Carathéodory existence theorem. Carathéodory's theorem is a generalization of Picard-Lindelöf existence-uniqueness theorem of problem (3.2), but with weaker conditions on $\vec{g}$.*

The following theorem has been taken from Chapter 5 in [47]. Theorem 3.2 guarantees the solution of the initial value problem in system (3.1) is non-negative given specific conditions on $\vec{g}$ and a non-negative initial conditions.

Theorem 3.2. (From [47]) *Assume that $\vec{g}$ satisfies the same assumptions as in Theorem 3.1 and when $\vec{y}_0 \in \mathbb{R}^n$ satisfies $\vec{y}_0 \geq 0$ with $\vec{y}_{0i} = 0$ for some i , then $\vec{g}_i(t, y) \geq 0$. Then, if $\vec{y} \in \mathbb{R}^n$ satisfies that $\vec{y}_0 \geq 0$ and $t_0 \geq 0$, the solution of (3.2) is non-negative for all $t \geq t_0$.*

In the next two theorems we state the existence, uniqueness of non-negative solution to our ZIKV system (3.1) given that the initial conditions are non-negative.

Theorem 3.3. *The ZIKV system (3.1) has a non-negative solution given a non-negative initial condition.*

Proof. In order to show that the solution for ZIKV system (3.1) is non-negative we check the conditions on Theorem 3.2. Let $\vec{y}_0 = (S_0, V_0, E_0, I_0, R_0, S_{v0}, E_{v0}, I_{v0}) \geq 0$ be a non-negative vector of initial condition with $\vec{y}_0 = \vec{y}(t_0)$ and $t_0 \geq 0$.

Suppose that $\vec{y}_0 = (0, V_0, E_0, I_0, R_0, S_{v0}, E_{v0}, I_{v0}) \geq 0$. Then,

$$g_1(t_0, \vec{y}_0) = \mu N + \omega V_0 \geq 0.$$

Suppose that $\vec{y}_0 = (S_0, 0, E_0, I_0, R_0, S_{v0}, E_{v0}, I_{v0}) \geq 0$. Then,

$$g_2(t_0, \vec{y}_0) = \phi(t_0) f S_0 \geq 0.$$

Suppose that $\vec{y}_0 = (S_0, V_0, 0, I_0, R_0, S_{v0}, E_{v0}, I_{v0}) \geq 0$. Then,

$$g_3(t_0, \vec{y}_0) = \beta S_0 \frac{I_{v0}}{N_v} + \alpha S_0 \frac{I_0}{N_0} \geq 0.$$

Suppose that $\vec{y}_0 = (S_0, V_0, E_0, 0, R_0, S_{v0}, E_{v0}, I_{v0}) \geq 0$. Then,

$$g_4(t_0, \vec{y}_0) = \kappa E_0 \geq 0.$$

Suppose that $\vec{y}_0 = (S_0, V_0, E_0, I_0, 0, S_{v0}, E_{v0}, I_{v0}) \geq 0$. Then,

$$g_5(t_0, \vec{y}_0) = \gamma I_0 \geq 0.$$

Suppose that $\vec{y}_0 = (S_0, V_0, E_0, I_0, R_0, 0, E_{v0}, I_{v0}) \geq 0$. Then,

$$g_6(t_0, \vec{y}_0) = \mu_v N_v \geq 0.$$

Suppose that $\vec{y}_0 = (S_0, V_0, E_0, I_0, R_0, S_{v0}, 0, I_{v0}) \geq 0$. Then,

$$g_7(t_0, \vec{y}_0) = \beta_v S_{v0} \frac{I_0}{N} \geq 0.$$

Suppose that $\vec{y}_0 = (S_0, V_0, E_0, I_0, R_0, S_{v0}, E_{v0}, 0) \geq 0$. Then,

$$g_8(t_0, \vec{y}_0) = \eta E_{v0} \geq 0.$$

Hence, we have shown that $\vec{g}_i(t_0, \vec{y}_0) \geq 0$ as long as $\vec{y}_0 \geq 0$ and $t_0 \geq 0$ with $y_{0i} = 0$ for some i . Thus, by Theorem 3.2, if a solution to the ZIKV system (3.1) exists, the solution is non-negative for all $t \geq t_0$. $\square$

Remark 3.2.2. *Note that since $N'(t) = 0$ and $N_v'(t) = 0$, then the total human and mosquito population remain constant for all time, that is $N(t) = N$ and $N_v(t) = N_v$. Thus, if a solution of system (3.1) exists we must have that each component of the state solution satisfies*

$$0 \leq S(t), V(t), E(t), I(t), R(t), S_v(t), E_v(t), I_v(t) \leq C \quad (3.4)$$

where $C = \max\{N, N_v\}$. Therefore, in case a solution exists, they are uniformly bounded.

Theorem 3.4. *There exists a unique solution of the ZIKV system (3.1) with corresponding initial condition.*

Proof. Let $\vec{y}(t) = (S(t), V(t), E(t), I(t), R(t), S_v(t), E_v(t), I_v(t))$ and define

$$\begin{aligned} S'(t) &= g_1(t, \vec{y}(t)), \\ V'(t) &= g_2(t, \vec{y}(t)), \\ E'(t) &= g_3(t, \vec{y}(t)), \\ I'(t) &= g_4(t, \vec{y}(t)), \\ R'(t) &= g_5(t, \vec{y}(t)), \\ S_v'(t) &= g_6(t, \vec{y}(t)), \\ E_v'(t) &= g_7(t, \vec{y}(t)), \\ I_v'(t) &= g_8(t, \vec{y}(t)). \end{aligned} \quad (3.5)$$

subject to the initial condition $\vec{y}_0 = (S_0, V_0, E_0, I_0, R_0, S_{v0}, E_{v0}, I_{v0})$. Note that all the entries of $\vec{g}$ are real-valued and continuous. We must show now that $\vec{g} = (g_1, g_2, g_3, g_4, g_5, g_6, g_7, g_8)$ is Lipschitz. To do so, we show that each g_i for $i = 1, 2, \dots, 8$ is Lipschitz. Recall that a

real-valued function with bounded derivative is Lipschitz. Consequently, one can show that g_i is Lipschitz in each of the eight states by showing that the derivative of g_i with respect to the j -th state are bounded for $i, j = 1, 2, \dots, 8$. We start off by taking the partial derivatives of g_1 with respect to each state variable:

$$\begin{aligned}\frac{\partial g_1}{\partial S} &= -\beta \frac{I_v(t)}{N_v} (1 - u_2(t)) - \alpha \frac{I(t)}{N} (1 - u_1(t)) - \phi(t)f - \mu, \\ \frac{\partial g_1}{\partial V} &= \omega, \\ \frac{\partial g_1}{\partial I} &= -\alpha \frac{S(t)}{N} (1 - u_1(t)), \\ \frac{\partial g_1}{\partial I_v} &= \beta \frac{S(t)}{N_v} (1 - u_2(t)), \\ \frac{\partial g_1}{\partial E} &= \frac{\partial g_1}{\partial R} = \frac{\partial g_1}{\partial S_v} = \frac{\partial g_1}{\partial E_v} = 0.\end{aligned}$$

Observe that all the partial derivatives of g_1 are bounded since all the parameter values are bounded, the terms $(1 - u_i(t)) \leq 1$ for $i = 1, 2$ and each state is bounded above by C as shown in remark 3.2.2. Similarly, we can find the partial derivatives of g_4 :

$$\begin{aligned}\frac{\partial g_4}{\partial E} &= \kappa, \\ \frac{\partial g_4}{\partial I} &= -(\gamma + \mu), \\ \frac{\partial g_1}{\partial S} &= \frac{\partial g_4}{\partial V} = \frac{\partial g_4}{\partial R} = \frac{\partial g_4}{\partial S_v} = \frac{\partial g_4}{\partial E_v} = \frac{\partial g_4}{\partial I_v} = 0.\end{aligned}$$

One can see that all the partial derivatives of g_4 are bounded due to the right hand sides depend only on parameter values which are bounded. In the same fashion as we have shown that the partial derivatives of g_1 and g_4 are bounded, we can show that the partial derivatives of g_i for $i = 2, 3, 5, 6, 7, 8$ are bounded as well, since they depend only on parameters values or the product of parameters with a state variable. On a compact subset of $\mathbb{R}^n$, g_i is Lipschitz in each of the state variables for every i . Therefore, $\vec{g}$ is Lipschitz. In addition, all functions g_i 's are bounded above by a constant due to bounds on states. Therefore by Theorem 3.1 and the Lipschitz property on $\vec{g}$, there exists a non-negative unique solution to the initial value problem in (3.1). Observe that the non-negativity of the solution is obtained by Theorem 3.3. □

In the next section we examine the basic reproductive number of model (3.1) in absence of the controls u_1 and u_2 , but a constant vaccination rate ϕ .

3.2.2 The Basic Reproduction Number

The dynamics of system (3.1) in the absence of control strategies u_1 and u_2 , but constant vaccination rate, is determined by the basic reproduction number $\mathcal{R}_0$. To find $\mathcal{R}_0$, we use the Next Generation Matrix method [51], and our the population is divided into 6 compartments. Our infected compartments are E , I , E_v and I_v . The disease free equilibrium (DFE) of the model is giving by

$$\vec{x}_0 = (0, 0, 0, 0, \frac{N(\mu + \omega)}{\phi f + \mu + \omega}, \frac{N\phi f}{\phi f + \mu + \omega})$$

where $\vec{x} = (E, I, E_v, I_v, S, V)$. Using the infected compartments, the progression of an infected individual through various compartments is given by:

$$\mathcal{F}(x) = \begin{pmatrix} S \left(\frac{\beta I_v}{N_v} + \frac{\alpha I}{N} \right) \\ 0 \\ 0 \\ 0 \end{pmatrix} \text{ and } \mathcal{V}(x) = \begin{pmatrix} (\kappa + \mu) E \\ (\gamma + \mu) I - E\kappa \\ -\frac{\beta_v S_v I}{N} + (\mu_v + \eta) E_v \\ -E_v \eta + \mu_v I_v \end{pmatrix}.$$

To calculate $\mathcal{R}_0$, we determine the Jacobian matrices F and V , given by

$$F(x_0) = \begin{pmatrix} 0 & \frac{S\alpha}{N} & 0 & \frac{S\beta}{N_v} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \text{ and } V(x_0) = \begin{pmatrix} \kappa + \mu & 0 & 0 & 0 \\ -\kappa & \gamma + \mu & 0 & 0 \\ 0 & -\frac{\beta_v S_v}{N} & \mu_v + \eta & 0 \\ 0 & 0 & -\eta & \mu_v \end{pmatrix}.$$

Using matrix algebra to calculate V^{-1} we obtain

$$V^{-1}(x_0) = \begin{pmatrix} \frac{1}{(\kappa+\mu)} & 0 & 0 & 0 \\ \frac{\kappa}{(\kappa+\mu)(\gamma+\mu)} & \frac{1}{(\gamma+\mu)} & 0 & 0 \\ \frac{\beta_v N_v \kappa}{N(\gamma+\mu)(\kappa+\mu)(\mu_v+\eta)} & \frac{\beta_v N_v}{N(\gamma+\mu)(\mu_v+\eta)} & \frac{1}{(\mu_v+\eta)} & 0 \\ \frac{\eta \beta_v N_v \kappa}{N(\gamma+\mu)(\kappa+\mu)(\mu_v+\eta)\mu_v} & \frac{\eta \beta_v N_v}{N(\gamma+\mu)(\mu_v+\eta)\mu_v} & \frac{\eta}{(\mu_v+\eta)\mu_v} & \frac{1}{\mu_v} \end{pmatrix}$$

and the next generation matrix of the model with vaccination is given by

$$FV^{-1}(x_0) = \begin{pmatrix} \frac{S\alpha\kappa}{N(\kappa+\mu)(\gamma+\mu)} + \frac{S\beta\eta\beta_v\kappa}{(\mu_v+\eta)N(\gamma+\mu)(\kappa+\mu)\mu_v} & \frac{S\alpha}{N(\gamma+\mu)} + \frac{S\beta\eta\beta_v}{(\mu_v+\eta)N(\gamma+\mu)\mu_v} & \frac{S\beta\eta}{(\mu_v+\eta)\mu_v} & \frac{S\beta}{\mu_v} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

where $\mathcal{R}_0 = \rho(FV^{-1})$ and thus

$$\mathcal{R}_0 = \frac{(\mu + \omega) \alpha \kappa}{(\phi f + \mu + \omega) (\kappa + \mu) (\gamma + \mu)} + \frac{(\mu + \omega) \beta \eta \beta_v \kappa}{(\phi f + \mu + \omega) (\mu_v + \eta) (\gamma + \mu) (\kappa + \mu) \mu_v}. \quad (3.6)$$

The $\mathcal{R}_0$ found in equation (3.6) can be rewritten as

$$\mathcal{R}_0 = (1 - \rho) (R_d + R_v)$$

where

$$R_d = \left(\frac{\alpha}{\mu + \gamma} \right) \left(\frac{\kappa}{\kappa + \mu} \right)$$

is the basic reproductive number of direct human transmission and

$$R_v = \left(\frac{\beta}{\mu + \gamma} \right) \left(\frac{\kappa}{\kappa + \mu} \right) \left(\frac{\beta_v}{\mu_v + \eta} \right) \left(\frac{\eta}{\mu_v} \right)$$

is the basic reproductive number associated with mosquito transmission. Here,

$$\rho = \frac{\phi f}{\mu + \omega + \phi f}$$

($0 \leq \rho \leq 1$) represents the vaccination effort which is the product of the effective vaccination ϕf and the average time ($\frac{1}{\mu + \omega + \phi f}$) that new susceptible humans occurred due to waning

vaccination. Observe that in absence of a vaccine ($\phi = 0$), there is no vaccination effort ($\rho = 0$). The direct transmission threshold (R_d) is the product between the average time a susceptible human takes to get infected by an infected human and the average time that it takes for an infected individual to become infectious. Moreover, the vector transmission threshold (R_v) is the product among four different average times. The first two factors correspond to the average time from a susceptible human to become infected by the bites of an infected mosquito and the time it takes from an infected human to become infectious. The last two factors are the average time from a susceptible mosquito to become infected after being bitten by an infected human and the time a mosquito takes to become infectious.

In the next section we describe the six scenarios from a mathematical and epidemiological viewpoint to reduce the spread of the epidemic. We also propose two optimal control problems associated with system (3.1) whose goals are to minimize the cost associated with control strategies while minimizing the burden of the disease or the total incidence.

3.3 Optimal Control Problem Formulation

In the present section we examine the application of different scenarios to decrease a ZIKV epidemic in a short period of time. The following scenarios are proposed in order to control the number of ZIKV infections and study the reduction of cases by the best plan. Table 3.3 summarizes the scenarios to be considered in terms of number of control strategies and public policy action.

- 1 Inform people about the use of condoms to avoid getting infected by sexual transmission (only control u_1 is applied).
- 2 Inform people about the use of mosquito repellents to avoid humans getting bitten by mosquitoes (only control u_2 is applied).
- 3 Inform people about the use of condoms to prevent new infections between humans and the use of insect repellents to prevent mosquito bites (two controls applied, u_1 and u_2).

Table 3.3: Six scenarios to prevent the spread of ZIKV.

Scenario	Controls	Policy
0	None	No campaigns
1	Only u_1	Condom campaigns
2	Only u_2	Insect repellent campaigns
3	Only u_1 and u_2	Condom and insect repellent campaigns
4	Only u_1 and ϕ	Condom and vaccination campaigns
5	Only u_2 and ϕ	Insect repellent and vaccination campaigns
6	u_1, u_2 and ϕ	Condom, insect repellent and vaccination campaigns

- 4 Vaccinate susceptible humans to provide them with some immunity against ZIKV and inform them about the use of condoms (only controls ϕ and u_1 are applied).
- 5 Vaccinate susceptible humans to provide them with some immunity against ZIKV and inform about the use of insect repellents (only controls ϕ and u_2 are applied).
- 6 Inform the public of two personal protection measures with an available vaccine (three controls applied, u_1 , u_2 , and ϕ).

In this work we want to asses the impact of increasing the awareness of personal protection measures such as condoms. insect repellent and vaccination by implementing social campaigns programs to reduce a ZIKV epidemic. We propose two optimal control problems to be minimized. The objective functional J_i with $i = 1, 2$ formulates the optimization problem (minimization) of interest which determines the most effective strategies to be implemented. The overall objective functional, J_1 , entails the minimization of the infected humans with ZIKV and the cost to implement each control over $(0, T)$. On the other hand, with J_2 , we want to minimize the total number of new ZIKV infections (incidence) and the cost associated to each control strategy over the entire time domain. Thus, we proposed the following two objective functionals J_i for $i = 1, 2$ given by

$$J_1(u_1, u_2, \phi) = \hat{J}_1 + \hat{J}_2 \quad (3.7)$$

$$J_2(u_1, u_2, \phi) = \hat{J}_3 + \hat{J}_2 \quad (3.8)$$

where

$$\hat{J}_1 = \int_0^T A_1 I(t) dt$$

and

$$\hat{J}_3 = \int_0^T A_2 \left(\beta S(t) \frac{I_v(t)}{N_v(t)} (1 - u_2(t)) + \alpha S(t) \frac{I(t)}{N(t)} (1 - u_1(t)) \right) dt$$

correspond to the cost of the epidemiological strategy while

$$\hat{J}_2 = \int_0^T B_1 u_1(t) S(t) + C_1 u_1^2(t) + B_2 u_2 S(t) + C_2 u_2^2(t) + B_3 \phi(t) S(t) + C_3 \phi^2(t) dt.$$

is the cost associated to the prevention measures. The constant A_1 is the relative cost of an infected human and A_2 is the cost of a new case. The relative costs associated with the nonlinear controls, $u_1^2(t)$, $u_2^2(t)$, and $\phi^2(t)$ are given by C_1 , C_2 and C_3 . The constants B_1 , B_2 , and B_3 are the relative cost of interventions to apply each control campaign over $[0, T]$, respectively. Table 3.4 provides a unit description and short definition of weight parameters. Therefore, for each optimization problem, we need to find optimal controls $(u_1^*(t), u_2^*(t), \phi^*(t))$ such that

$$J_i(u_1^*, u_2^*, \phi^*) = \min_{\Omega} J_i(u_1, u_2, \phi) \text{ for } i = 1, 2 \quad (3.9)$$

subject to the state system (3.1) and appropriate initial conditions. The set of admissible controls is given by

$$\Omega = \{(u_1, u_2, \phi) \in L^\infty[0, T]^3 : 0 \leq u_i(t) \leq b_i, i = 1, 2, 0 \leq \phi(t) \leq b_3\}.$$

The value of the upper bounds for the rates of using condoms, repellents and vaccination campaigns satisfy $0 \leq b_i \leq 1$ for $i = 1, 2, 3$ are selected depending on the circumstances of the problem. For instance, developed countries are more likely to allocate resources to each mitigation campaign in order to stop the spread of the epidemic rather than those developing countries where budgets are tighter to take timely actions. In the next subsection we prove the existence of an optimal control problem for each objective functional subject to our ZIKV model.

3.3.1 Existence of an Optimal Control

The next theorem guarantees the existence of an optimal control triple of the objective functional in (3.7) subject to system (3.1). We denote by $y = y(u_1, u_2, \phi)$ the state solution corresponding to the control triple (u_1, u_2, ϕ) .

Theorem 3.5. *There exists an optimal control triple (u_1^*, u_2^*, ϕ^*) that minimizes the objective functional $J_1(u_1, u_2, \phi)$ in (3.7) subject to the state system (3.1) and non-negative initial conditions.*

Table 3.4: Description of Weight parameters.

Parameter	Definition	Units
A_1	Weight constant on I class	$\$ \times \text{week}^{-1}$
A_2	Weight constant on Incidence	$\$$
B_i	Weight constants on linear controls $i = 1, 2$	$\$ \times \text{week}^{-1}$
B_3	Weight constant on linear vaccination rate	$\$$
C_i	Weight constants on controls $i = 1, 2$	$\$ \times \text{week}^{-1}$
C_3	Weight constant on vaccination rate	$\$ \times \text{week}$
b_i	Upper bound on controls $i = 1, 2$	dimensionless
b_3	Upper bound on vaccination rate	week^{-1}

Proof. Note that the state solutions are uniformly bounded for all $t \in [0, T]$ by remark 3.2.2 and Theorem 3.4. Since the control triple are also uniformly bounded, one can see that the objective functional is bounded below by 0, and thus, a minimum exists. Therefore, there exists a minimizing sequence $\{v_n\}_{n=1}^\infty$ where $v_n = (u_{1n}, u_{2n}, \phi_n)$ such that

$$\min_{v \in \Omega} J_1(v) = \lim_{n \rightarrow \infty} J_1(v_n).$$

Moreover, let $y_n = (S_n, V_n, E_n, I_n, R_n, S_{v_n}, E_{v_n}, I_{v_n})$ be the state sequence corresponding to the control v_n , that is $y_n = y(v_n)$. The time derivatives corresponding to each state are also bounded since the sequence of controls and state solutions are bounded for all $t \in [0, T]$. This implies that each state is Lipschitz continuous for each n due to boundedness of its derivatives. Thus, the state sequences are equicontinuous. We invoke Arzela-Ascoli Theorem to guarantee that our state sequence has a uniformly convergent subsequence since the state sequence is uniformly bounded and equicontinuous on a compact set. Let $\{y_{n_k}\}_{k=1}^\infty \subset \{y_n\}_{n=1}^\infty$ be the uniformly convergent subsequence such that:

$$y_{n_k} \rightarrow y^*$$

where $y^* = (S^*, V^*, E^*, I^*, R^*, S_v^*, E_v^*, I_v^*)$.

Let $C_1 = \max\{b_1, b_2, b_3\}$ so that $\|v_n\|_{L^\infty(0,T)} \leq C_1$ for all $n \in \mathbb{N}$. By equivalent norms, there exists a positive constant C_2 independent of n that guarantees

$$\|v_n\|_{L^2(0,T)} \leq C_2 \tag{3.10}$$

where C_2 depends only on C_1 and T . Hence, $v_n \in (L^2(0, T))^3$ for all n . The Banach-Alaoglu Theorem [20] states that every bounded sequence in L^2 has a weakly convergent subsequence. As a result of Banach-Alaoglu Theorem, there exists $v^* \in L^2(0, T)^3$ so that

$$v_{n_k} \rightharpoonup v^* \in (L^2(0, T))^3.$$

One still needs to show that y^* is the vector solution with corresponding state solutions associated with the optimal control triple v^* , that is $y^* = y(v^*)$. Using the S -equation from

system (3.1) after integrating over the interval $(0, t)$ and taking absolute values of both sides:

$$\begin{aligned}
\left| S_{nk}(t) - S^*(t) \right| &\leq \beta \left| \int_0^t S_{nk}(\tau) \frac{I_{vnk}(\tau)}{N_v} (1 - u_{2nk}(\tau)) - S^*(\tau) \frac{I_v^*(\tau)}{N_v} (1 - u_2^*(\tau)) d\tau \right| \\
&\quad + \alpha \left| \int_0^t S_{nk}(\tau) \frac{I_{nk}(\tau)}{N} (1 - u_{1nk}(\tau)) - S^*(\tau) \frac{I^*(\tau)}{N} (1 - u_1^*(\tau)) d\tau \right| \\
&\quad + f \left| \int_0^t \phi_{nk}(\tau) S_{nk}(\tau) - \phi^*(\tau) S^*(\tau) d\tau \right| \\
&\quad + \omega \int_0^t \left| V_{nk}(\tau) - V^*(\tau) \right| d\tau + \int_0^t \mu \left| S_{nk}(\tau) - S^*(\tau) \right| d\tau.
\end{aligned}$$

Observe that the following inequalities hold

$$\begin{aligned}
&\left| \int_0^t S_{nk}(\tau) \frac{I_{vnk}(\tau)}{N_v} (1 - u_{2nk}(\tau)) - S^*(\tau) \frac{I_v^*(\tau)}{N_v} (1 - u_2^*(\tau)) d\tau \right| \\
&\leq \left| \int_0^t \left(S_{nk}(\tau) \frac{I_{vnk}(\tau)}{N_v(\tau)} - S^*(\tau) \frac{I_v^*(\tau)}{N_v} \right) (1 - u_{2nk}(\tau)) - \left(S^*(\tau) \frac{I_v^*(\tau)}{N_v} \right) (u_{2nk} - u_2^*(\tau)) d\tau \right| \\
&\leq \int_0^t \left| S_{nk}(\tau) \frac{I_{vnk}(\tau)}{N_v} - S^*(\tau) \frac{I_v^*(\tau)}{N_v} \right| d\tau + \left| \int_0^t \left(S^*(\tau) \frac{I_v^*(\tau)}{N_v} \right) (u_{2nk} - u_2^*(\tau)) d\tau \right| \\
&\rightarrow 0 \text{ as } k \rightarrow \infty.
\end{aligned}$$

Note that in the above inequality, we invoked the uniform convergence associated to the state sequences S_{nk} , I_{nk} and I_{vnk} for the first integral while on the second integral we used the weak convergence of the sequence u_{2nk} . Recall that the product of two sequences that converge uniformly also converges uniformly. By a similar convergence argument to the one illustrated above, it can be shown that

$$\begin{aligned}
\int_0^t \left| S_{nk}(t) \frac{I_{nk}(t)}{N(t)} (1 - u_{1nk}(t)) - S^*(t) \frac{I^*(t)}{N(t)} (1 - u_1^*(t)) \right| dt &\rightarrow 0 \text{ as } k \rightarrow \infty, \\
\int_0^t \left| \phi_{nk}(t) S_{nk}(t) - \phi^*(t) S^*(t) \right| dt &\rightarrow 0 \text{ as } k \rightarrow \infty
\end{aligned}$$

By our last three convergence results as well as uniform convergence of V_{nk} , we obtain that

$$S(v_{nk}) \rightarrow S^* \text{ as } v_{nk} \rightarrow v^*$$

and with similar results for each state equation, we can show that

$$y^* = y(v^*).$$

Using the lower-semicontinuity of L^2 -norms with respect to weak convergence (see Theorem 4.10.7 in [20]), we obtain that

$$\|v^*\|_{L^2(0,T)} \leq \liminf_{k \rightarrow \infty} \|v_{nk}\|_{L^2(0,T)}. \quad (3.11)$$

Observe that since $J(v_n)$ converges to $\min_{v \in \Omega} J(v)$, thus any subsequence of $J(v_n)$ has to converge to the same limit. Since $v_{nk} \rightharpoonup v^*$ in $L^2(0, T)$ and the state subsequences converge uniformly in $L^2(0, T)$, we have that

$$\int_0^T B_1 u_{1nk} S_{nk} + B_2 u_{2nk} S_{nk} + B_3 \phi_{nk} S_{nk} dt \rightarrow \int_0^T B_1 u_1^* S^* + B_2 u_2^* S^* + B_3 \phi^* S^* dt. \quad (3.12)$$

Considering all the aforementioned results, we have that:

$$\begin{aligned} \min_{v \in \Omega} J_1(v) &= \lim_{n \rightarrow \infty} J_1(v_n) \\ &= \lim_{k \rightarrow \infty} J_1(v_{nk}) \\ &= \liminf_{k \rightarrow \infty} J_1(v_{nk}) \\ &\geq \liminf_{k \rightarrow \infty} \int_0^T (A_1 I_{nk} + B_1 u_{1nk} S_{nk} + B_2 u_{2nk} S_{nk} + B_3 \phi_{nk} S_{nk} dt \\ &\quad + C_1 \liminf_{k \rightarrow \infty} \|u_{1nk}\|_{L^2(0,T)}^2 + C_2 \liminf_{k \rightarrow \infty} \|u_{2nk}\|_{L^2(0,T)}^2 + C_3 \liminf_{k \rightarrow \infty} \|\phi_{nk}\|_{L^2(0,T)}^2) \\ &\geq \int_0^T (A_1 I^* + B_1 u_1^* S^* + B_2 u_2^* S^* + B_3 \phi^* S^* dt \\ &\quad + C_1 \|u_1^*\|_{L^2(0,T)}^2 + C_2 \|u_2^*\|_{L^2(0,T)}^2 + C_3 \|\phi^*\|_{L^2(0,T)}^2) \\ &= J_1(u_1^*, u_2^*, \phi^*) \\ &= J_1(v^*). \end{aligned} \quad (3.13)$$

Therefore, $\min_{v \in \Omega} J_1(v) = J_1(v^*)$ and v^* is an optimal control. $\square$

Remark 3.3.1. Using similar techniques to those used in the proof of Theorem 3.5, one can show the existence of an optimal control triple given the objective functional J_2 .

3.3.2 Optimal Control Characterization

We use Pontryagin's Maximum Principle [42] to derive the necessary conditions that the optimal control triple should satisfy for each minimization problem. Thus, from Pontryagin's Maximum Principle, problem (3.9) turns into minimizing the following two Hamiltonians over the controls at each t ,

$$H_1(t, x, v, \lambda) = A_1 I + B_1 u_1 S + C_1 u_1^2 + B_2 u_2 S + C_2 u_2^2 + B_3 \phi S + C_3 \phi^2 + \lambda_s S' + \lambda_v V' + \lambda_e E' + \lambda_i I' + \lambda_r R' + \lambda_{s_v} S'_v + \lambda_{e_v} E'_v + \lambda_{i_v} I'_v \quad (3.14)$$

$$H_2(t, x, v, \lambda) = A_2 \left(\beta S(t) \frac{I_v(t)}{N_v(t)} (1 - u_2(t)) + \alpha S(t) \frac{I(t)}{N(t)} (1 - u_1(t)) \right) + B_1 u_1 S + C_1 u_1^2 + B_2 u_2 S + C_2 u_2^2 + B_3 \phi S + C_3 \phi^2 + \lambda_s S' + \lambda_v V' + \lambda_e E' + \lambda_i I' + \lambda_r R' + \lambda_{s_v} S'_v + \lambda_{e_v} E'_v + \lambda_{i_v} I'_v \quad (3.15)$$

where $x = (S, V, E, I, R, S_v, E_v, I_v)$ is the vector of state variables, $v = (u_1, u_2, \phi)$ is the control triple, and $\lambda = (\lambda_s, \lambda_v, \lambda_i, \lambda_e, \lambda_r, \lambda_{s_v}, \lambda_{e_v}, \lambda_{i_v})$ represents the vector of adjoint variables. The values of λ 's are the associated adjoints for the state variables. The following two Theorems, 3.6 and 3.7, give the existence of continuous adjoint functions λ_i , and the characterization of the optimal control triple for each optimization problem.

Theorem 3.6. Given an optimal triple $v^*(t) = (u_1^*, u_2^*, \phi^*) \in \Omega$ with its respective states $x^* = (S^*, V^*, E^*, I^*, R^*, S_v^*, E_v^*, I_v^*)$, then there exist adjoint functions satisfying

$$\begin{aligned} \lambda'_s &= - \left(\beta \frac{I_v^*}{N_v} (1 - u_2^*) + \alpha \frac{I^*}{N} (1 - u_1^*) \right) \lambda_e + \left(\beta \frac{I_v^*}{N_v} (1 - u_2^*) + \alpha \frac{I^*}{N} (1 - u_1^*) + \phi^* f + \mu \right) \lambda_s \\ &\quad - \phi^* f \lambda_v - B_1 u_1^* - B_2 u_2^* - B_3 \phi^* \\ \lambda'_v &= -\omega \lambda_s + (\mu + \omega) \lambda_v \\ \lambda'_e &= (\kappa + \mu) \lambda_e - \kappa \lambda_i \\ \lambda'_i &= -\alpha \frac{S^*}{N} (1 - u_1^*) \lambda_e + (\mu + \gamma) \lambda_i - \gamma \lambda_r + \alpha \frac{S^*}{N} (1 - u_1^*) \lambda_s - \beta_v \frac{S_v^*}{N} \lambda_{e_v} \end{aligned}$$

$$\begin{aligned}
& + \beta_v \frac{S_v^*}{N} \lambda_{s_v} - A_1, \\
\lambda_r' & = \mu \lambda_r, \\
\lambda_{s_v}' & = -\beta_v \frac{I^*}{N} \lambda_{e_v} + \left(\beta_v \frac{I^*}{N} + \mu_v \right) \lambda_{s_v} \\
\lambda_{e_v}' & = (\mu_v + \eta) \lambda_{e_v} - \eta \lambda_{i_v} \\
\lambda_{i_v}' & = -\beta \frac{S^*}{N_v} (1 - u_2^*) \lambda_e + \beta \frac{S^*}{N_v} (1 - u_2^*) \lambda_s + \mu_v \lambda_{i_v},
\end{aligned}$$

with transversality conditions

$$\lambda_s(T) = \lambda_i(T) = \lambda_v(T) = \lambda_r(T) = \lambda_e(T) = \lambda_{s_v}(T) = \lambda_{e_v}(T) = \lambda_{i_v}(T) = 0.$$

Moreover, we obtain these optimal control characterizations

$$\begin{aligned}
u_1^* & = \min \left[b_1, \max \left[0, \frac{S^* (I^* \alpha (\lambda_e - \lambda_s) - B_1 N)}{2NC_1} \right] \right], \\
u_2^* & = \min \left[b_2, \max \left[0, \frac{S^* \beta I_v^* (\lambda_e - \lambda_s) - B_2 S^* N_v}{2N_v C_2} \right] \right], \\
\phi^* & = \min \left[b_3, \max \left[0, \frac{S^* (f(\lambda_s - \lambda_v) - B_3)}{2C_3} \right] \right].
\end{aligned}$$

Proof. The differential equations for the adjoint system follow from Pontryagin's Maximum Principle [42]. After differentiating the Hamiltonian (3.14) with respect to each state variable, we find the differential equations for the associated adjoint:

$$\begin{aligned}
\lambda_s' & = -\frac{\partial H_1}{\partial S}, & \lambda_r' & = -\frac{\partial H_1}{\partial R}, \\
\lambda_v' & = -\frac{\partial H_1}{\partial V}, & \lambda_{s_v}' & = -\frac{\partial H_1}{\partial S_v}, \\
\lambda_e' & = -\frac{\partial H_1}{\partial E}, & \lambda_{e_v}' & = -\frac{\partial H_1}{\partial E_v}, \\
\lambda_i' & = -\frac{\partial H_1}{\partial I}, & \lambda_{i_v}' & = -\frac{\partial H_1}{\partial I_v}.
\end{aligned}$$

The final conditions are set to zero due to the transversality conditions. Since the Hamiltonian attains its minimum value at the optimal control v^* , we differentiate H_1 with

respect to each control on the interior of the control set, and obtain

$$\begin{aligned}\frac{\partial H_1}{\partial u_1} &= -\frac{S\alpha I \lambda_e}{N} + \frac{S\alpha I \lambda_s}{N} + B_1 S + 2C_1 u_1 = 0, \\ \frac{\partial H_1}{\partial u_2} &= -\frac{S\beta I_v \lambda_e}{N_v} + \frac{S\beta I_v \lambda_s}{N_v} + B_2 S + 2C_2 u_2 = 0, \\ \frac{\partial H_1}{\partial \phi} &= -Sf\lambda_s + Sf\lambda_v + B_3 S + 2C_3 \phi = 0.\end{aligned}$$

On the interior of the control set, we deduce our optimal triple (u_1^*, u_2^*, ϕ^*) to be

$$\begin{aligned}u_1 &= \frac{S(I\alpha(\lambda_e - \lambda_s) - B_1 N)}{2NC_1}, \\ u_2 &= \frac{S\beta I_v(\lambda_e - \lambda_s) - B_2 S N_v}{2N_v C_2}, \\ \phi &= \frac{S(f(\lambda_s - \lambda_v) - B_3)}{2C_3},\end{aligned}$$

and taking into account the bounds, we conclude:

$$\begin{aligned}u_1^* &= \min \left[b_1, \max \left[0, \frac{S^*(I^*\alpha(\lambda_e - \lambda_s) - B_1 N)}{2NC_1} \right] \right], \\ u_2^* &= \min \left[b_2, \max \left[0, \frac{S^*\beta I_v^*(\lambda_e - \lambda_s) - B_2 S^* N_v}{2N_v C_2} \right] \right], \\ \phi^* &= \min \left[b_3, \max \left[0, \frac{S^*(f(\lambda_s - \lambda_v) - B_3)}{2C_3} \right] \right].\end{aligned}$$

□

In the next theorem, the existence of adjoint functions and optimal control characterization associated to objective functional J_2 follow similarly as in Theorem 3.6.

Theorem 3.7. *Given an optimal triple $v^*(t) = (u_1^*, u_2^*, \phi^*) \in \Omega$ with its respective states $x^* = (S^*, V^*, E^*, I^*, R^*, S_v^*, E_v^*, I_v^*)$, then there exist adjoint functions satisfying*

$$\begin{aligned}\lambda'_s &= -\left(\beta \frac{I_v^*}{N_v} (1 - u_2^*) + \alpha \frac{I^*}{N} (1 - u_1^*)\right) \lambda_e + \left(\beta \frac{I_v^*}{N_v} (1 - u_2^*) + \alpha \frac{I^*}{N} (1 - u_1^*) + \phi^* f + \mu\right) \lambda_s \\ &\quad - \phi^* f \lambda_v - A_2 \left(\beta \frac{I_v^*}{N_v} (1 - u_2^*) + \alpha \frac{I^*}{N} (1 - u_1^*)\right) - B_1 u_1^* - B_2 u_2^* - B_3 \phi \\ \lambda'_v &= -\omega \lambda_s + (\mu + \omega) \lambda_v\end{aligned}$$

$$\lambda'_e = (\kappa + \mu) \lambda_e - \kappa \lambda_i$$

$$\begin{aligned} \lambda'_i = & -\alpha \frac{S^*}{N} (1 - u_1^*) \lambda_e + (\mu + \gamma) \lambda_i - \gamma \lambda_r + \alpha \frac{S^*}{N} (1 - u_1^*) \lambda_s - \beta_v \frac{S_v^*}{N} \lambda_{e_v} \\ & + \beta_v \frac{S_v^*}{N} \lambda_{s_v} - A_2 \left(\alpha \frac{S^*}{N} (1 - u_1^*) \right), \end{aligned}$$

$$\lambda'_r = \mu \lambda_r,$$

$$\lambda'_{s_v} = -\beta_v \frac{I^*}{N} \lambda_{e_v} + \left(\beta_v \frac{I^*}{N} + \mu_v \right) \lambda_{s_v}$$

$$\lambda'_{e_v} = (\mu_v + \eta) \lambda_{e_v} - \eta \lambda_{i_v}$$

$$\lambda'_{i_v} = -\beta \frac{S^*}{N_v} (1 - u_2^*) \lambda_e + \beta \frac{S}{N_v} (1 - u_2^*) \lambda_s + \mu_v \lambda_{i_v} - A_2 \left(\beta \frac{S^*}{N_v} (1 - u_2^*) \right),$$

with transversality conditions

$$\lambda_s(T) = \lambda_i(T) = \lambda_v(T) = \lambda_r(T) = \lambda_e(T) = \lambda_{s_v}(T) = \lambda_{e_v}(T) = \lambda_{i_v}(T) = 0.$$

Moreover, we obtain the following optimal control characterizations

$$\begin{aligned} u_1^* &= \min \left[b_1, \max \left[0, \frac{S^* (I^* \alpha (A_2 + \lambda_e - \lambda_s) - B_1 N)}{2NC_1} \right] \right], \\ u_2^* &= \min \left[b_2, \max \left[0, \frac{S^* \beta I_v^* (A_2 + \lambda_e - \lambda_s) - B_2 S^* N_v}{2N_v C_2} \right] \right], \\ \phi^* &= \min \left[b_3, \max \left[0, \frac{S^* (f(\lambda_s - \lambda_v) - B_3)}{2C_3} \right] \right]. \end{aligned}$$

In the next section we explain two data sets of ZIKV epidemics to estimate parameters of the model such that numerical simulations are more realistic.

3.4 Data Collection from 2015-2016 ZIKV Epidemic in Colombia and 2016 ZIKV Outbreak in Puerto Rico

Now we present the data collected from corresponding ZIKV epidemics in Colombia and Puerto Rico. Later, in Sections 3.5, 3.6 and 3.7, we use these data to estimate some of the

parameters in our model as well as to perform numerical simulations of our optimal control problem applied to each country.

Data from Colombia were collected from the National Institute of Health of Colombia or Instituto Nacional de Salud (INS), its official name in Spanish. The INS is the health agency in charge of the health surveillance system of Colombia that reports and publishes results for the nation each week. The INS began to monitor ZIKV disease in August 2015 after outbreaks of the virus were detected earlier in Brazil. In October 2015, ZIKV disease was declared an outbreak until July 2016 when Colombia announced an end to the ZIKV epidemic [40]. We obtained weekly data of confirmed and suspicious cases from week 42 of 2015 to week 52 of 2019. However, we only use data from week 42 of 2015 until week 52 of 2016 since the incidence of ZIKV dropped drastically between 2017 and 2019 with less than 1000 confirmed cases per year. Table 3.5 shows the incidence data that later are used to estimate some key parameters of the model corresponding to Colombia.

We collected available data for the 2016 ZIKV outbreak in Puerto Rico from the Department of Health of Puerto Rico (PRDH). One of the many functions of PRDH is to gather weekly data provided by all health care providers on the island of arboviral diseases such as dengue, chikungunya and zika. We collected data from 2016 to 2017 of cumulative cases, but later we only considered the 52 weeks of 2016 due to very low numbers of weekly ZIKV infections reported in 2017. Table 3.6 shows the incidence number of confirmed ZIKV cases for each epidemiological week of 2016.

3.5 Parameter Estimation Scheme

To make qualitative and quantitative predictions of the vaccination model applied to ZIKV epidemics in Colombia and Puerto Rico, it is necessary to estimate some of the epidemiological parameters described in the model. In this section we explain the strategy to estimate these parameters using the data collected from Colombia and Puerto Rico. In absence of controls, the incidence or number of new infected cases of our ZIKV vaccination

Table 3.5: Incidence Data from 2015-2016 ZIKV Epidemic in Colombia.

2015

Week		42	43	44	45	46	47	48
Cases		389	438	414	836	1136	1065	1400
Week	49	50	51	52				
Cases	1838	1476	876	158				

2016

Week	1	2	3	4	5	6	7	8
Cases	3505	2888	3878	5348	5910	5456	5695	5083
Week	9	10	11	12	13	14	15	16
Cases	3684	4251	3114	2555	3446	3791	3322	3235
Week	17	18	19	20	21	22	23	24
Cases	2898	2708	3096	3466	1590	2211	2086	1704
Week	25	26	27	28	29	30	31	32
Cases	1548	1134	1160	933	745	679	523	439
Week	33	34	35	36	37	38	39	40
Cases	234	313	284	612	405	283	227	154
Week	41	42	43	44	45	46	47	48
Cases	105	31	330	162	125	146	37	309
Week	49	50	51	52				
Cases	98	596	4	97				

Table 3.6: Incidence Data from 2016 ZIKV Puerto Rico Outbreak.

2016

Week	1	2	3	4	5	6	7	8
Cases	4	9	12	21	54	97	139	179
Week	9	10	11	12	13	14	15	16
Cases	215	287	274	315	414	484	478	551
Week	17	18	19	20	21	22	23	24
Cases	717	882	850	967	1160	1330	1522	1562
Week	25	26	27	28	29	30	31	32
Cases	2056	3063	3644	4936	6030	7274	7822	9295
Week	33	34	35	36	37	38	39	40
Cases	10389	11828	12710	14539	15004	16762	18027	18938
Week	41	42	43	44	45	46	47	48
Cases	19176	20756	21402	21643	21397	22420	22711	22819
Week	49	50	51	52				
Cases	22334	23203	23222	23753				

2017

Week	1	2	3	4	5	6	7	8
Cases	1113	289	408	164	272	207	399	190
Week	9	10	11	12	13	14	15	16
Cases	30	77	179	24	145	83	67	5
Week	17	18	19	20	21	22	23	24
Cases	1	134	27	29	68	0	0	8
Week	25	26	27	28	29	30	31	32
Cases	18	9	29	6	33	85	24	1
Week	33	34	35	36	37	38	39	40
Cases	6	6	6	0	0	0	0	0
Week	41	42	43	44	45	46	47	48
Cases	0	0	2	9	0	28	9	20
Week	49	50	51	52				
Cases	0	0	0	0				

model in (t_i, t_{i+1}) is given by

$$\mathcal{Y}_{i+1} = \int_{t_i}^{t_{i+1}} \left(\beta S(t) \frac{I_v(t)}{N_v} + \alpha S(t) \frac{I(t)}{N} \right) dt \quad (3.16)$$

where (t_i, t_{i+1}) represents the time interval between weeks t_i and t_{i+1} and the integrand represents the rate at which susceptible individuals become infected either by the bite of an infected mosquito or sexual contact with an infected human. We let $\bar{\mathcal{Y}}_{i+1}$ be the incidence from the data between weeks t_i and t_{i+1} . We define the normalized $\ell^2(0, T)$ error between the incidences of the model and the data as

$$\mathcal{E} = \sqrt{\frac{\sum_i (\bar{\mathcal{Y}}_{i+1} - \mathcal{Y}_{i+1})^2}{\sum_i (\bar{\mathcal{Y}}_{i+1})^2}}. \quad (3.17)$$

We want to minimize the square error $\mathcal{E}$ to obtain parameters for the model that best fit the data. Since we have two different sets of data, one from Colombia and one from Puerto Rico, two minimization problems are considered, that is, one minimization problem for each data set. The goal of the minimization problem is to estimate the parameters β , β_v , α , κ , η and r (where r is the reporting rate) that can minimize $\mathcal{E}$ subject to the ZIKV vaccination model in absence of control strategies [34, 44]. We chose lower bounds for the parameters near zero while upper bounds are adjusted based on other estimates for the same parameters [21, 44]. Initial guesses on the parameters were randomly chosen to find an absolute minimum instead of a local minimum. The estimation of parameters was performed in MATLAB using the MultiStart algorithm with the fmincon function adjusted to our problem. The multistart algorithm starts the solver from different initial points to find many local solutions and the fmincon function is a gradient-based method where the objective and constraint functions are both C^1 functions. Table 3.7 displays parameter bounds based on assumptions and statistical data from different ZIKV models [49, 27, 54, 21, 53].

There have been studies [27, 2, 8, 25] showing that ZIKV disease is highly underreported since infected individuals are mostly asymptomatic or have mild symptoms. For example, it was estimated that only 10.4% of the total infections for 2015 - 2016 ZIKV epidemic in Rio

Table 3.7: Parameter ranges for ZIKV model.

Parameter	Baseline Value	Reference
μ	$[\frac{1}{(52*81)}, \frac{1}{(52*77)}]$ week ⁻¹	[53]
β	$[0.7, 15]$ week ⁻¹	[21]
α	$[0.007, 2]$ week ⁻¹	[49]
κ	$[1, \frac{7}{2}]$ week ⁻¹	[21]
f	$[0, 1]$ dimensionless	assumed
ω	$[0, 0.1]$ week ⁻¹	assumed
γ	$[1, \frac{7}{3}]$ week ⁻¹	[27]
μ_v	$[\frac{7}{21}, \frac{7}{10}]$ week ⁻¹	[54]
β_v	$[0.7, 14]$ week ⁻¹	[21]
η	$[\frac{7}{13}, \frac{7}{8}]$ week ⁻¹	[27]
r	$[0.01, 0.5]$	[8, 25]

de Janeiro were reported [2]. Thus, dividing the data by the reporting rate we obtain the data to be estimated accounting for both confirmed and underreported cases:

$$(\text{Reporting Rate}) \times (\text{Total Number of cases}) = \text{Total Number of Reported cases}.$$

We estimate the reporting rate for each data set since neither Colombia or Puerto Rico health systems indicated an underreporting rate.

For both countries we assumed that the average human lifespan ($1/\mu$) is 80 years, average mosquito lifespan ($1/\mu_v$) is 3 weeks and humans recover from ZIKV ($1/\gamma$) after 5 days [53, 27].

3.5.1 Parameter Estimation for 2015-2016 ZIKV Epidemic in Colombia

The altitude across Colombia's cities varies from 0 to 18,045 feet above the sea level. The mosquito that transmits the disease is very unlikely to be found in places above 6,500 feet above sea level [11, 25]. In Table 3.8 we illustrate the elevation and population of some cities in Colombia where *Aedes aegypti* mosquitoes are unlikely to survive. We estimate that nearly 12 million individuals were living in areas above 6,500 ft. These individuals were not affected with ZIKV unless they traveled to regions with lower elevation. The average population of Colombia in 2016 was estimated to be near 47 million from which we believe that less than 35 million were actually at risk of ZIKV. For instance, Hernández-Ávila et al. [25] calculate the magnitude of the Mexican ZIKV epidemic in 2015-16 by stratifying data corresponding to birth certificates according to places with altitudes of 2,200 meters (7,217 feet) below and above sea level. They compared the results with the mean monthly incidence of congenital microcephaly before the introduction of the virus to determine the actual size of their epidemic.

In Figure 3.2 we illustrate the best numerical fit that we obtained (red curve) to the data (blue circles) from Colombia with incidence error of $\mathcal{E} = 0.279$. The estimated parameters are given by

$$(\beta, \beta_v, \alpha, \kappa, \eta, r) = (0.707, 1.513, 0.874, 3.395, 0.546, 0.015).$$

Table 3.8: Cities in Colombia by population and elevation in 2015-16 based on their National Administrative Department of Statistics (DANE in Spanish).

City	Elevation (feet)	Population
Vetas	10,991	2,114
IpiALES	9,508	123,341
Tunja	9,259	172,548
Zipaquirá	8,694	130,432
Bogotá	8,661	7,181,000
Soacha	8,576	522,442
Duitama	8,497	126,670
Facatativá	8,484	141,762
Sogamoso	8,428	111,336
Chiquinquirá	8,386	72,274
Pasto	8,291	392,930
Manizales	7,087	434,403
Rionegro	6,972	128,153
Total		9,539,405

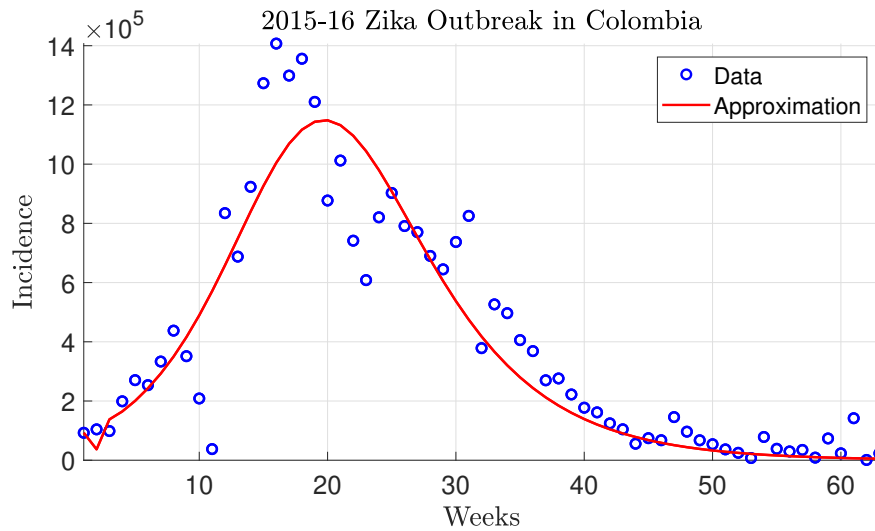


Figure 3.2: Colombian data with 1.5% reporting rate and simulation results from best numerical approximation. Incidence error of $\mathcal{E} = 0.279$. The parameters with the best fit are given by $(\beta, \beta_v, \alpha, \kappa, \eta) = (0.707, 1.513, 0.874, 3.395, 0.546)$. The basic reproductive number was $\mathcal{R}_0 = 1.727$. Initial population of Colombia was assumed to be $S_0 = 35,000,000$. Week zero corresponds to week 42 in 2015.

Later in Section 3.6 we will use these parameter values to explore different numerical scenarios.

3.5.2 Parameter Estimation for 2016-17 Puerto Rico Outbreak

We estimate the parameters β , β_v , α , κ , η and r without optimal controls such that the error in equation (3.17) is minimized using the data from Puerto Rico (see Table 3.6). In Figure 3.3 we depict the best numerical approximation of daily new infections in Puerto Rico with an incidence error of $\mathcal{E} = 0.359$. The parameters obtained by the estimation are given by

$$(\beta, \beta_v, \alpha, \kappa, \eta, r) = (0.701, 2.823, 0.007, 1, 0.634, 0.02)$$

The next sections we explore numerical simulations for each country regarding the mitigation effects that different scenarios can produce.

3.6 Numerical Simulations: Colombia

In this section and the next one, we numerically show the results of a single and multiple optimal control strategies (see Table 3.3) in controlling ZIKV spread for Colombia and Puerto Rico. Such scenarios can be seen as modifications from the overall objective functionals (see equations (3.7) and (3.8)) with the solution of state and associate adjoint equations, respectively. In order to solve the state equations (3.1) we implement a Forward Sweep method with its respective initial conditions for the state equations. The adjoint equations (in Theorems 3.6 and 3.7) are solved implementing a Backward Sweep routine with its respective transversality conditions. The optimal controls are updated by using the solutions of the state and adjoint system in their corresponding characterization and doing a convex combination between old and new controls. For a better understanding of Forward-Backward Sweep algorithm see Chapter 4 of [28]. In addition, we compute the objective functionals for each strategy where we specify the cost of the prevention ($\hat{J}_2$) and epidemiological integrals ($\hat{J}_1$ and $\hat{J}_3$) to indicate the strategy that does better in minimizing the objective functional.

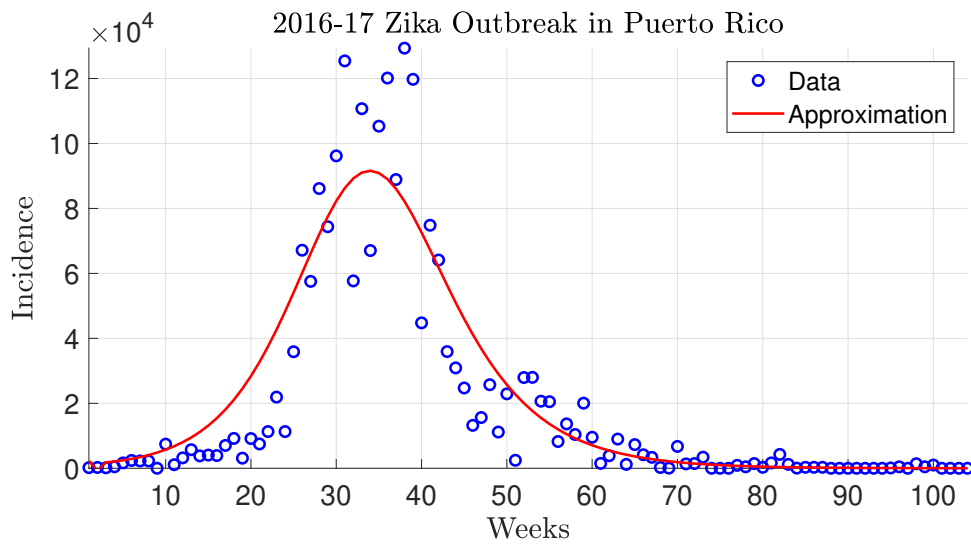


Figure 3.3: Puerto Rico data with 2% reporting rate and simulation results from best numerical approximation. Incidence error of $\mathcal{E} = 0.359$. The parameters with the best fit are given by $(\beta, \beta_v, \alpha, \kappa, \eta) = (0.701, 2.823, 0.007, 1, 0.634)$. The basic reproductive number in absence of control was $\mathcal{R}_0 = 2.227$. Initial susceptible population of Puerto Rico to ZIKV disease was $S_0 = 2,800,000$. Week zero corresponds to week 1 in 2016.

Total number of ZIKV cases and total number of vaccinated individuals (if applicable) are also given for each control strategy.

In this section, we provide an assessment of the impact of implementing different measures, as described in Section 3.3, on controlling a possible ZIKV epidemic in Colombia. The baseline parameter values and initial conditions used for the simulations are displayed in Tables 3.9 and 3.10. These values were selected according to the parameter estimation in Section 3.5. The initial infected population is equal to the number of people infected at week 42 (389) scaled by the reporting rate ($r = 0.015$). The initial number of exposed individuals was approximately a third of the initial number of infected people. The initial number of infected mosquitoes is nearly twice the number of infected individuals at time zero, and the initial number of mosquitoes exposed was almost a third of the initial number of infected mosquitoes.

Without any controls, Figure 3.4 illustrates the dynamics of the populations for all human and mosquito compartments. Both of them also emphasize the burden corresponding to the exposed and infected human classes. Note that vaccinated individuals are not considered at this point. For all the numerical scenarios the final time corresponds to 63 weeks. This time period represents when Colombia reported to be during the ZIKV epidemic. The value of the upper bounds for u_1 and u_2 are assumed 0.2. This assumption simply means that at most 20% of the total population could be informed about the controls and perform corresponding control actions. The upper bound for the vaccination is selected to be 0.01 without waning immunity ($\omega = 0$). Thus, if a vaccine is fully effective ($f = 1$), at most 1% of the population can be vaccinated weekly. The value for the weight parameters are given at the beginning of each numerical scenario.

The basic reproduction number for the ZIKV model in absence of controls for Colombia is 1.728 as found in Table 3.11. Moreover, we also show the contribution to $\mathcal{R}_0$ from the direct and vector transmission thresholds. In this case, we can observe that the contribution from mosquito transmission is higher than from sexual contact.

In the subsequent parts we analyze the impact of different control scenarios with and without vaccination.

Table 3.9: Initial condition values for ZIKV outbreak in Colombia to create Figures 3.4, 3.5, 3.6 and 3.7.

$S(0)$	$V(0)$	$E(0)$	$I(0)$	$R(0)$	$S_v(0)$	$E_v(0)$	$I_v(0)$
35 M	0	30,874	92,620	0	90 M	62,100	185,715

Table 3.10: Parameter values for ZIKV outbreak in Colombia to create Figures 3.4, 3.5, 3.6 and 3.7.

μ	β	α	κ	γ	μ_v	β_v	η	ω	f
$\frac{1}{52 \times 80}$	0.7073	0.8745	3.3951	1.40	0.4	1.5138	0.5463	0	0.9

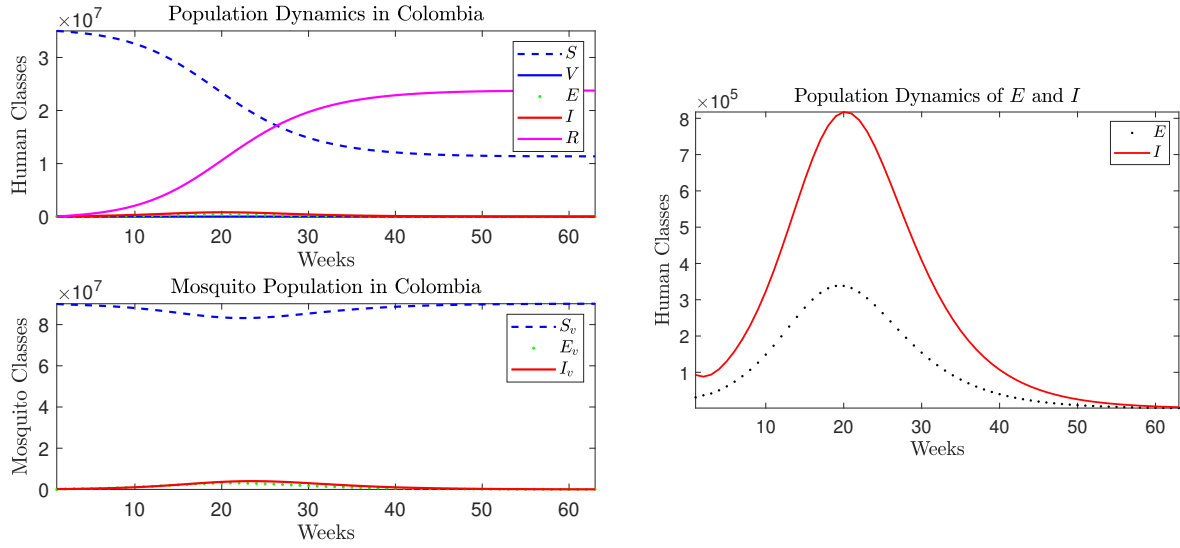


Figure 3.4: **Left:** Human-Mosquito population dynamics for 2015-16 ZIKV epidemic in Colombia in absence of control strategies. **Right:** Only E and I populations at a lower population scale.

Table 3.11: Basic Reproductive Number of Colombia using estimated parameters.

	$\mathcal{R}_v$	$\mathcal{R}_d$	$\mathcal{R}_0$
Colombia	1.103	0.624	1.727

3.6.1 Implementation of Personal Protection Controls without Vaccination

The impact of optimally informing the population about the use of condoms (scenario 1), insect repellent (scenario 2) and both condom and insect repellent at the same time (scenario 3) for the dynamics of the ZIKV spread in absence of vaccination are evaluated in Figure 3.5. The value of upper bounds on the controls (b_i 's) as well as the weight parameters for Figure 3.5 are in Table 3.12.

The controls u_1 and u_2 model the importance of personal protection efforts against ZIKV to avoid being infected by sexual contact and mosquito bites, respectively. The two graphs at the left side on Figure 3.5a display the two optimal control functions analyzed for scenarios 1 and 2, while the results of implementing two controls simultaneously (scenario 3) are displayed in the two graphs at the right of Figure 3.5a. The graphs on Figure 3.5b measure the impact of each strategy against the scenario in absence of controls. Further, each graph represents the number of weekly new cases of humans with ZIKV under scenarios 1, 2, 3, and no controls. The dynamic of new infected humans under no interventions (no condoms, repellents and vaccination) are compared with those where optimal control strategies are implemented.

Tables 3.13 and 3.14 show the costs associated to the prevention measures and epidemiological strategies for objective functionals J_1 and J_2 . Further, both tables provide the total number of ZIKV cases at the final time in presence of each strategy. In this situation, the best strategy to decrease the total number of infections is to inform the public about condoms and insect repellents.

In the next section we explore strategies 4, 5 and 6 where an effective vaccine is available to protect the population against ZIKV.

3.6.2 Personal Protection Controls along with an Effective Vaccine

In the scenarios 4, 5 and 6, we evaluate the use of personal protection efforts when an available vaccine is ready to be rolled out. The value corresponding to control upper bounds

Table 3.12: Values for upper bounds on the controls and weight parameters for Figure 3.5.

A_1	A_2	B_1	B_2	B_3	C_1	C_2	C_3	b_1	b_2	b_3
10	10	0.01	0.01	0	3	5	0	0.2	0.2	0

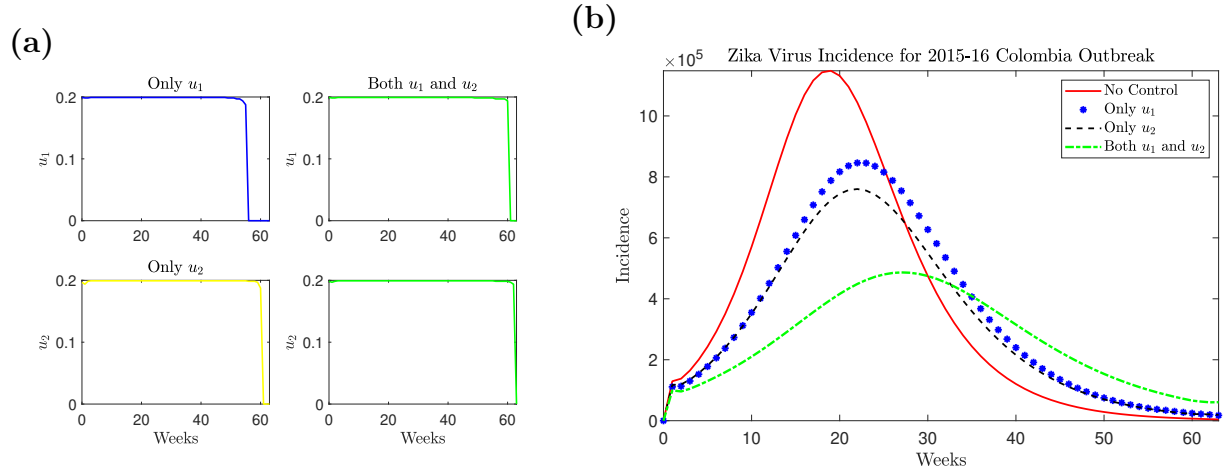


Figure 3.5: a) The two figures on the left display the optimal control functions for scenarios 1 and 2. The two figures on the right represent optimal control functions implemented for scenario 3. b) Incidence corresponding to scenarios 0, 1, 2 and 3. Graphs correspond to solutions of the optimization problem with objective functional J_2 .

Table 3.13: Cost in millions and total number of cases in millions corresponding to scenarios 0, 1, 2 and 3 using objective functional J_1 with $\hat{J}_1$ representing the cost associated to infected humans and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario	$\hat{J}_1$	$\hat{J}_2$	$J_1 = \hat{J}_1 + \hat{J}_2$	Total Cases
No Control	171.3	0	171.3	23.8
Only u_1	156.6	2.5	159.1	21.8
Only u_2	143.6	2.6	146.3	20.1
Both u_1 and u_2	119.8	6.2	126	16.7

Table 3.14: Cost in millions and total number of cases in millions corresponding to scenarios 0, 1, 2 and 3 using objective functional J_2 where $\hat{J}_1$ representing the cost associated to new cases and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario	$\hat{J}_3$	$\hat{J}_2$	$J_2 = \hat{J}_3 + \hat{J}_2$	Total Cases
No Control	238.7	0	238.7	23.8
Only u_1	218.1	2.5	220.6	21.8
Only u_2	200.2	2.7	202.9	20.1
Both u_1 and u_2	166.8	6.3	173.1	16.6

and weight parameters are given in Table 3.15. The cost associated with vaccination ($C_3 = 1$) was chosen to be smaller than the cost related to the other two controls.

Figure 3.6a depicts the dynamics of optimal control strategies when one and both personal protection efforts are combined with vaccination. Moreover, Figure 3.6b illustrates the number of weekly new cases corresponding to each strategy. It can be seen that any of the control measures does enormously better in reducing the peak of the incidence than no control. In Tables 3.16 and 3.17 we report the cost of implementing objective functionals J_1 and J_2 with their corresponding contributions to the prevention and epidemiological integrals. We also report the total number of vaccinated and infected cases at the end of the epidemic for each of the scenarios. As expected, the best scenario in mitigating the impact of a ZIKV epidemic is to implement all three controls simultaneously. The reduction in the total number of cases is notably from around 23 million to 6 million people. The second best scenario is simply to promote the use of mosquito repellent along with vaccination. Second best scenario can produce nearly 10 million total cases by the end of week 63 which it is still considerably better if compared with 23 million individuals infected when no measures are taken. Observe that for the best plan, it was enough to vaccinate nearly 10% of the total population at risk to achieve a significant decrease in total number of cases. Moreover, vaccination was not needed until the final time as seen in Figure 3.6a, but it stopped around 10 weeks earlier.

In our next section we study the scenario of implementing the best mitigation plan starting at different times once a ZIKV epidemic has been declared.

3.6.3 Personal Protection and Effective Vaccine at Different Times

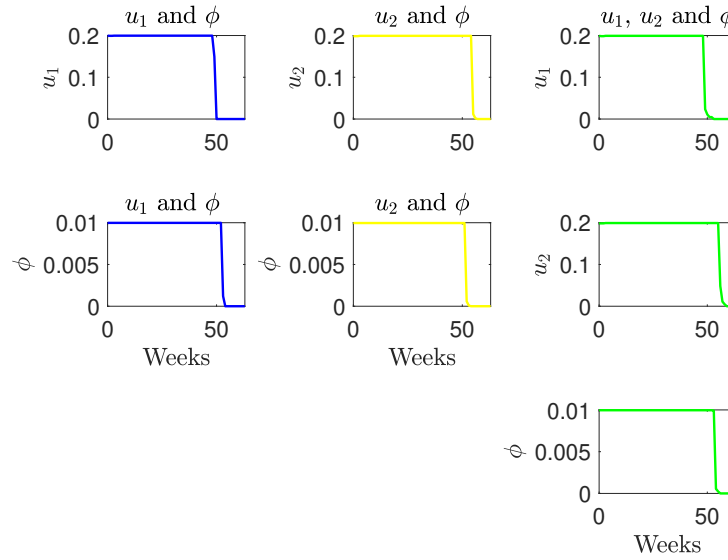
In this section we explore the benefits of incorporating the best control strategy even at a later time after a ZIKV emergency has been declared. The best control strategy in order to mitigate the ZIKV disease in Colombia is to vaccinate susceptible individuals and inform them of personal protections measures such as condoms and insect repellent. This best strategy was chosen based on our results in Section 3.5.

In Figure 3.7a we show the evolution of each control starting at the beginning of the epidemic, week 10 and week 20. In the case all three controls are available by week 10, they

Table 3.15: Value for upper bounds on the controls and weight parameters for Figures 3.6 and 3.7.

A_1	A_2	B_1	B_2	B_3	C_1	C_2	C_3	b_1	b_2	b_3
10	10	0.01	0.01	0.1	3	5	1	0.2	0.2	0.01

(a)



(b)

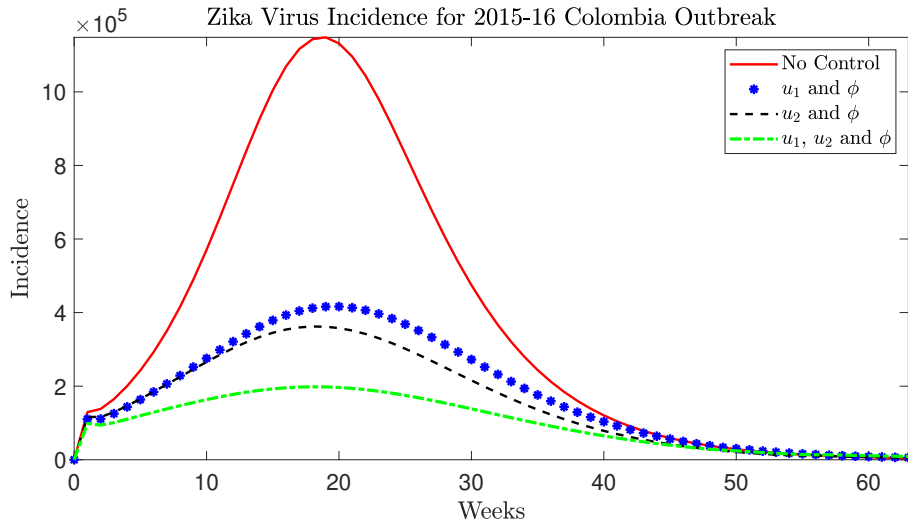


Figure 3.6: a) The two figures to the left and middle display the optimal control functions for scenarios 4 and 5. The three figures on the right correspond to optimal control functions implemented for scenario 6. b) Number of weekly new cases in absence of controls and for scenarios 4, 5 and 6. Graphs correspond to solutions of the optimization problem with objective functional J_2 .

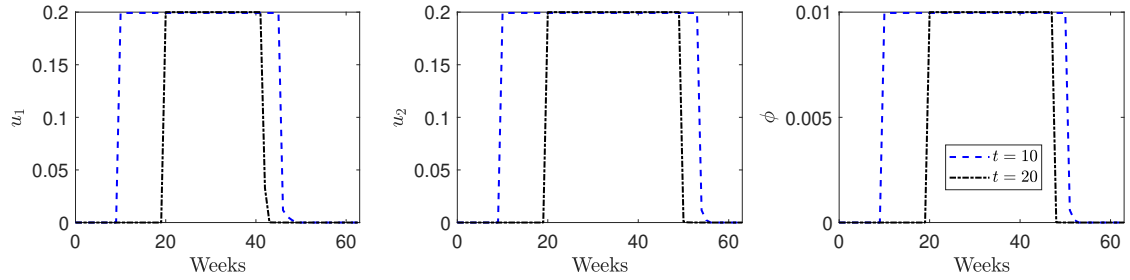
Table 3.16: Costs in millions, total number of vaccinated individuals and total number of cases in millions corresponding to scenarios 4, 5 and 6 using objective functional J_1 with $\hat{J}_1$ representing the cost associated to infected humans and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario	$\hat{J}_1$	$\hat{J}_2$	$J_1 = \hat{J}_1 + \hat{J}_2$	Total Vacc.	Total Cases
No Control	171.3	0	171.3	0	23.8
u_1 and ϕ	85.3	3.2	88.5	3.4	11.8
u_2 and ϕ	74.3	3.4	77.7	3.3	10.2
u_1, u_2 and ϕ	48.3	6.2	54.5	3.6	6.6

Table 3.17: Costs in millions, total number of vaccinated individuals and total number of cases in millions corresponding to scenarios 4, 5 and 6 using objective functional J_2 with $\hat{J}_3$ representing the cost associated to new cases and $\hat{J}_2$ and the cost associated with the prevention measures.

Scenario	$\hat{J}_3$	$\hat{J}_2$	$J_2 = \hat{J}_3 + \hat{J}_2$	Total Vacc.	Total Cases
No Control	238.7	0	238.7	0	23.8
u_1 and ϕ	118.2	3.3	121.5	3.6	11.8
u_2 and ϕ	101.7	3.5	105.3	3.4	10.1
u_1, u_2 and ϕ	66.3	6.3	72.6	3.9	6.6

(a)



(b)

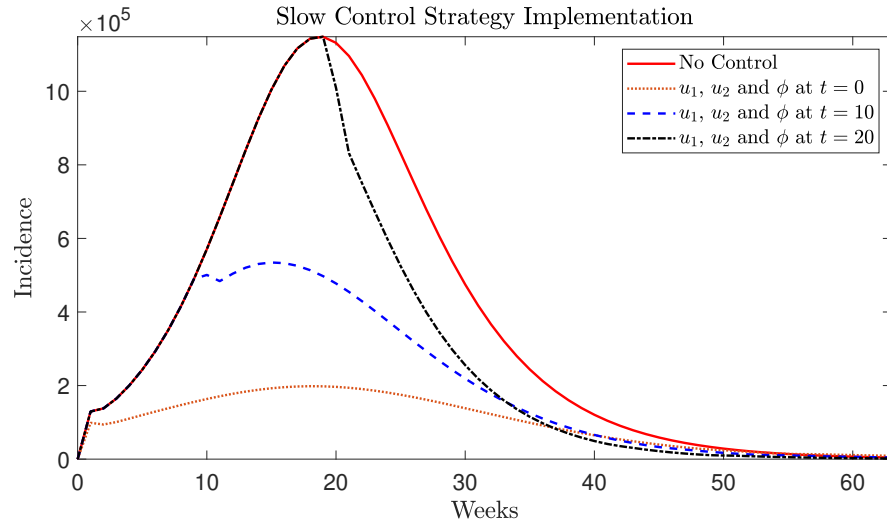


Figure 3.7: **a)** Graphs corresponding to each control starting at week 10 and 20. **b)** Number of weekly new cases in absence of controls and for scenario 6 starting at week 0, 10 and 20. Number of new cases correspond to outbreak in Colombia. Graphs correspond to solutions of the optimization problem with objective functional J_1 .

all should start at the highest level, but condom, insect repellent and vaccination information campaigns should no longer be needed by weeks 40, 50 and 48 respectively. Moreover, in Figure 3.7b the dynamics of weekly incidence for each strategy is illustrated and compared when no control is applied. From the graphs, it can be observed that as soon as the controls are put in place the weekly incidence start to shrink when compared to no control actions. In Table 3.18 we only provide the cost of the objective functional J_1 as well as the total number of vaccinated individuals and new cases by the end of week 63. By inspecting the total number of cases one can see that quicker control actions are able to produce more mitigation effects. Nonetheless, public health agencies should always consider to apply a later control strategy rather than taking no steps against the disease.

A significant reduction in the number of weekly new cases will be seen as long as the prevention measures are put in place before the peak of new cases. However, we omitted simulations after the peak of new cases since the implementation of controls show no significant reductions. One reason for this effect may be that most of the population has been infected and received natural immunity against the disease. Thus, when a control strategy is implemented after the peak of the epidemic there will be fewer susceptible individuals to reach which makes the control action to last less or even to go unseen if it is applied too late.

3.7 Numerical Simulations: Puerto Rico

In this section, we provide an assessment of the impact of implementing different scenarios to mitigate the impact of a possible ZIKV epidemic in Puerto Rico. The parameter values and initial conditions used for the simulations are displayed in Tables 3.19 and 3.20. The initial amount of infected individuals correspond to the total number of cases reported on the first month (46) scaled by the reporting rate ($r = 0.02$). The initial number of exposed is nearly a third of initial number of infected people. The initial number of infected mosquitoes is twice the initial number of infected people, and the initial number of exposed mosquito is only a third of the initial number of infected mosquitoes. These values were selected according to the parameter estimation in Section 3.5. Figure 3.8 depicts the dynamics of all

Table 3.18: Costs in millions, total number of vaccinated individuals and total number of cases in millions corresponding to scenario 6 at different starting times using objective functional J_1 with $\hat{J}_1$ representing the cost associated to infected people and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario at	$\hat{J}_1$	$\hat{J}_2$	$J_1 = \hat{J}_1 + \hat{J}_2$	Total Vacc.	Total Cases
$t = 0$	48.3	6.1	54.4	3.6	6.6
$t = 10$	94.2	4.1	98.3	1.9	13.1
$t = 20$	138.2	2.1	140.3	654,368	19.2
No Control	171.3	0	171.3	0	23.8

Table 3.19: Initial condition values for ZIKV outbreak in Puerto Rico to create Figures 3.8, 3.9, 3.10, and 3.11.

$S(0)$	$V(0)$	$E(0)$	$I(0)$	$R(0)$	$S_v(0)$	$E_v(0)$	$I_v(0)$
2.8 M	0	763	2,312	0	6 M	1,541	4,624

Table 3.20: Parameter values for ZIKV outbreaks in Puerto Rico to create Figures 3.8, 3.9, 3.10, and 3.11.

μ	β	α	κ	γ	μ_v	β_v	η	ω	f
$\frac{1}{52 \cdot 80}$	0.701	0.007	1	1.40	0.4	2.823	0.634	0	0.9

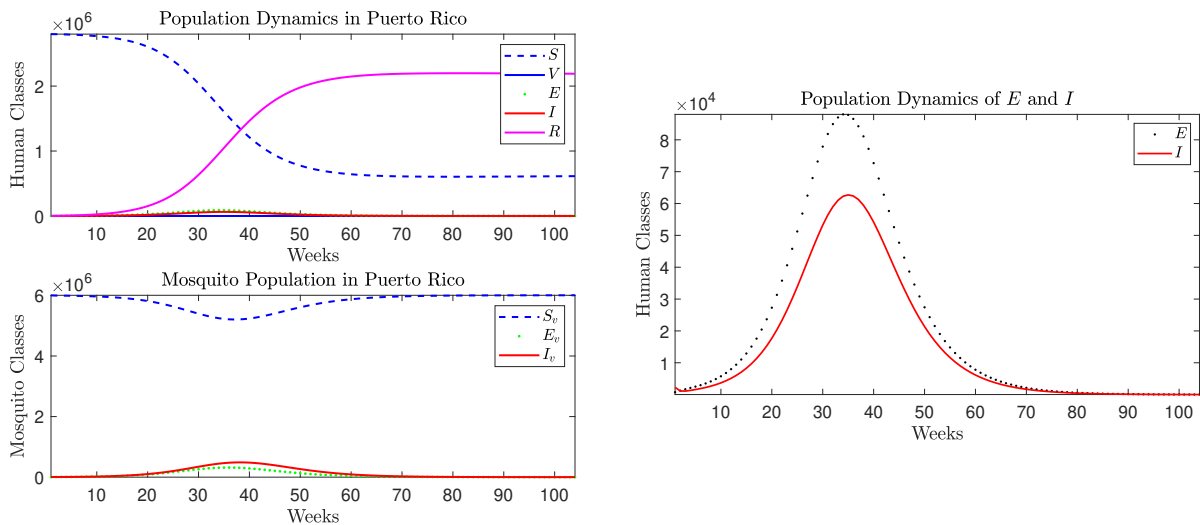


Figure 3.8: Left: Human-Mosquito population dynamics for 2016-17 ZIKV epidemic in Puerto Rico in absence of control strategies. **Right:** Only E and I populations at a lower population scale.

human and mosquito populations. We also highlighted the burden corresponding to those individuals in the exposed and infected human classes. Observe that vaccination has not been incorporated in these simulations.

We simulate a ZIKV epidemic within 104 weeks to represent the outbreak occurred in Puerto Rico. The value of the upper bounds for the controls u_1 and u_2 are assumed 0.2. This assumption simply means that at most 20% of the total population could be informed about the controls and perform control actions. The upper bound for the vaccination is selected to be 0.01 which represents that at most 1% of the population will be able to get vaccinated weekly if the vaccine is fully effective. We assume vaccine protection does not wane and it's mostly effective ($f = 0.9$). In Table 3.22 we show the values used for the upper bounds and weight parameters.

The basic reproduction number for the ZIKV model in absence of optimal controls for Puerto Rico is 2.1739 as shown in Table 3.21. Further, it can be seen that the contribution to $\mathcal{R}_0$ from the direct transmission is much lower than the vector transmission. In this case, the vast majority of weekly ZIKV cases are associated to mosquitoes and not to humans. This basic reproduction number was larger than the one found for Colombia on Section 3.6.

Next we explore the impact of a ZIKV epidemic in Puerto Rico in presence of different control strategies.

3.7.1 Implementation of Personal Protection Controls without Vaccination

The impact of optimally informing the population about the use of condoms (scenario 1), insect repellent (scenario 2) and both condom and insect repellent at the same time (scenario 3) for the dynamics of the ZIKV spread in absence of vaccination are evaluated in Figure 3.9. The values of upper bounds on the controls (b_i 's) as well as the weight parameters for Figure 3.9 are in Table 3.22.

The controls u_1 and u_2 represent the importance of personal protection efforts against ZIKV to avoid being infected by sexual contact and mosquito bites, respectively. The two graphs at the left side on Figure 3.9a display the two optimal control functions analyzed for

Table 3.21: Basic Reproductive Number of Puerto Rico using estimated parameters.

	$\mathcal{R}_v$	$\mathcal{R}_d$	$\mathcal{R}_0$
Puerto Rico	2.222	0.005	2.227

Table 3.22: Values for upper bounds on the controls and weight parameters for Figure 3.9.

A_1	A_2	B_1	B_2	B_3	C_1	C_2	C_3	b_1	b_2	b_3
10	10	0.1	0.01	0	0.1	0.01	0	0.2	0.2	0

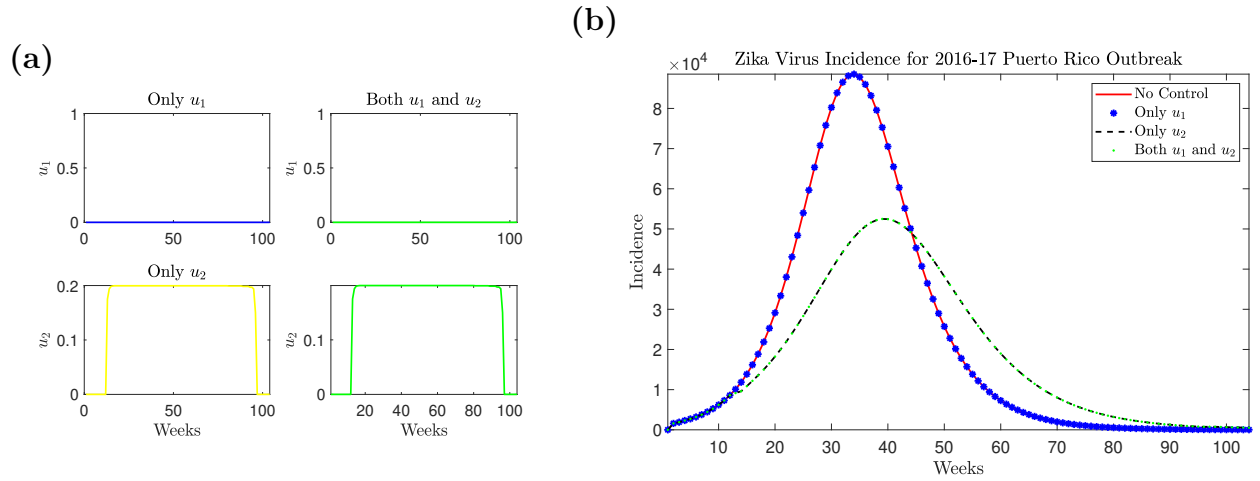


Figure 3.9: **a)** The two figures on the left display the optimal control functions for scenarios 1 and 2. The two figures on the right represent optimal control functions implemented for scenario 3. **b)** Incidence corresponding to scenario 1, 2 and 3 as well as when no strategy is used. Graphs correspond to solutions of the optimization problem with objective functional J_2 .

scenarios 1 and 2, while the results of implementing two controls simultaneously (scenario 3) are displayed in the two graphs at the right of Figure 3.9a. The graphs on Figure 3.9b measure the impact of each strategy against the scenario in absence of controls. Further, each graph represents the number of weekly new cases of humans with ZIKV under scenarios 1, 2, 3, and no controls. The dynamics of new infected humans under no interventions (no condoms, repellents and vaccination) are compared with those where optimal control strategies are implemented.

The implementation of scenarios 2 or 3 (black dashed and green dotted lines) bring a notable reduction in the peak of number of new cases from nearly 100,000 (around week 30) when no controls are used to 55,000 (near week 42). For these scenarios, the optimal control u_2 stayed positive at the highest level from nearly week 11 to week 100 and it was zero outside this timeline. However, informing the public about the use of condoms does not seem to have any effect in diminishing the number of new cases. We believe the lack of effect on scenario 1 is due to most of the ZIKV transmission is associated to the mosquitoes and not the direct transmission (see Table 3.11). One can also associate the lack of u_1 control to the weight parameters B_1 and C_1 , but after running several simulations with high and low weights, the results were the same. Thus, when scenario 3 is implemented, it reduces to implement scenario 2 since u_1 is not necessary.

Tables 3.23 and 3.24 show the cost associated to the prevention measures and epidemiological strategies for objective functionals J_1 and J_2 . Both tables provide the total number of ZIKV cases at the final time in presence of each scenario. In this situation, the best strategy to decrease the total number of infections is clearly to inform the public about the use of insect repellents to prevent mosquito bites. In this case, regardless of which epidemiological strategy is used, one can see that the total number of new cases will drop to near 1.8 from 2.22 millions. In the next section we examine some scenarios when an effective vaccine is available to protect the population against ZIKV.

Table 3.23: Costs in millions and total number of cases in millions corresponding to scenarios 1, 2 and 3 using objective functional J_1 with $\hat{J}_1$ representing the cost associated to infected people and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario	$\hat{J}_1$	$\hat{J}_2$	$J_1 = \hat{J}_1 + \hat{J}_2$	Total Cases
No Control	15.9	0	15.9	2.2
Only u_1	15.9	0	15.9	2.2
Only u_2	13.4	26,150	13.6	1.8
Both u_1 and u_2	13.4	26.1	13.6	1.8

Table 3.24: Costs in millions and total number of cases in millions corresponding to scenarios 1, 2 and 3 using objective functional J_2 with $\hat{J}_3$ representing the cost associated to new cases and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario	$\hat{J}_3$	$\hat{J}_2$	$J_2 = \hat{J}_3 + \hat{J}_2$	Total Cases
No Control	22.2	0	22.2	2.2
Only u_1	22.2	0	22.2	2.2
Only u_2	18.7	28,261	19.1	1.8
Both u_1 and u_2	18.7	28,261	19	1.8

3.7.2 Personal Protection Controls along with an Effective Vaccine

In the scenarios 4, 5 and 6, we want to assess the use of personal protection efforts when an available vaccine is ready to be rolled out. The parameter values corresponding to control upper bounds and weights are given in Table 3.25. Here, we consider the cost associated with vaccination to be larger than the cost associated with the other two controls to illustrate an opposite case than the one study from Colombia in Section 3.6. These assumptions were simply made to capture a ZIKV epidemic with different cost features than those assumed for Colombia. Nothing should imply that these weights realistically match a possible ZIKV epidemic in either Puerto Rico or Colombia.

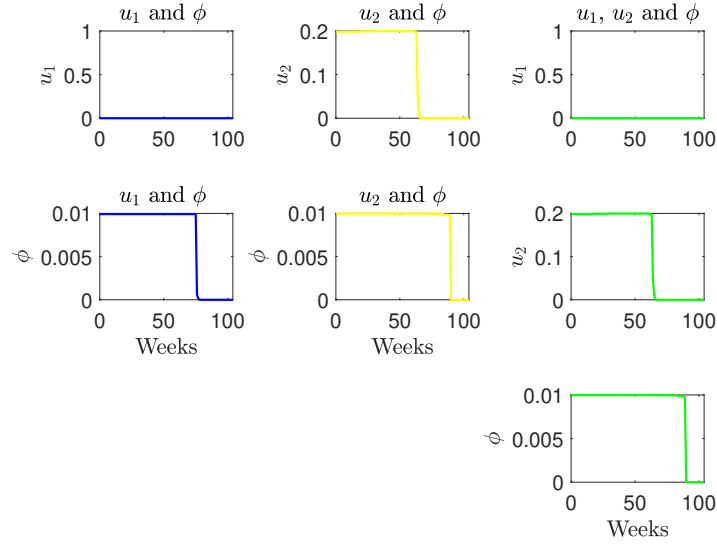
Figure 3.10a shows the dynamics of optimal control strategies when one or both personal protection efforts are used along with vaccination. Here we can observe the duration that each optimal control should last. For instance, when scenario 5 is used, both u_2 and ϕ should start at their highest level since week 0, but u_2 and ϕ should shut down near week 60 and 90, respectively. The number of weekly new cases corresponding to each scenario is illustrated in Figure 3.10b. It can be seen that when vaccination is available with one of the other control measures it reduces drastically the peak of the incidence than when no control is applied. Moreover, it can also be seen that prophylactic campaigns do not provide any contributions in reducing the peak of new infections regardless the scenario. Hence, the scenario 4 turn down to simply implement a vaccination campaign (blue asterisk graph) while the scenarios 5 and 6 become the same, that is, vaccination and insect repellent campaigns (black line and green dashed graphs) should be put in place.

Additionally, in Tables 3.26 and 3.27 we report the cost of implementing objective functionals J_1 and J_2 with their corresponding contributions to the prevention and epidemiological integrals. The total number of vaccinated and infected individuals at the end of the epidemic are also included for each of the scenarios. The best strategy in mitigating the impact of a ZIKV epidemic in Puerto Rico is to implement information campaigns to increase the use of insect repellent along with vaccination efforts. The reduction in the total number of cases is notably from around 2.2 million to 567 thousand individuals. The second

Table 3.25: Values for upper bounds on the controls and weight parameters for Figures 3.10 and 3.11.

A_1	A_2	B_1	B_2	B_3	C_1	C_2	C_3	b_1	b_2	b_3
10	10	0.1	0.1	0.1	1	2	5	0.2	0.2	0.01

(a)



(b)

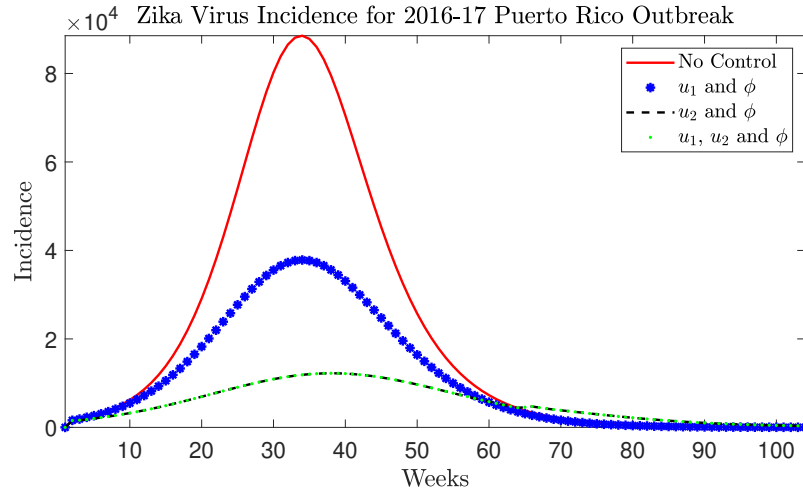


Figure 3.10: **a)** The two figures to the left and middle display the optimal control functions for scenarios 4 and 5. The three figures on the right correspond to optimal control functions implemented for scenario 6. **b)** Number of weekly new cases in absence of controls and for scenarios 4, 5 and 6. Graphs correspond to solutions of the optimization problem with objective functional J_2 .

Table 3.26: Costs in millions, total number of vaccinated individuals and total number of cases in millions corresponding to scenarios 4, 5 and 6 using objective functional J_1 with $\hat{J}_1$ representing the cost associated to infected people and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario	$\hat{J}_1$	$\hat{J}_2$	$J_1 = \hat{J}_1 + \hat{J}_2$	Total Vacc.	Total Cases
No Control	15.9	0	15.9	0	2.2
u_1 and ϕ	8.3	108,253	8.5	504,681	1.1
u_2 and ϕ	4	2.5	6.5	762,207	567,191
u_1, u_2 and ϕ	4	2.5	6.5	762,207	567,191

Table 3.27: Costs in millions, total number of vaccinated individuals and total number of cases in millions corresponding to scenarios 4, 5 and 6 using objective functional J_2 with $\hat{J}_3$ representing the cost associated to new cases and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario	$\hat{J}_3$	$\hat{J}_2$	$J_2 = \hat{J}_3 + \hat{J}_2$	Total Vacc.	Total Cases
No Control	22.2	0	22.2	0	2.2
u_1 and ϕ	11.7	109,760	11.8	533,089	1.1
u_2 and ϕ	5.4	2.7	8.1	792,450	549,746
u_1, u_2 and ϕ	5.4	2.6	8.1	792,450	549,746

best strategy is simply to promote vaccination campaigns. With only vaccination the number of individuals that can be prevented from becoming infected is close to 1 million.

According to our results, vaccination should be put in place since day one of the epidemic until week 90 to accomplish this significant reductions. Nonetheless, the implementation of vaccination campaigns since day one might not be realistic to achieve, in the next section we explore the impact of interventions starting at different times. Observe also that condom information campaigns are not demanded due to Puerto Rico's low direct transmission threshold ($\mathcal{R}_d$).

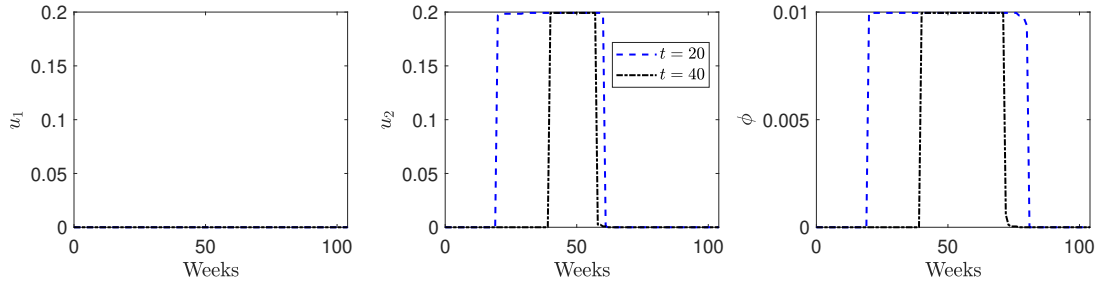
In the next section we explore what can occur when the controls u_2 and ϕ are implemented some time after the epidemic has begun.

3.7.3 Personal Protection and Effective Vaccine at Different Times

In this section we want to measure the benefits produced by the best mitigation plan even if applied at a later time after a ZIKV emergency has been announced. The best control strategy in order to mitigate the ZIKV disease in Puerto Rico is to tirelessly vaccinate susceptible individuals and inform them about the importance of insect repellent. This best strategy was selected based on our results in Section 3.5 due to the majority of new ZIKV cases in Puerto Rico were associated with mosquito transmission rather than sexual transmission (see Table 3.21).

In Figure 3.11a we show the evolution of each control starting at the beginning of the epidemic, week 20 and week 40. Moreover, in Figure 3.7b we display the dynamics of weekly incidence for each strategy and we compare when no control is applied. By looking at weekly incidence curves, it can be observed that as soon as the controls are put in place the weekly incidence start to shrink when compare to the no control curve. In Table 3.28 we provide the cost of only objective functional J_1 as well as the total number of individuals vaccinated and infected by the end of week 104. Looking at the total number of cases, one can see that faster control measures can produce more benefits mitigating the spread of the disease. Although, public health official should note that any control strategy regardless of starting time could be significantly better than taking no action at all.

(a)



(b)

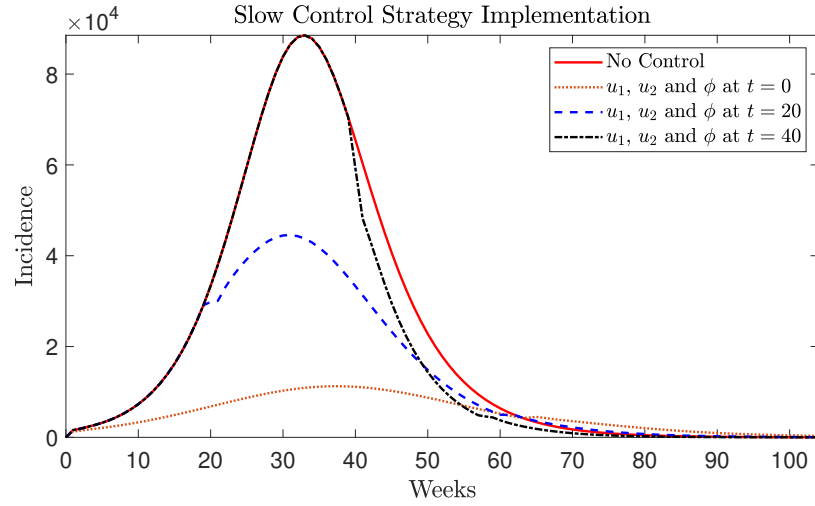


Figure 3.11: a) Graphs corresponding to each control starting at week 20 and 40. b) Number of weekly new cases in absence of controls and for scenario 6 starting at different weeks. Number of new cases correspond to outbreak in Puerto Rico. Graphs correspond to solutions of the optimization problem with objective functional J_1 .

Table 3.28: Costs in millions, total number of vaccinated individuals and total number of cases in millions corresponding to scenario 6 at different times using objective functional J_1 , with $\hat{J}_1$ representing the cost associated to infected humans and $\hat{J}_2$ the cost associated with the prevention measures.

Scenario at	$\hat{J}_1$	$\hat{J}_2$	$J_1 = \hat{J}_1 + \hat{J}_2$	Total Vacc.	Total Cases
$t = 0$	4	2.50	6.5	762,207	567,191
$t = 20$	9.9	1.3	11.2	287,480	1.3
$t = 40$	14.5	324,727	14.9	41,696	2.1
No Control	15.9	0	15.9	0	2.2

We could also see a significant reduction in the number of weekly new cases when control measures are put in place before the peak of new cases. However, the implementation of controls after the peak of new cases show no significant reductions as it can be seen when $t = 40$. One cause of this effect is that most of the population has been infected and obtained natural immunity against the disease once the incidence started to decrease. Hence, when a control strategy is implemented at a late stage of the epidemic there are fewer susceptible individuals to reach which makes the control action to last less or in the worst case scenario to go unnoticed.

3.8 Discussion

In this chapter, we have formulated a ZIKV vaccination model to understand the dynamics of a ZIKV epidemic under six different scenarios with three optimal controls. Two time dependent controls were implemented to reduce the mosquito transmission and direct transmission while incorporating the possibility of a time dependent vaccination rate. We computed the basic reproduction number (equation (3.6)) using the Next Generation Matrix approach when the controls are constant. Subsequently, we showed the existence, positivity and uniqueness of a solution to the model. There were two optimal control problems associated to the vaccination model. The first problem considered an objective functional to minimize the burden of infected humans and the cost of implement all three controls. The second objective functional was designed such that the total incidence of the epidemic and the cost associated with the all three control strategies were minimized. We proved the existence of optimal control solutions to each optimal control problem. Pontryagin's Maximum Principle was used to derive the necessary conditions that the optimal triple satisfies for each optimal control problem proposed. To illustrate numerical simulations of the model, we used data from previous ZIKV outbreaks in Colombia and Puerto Rico. We estimated parameters corresponding to each country by minimizing the incidence error between the data and the model. The parameter estimation showed that the data corresponded to very low reporting rates after the initial conditions corresponding to exposed and infected humans and mosquitoes were scaled up. Also, for each country we found that the incubation period

in humans (κ) always exceeded the birth/death rate of mosquitoes (μ_v). This situation will guarantee to have enough infected humans in the community for new susceptible mosquitoes to become infected since the progression from exposed to infected human individuals is shorter than the mosquitoes lifespan. For each country, we assessed six different scenarios to decrease the weekly number of infections of a possible ZIKV epidemic. First, we measured the implementation of isolated condom and insect repellent campaigns (scenarios 1 and 2) and the use of condom and insect repellent campaigns (scenario 3) combined. Second, the use of a personal protection and vaccination campaigns (scenarios 4 and 5) and all three controls at the same time (scenario 6). In addition, we analyzed the consequences of implementing the best optimal control strategy starting at different times after an epidemic has already been announced.

In general, the numerical results showed that any control strategy is better than letting the disease take its own course. The only exception to this was the use of condoms in Puerto Rico since the sexual transmission threshold was considerably low and most of the ZIKV infections were associated with the mosquito transmission as noticed in Table 3.21. As far as the values of the objective functionals, we could see for all the examples that reducing the weekly incidence was always more costly than reducing the cost of the disease burden. This could have happened due to our choice for weight parameters A_1 and A_2 being the same. In reality they can be different, but the question is then how much different and why. Our parameter choices for B_i 's and C_i 's in each scenario were intended to realistically capture the cost of each strategy. In some of the examples we chose the weight parameters associated with the controls near to zero to represent the low-cost associated with them. Note that if control weights are high, it is very unlikely to see a significant reduction in weekly new cases. We also found that the best strategies to mitigate a ZIKV epidemic in either Colombia or Puerto Rico are different. The best mitigation plan for Colombia is to implement all three time dependent controls at the same time. However, we found that the best strategy for Puerto Rico is to apply insect repellent and vaccination campaigns without advertising condoms. In absence of vaccination, Colombia should implement both personal protection controls while Puerto Rico should only advertise mosquito repellents to reduce the number of weekly infections.

In presence of optimal control strategies, we have also identified patterns in the delivery of both personal protection efforts to keep people safe from getting infected with ZIKV. In the case of Colombia, the use of isolated insect repellent and preservative controls (scenarios 1 and 2) are required intensively from the beginning of an epidemic. However, when both personal protection and vaccination campaigns are combined (scenario 6), it demands a high level of effort from each control since the beginning until approximately week 53 instead of week 63. We could also notice in the simulations that vaccination campaigns are not necessary throughout a complete ZIKV epidemic even if combined with the other two preventive measures. In the case of Puerto Rico, when controls are started at different times, one can see that vaccination campaigns do not have to be rolled out until the last week of the epidemic, but instead until weeks 75 to 80 depending on when the strategies began.

Although we truly believe our model can do well in capturing the dynamics of possible future ZIKV epidemics in presence of vaccination and personal protection controls, it has some limitations. Our model does not recognize if infected individuals are symptomatic or asymptomatic. Another limitation of our model is that mostly the entire population is considered homogeneous. Since most vaccines get approved by age group, it would be interesting to incorporate this feature into the model. Some new models where these features are added can provide public health managers with more new insights in understanding the evolution of ZIKV epidemics.

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Vita

Originally from Colombia, Wencel Valega-Mackenzie grew up in Barranquilla, Atlántico. After high school, he attended the Universidad Sergio Arboleda in Bogotá and received a Bachelor's degree in Mathematics. Before graduating with his undergraduate degree, he knew he wanted to attend graduate school. He first chose to attend The University of Puerto Rico at Mayagüez to pursue a Master's degree in Applied Mathematics. After his first master's degree, he chose to attend the University of Tennessee, Knoxville to pursue a Doctor of Philosophy degree in Mathematics with a concentration in Mathematical Biology under the advisement of Dr. Suzanne Lenhart. By the second year of his PhD, he received a second Master of Sciences. His research interest includes studying the implementation of optimal control theory applied to disease models, population dynamics and spatial ecology. After graduation, he will begin a postdoctoral position at the FDA-CBER in the Office of Biostatistics and Pharmacovigilance as an ORISE Fellow. He is incredibly grateful for all the support from his advisor, family and fiancée as he begins his new career.